TT 47: Correlated Electrons: Spin Systems and Itinerant Magnets 2

Time: Friday 9:30–12:45 Location: H 0104

TT 47.1 Fri 9:30 H 0104

Single-Crystal Growth and Low Temperature Properties of the Itinerant Antiferromagnet $Cr^{11}B_2$ — Andreas Bauer[1], •Alexander Regnat[1], Saskia Gottlieb-Schönmeyer[1], Michael Wagner[1], Christian Bluhm[2], Sabine Wurmehl[2], Bernd Büchner[2], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, James-Franck-Straße, D-85748 Garching, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany

We report the preparation and low temperature properties of the itinerant antiferromagnet $Cr^{11}B_2$. Large single crystals were grown by means of optical float-zoning, where the feed rods were prepared in a solid state reaction using high purity Cr and B powder in a bespoke tungsten crucible. ^{10}B depleted boron was used to permit detailed neutron scattering studies. The crystal grown has the highest residual resisitvity ratio reported to date in the literature of 31 and 11 for current along the crystallographic c- and a-directions, respectively [1]. Measurements of the low temperature specific heat, magnetization and electrical resistivity are consistent with SDW type antiferromagnetic order below T_N=88 K [2], which is remarkably insensitive to large applied magnetic fields.

[1] Tanaka et al., J Less-Comm Met, **50**, 15 (1967)
[2] Funhashi et al., Solid State Commun, **23**, 859 (1977)

TT 47.2 Fri 9:45 H 0104

The strength of frustration and quantum fluctuations in $LiVCuO_4$ — •Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Roman Kuzian[1,2], Johannes Richter[3], Jiři Málek[1,4], Miriam Schmitt[5], Jeroen van den Brink[1], and Helge Rosner[5] — [1]IFW Dresden — [2]Institute for Problems of Materials Science, Kiev, Ukraine — [3]Universität Magdeburg — [4]Institute of Physics, ASCR, Prague, Czech Republic — [5]MPI für Chemische Physik fester Stoffe

We present an empirical and microscopical analysis of the inchain exchange constants of the edge-shared frustrated chain cuprate $LiVCuO_4$. We argue that the ferromagnetic nearest neighbour coupling J_1 clearly exceeds the antiferromagnetic (AFM) next-nearest neighbour coupling J_2. The measured saturation field is significantly affected by a weak 3D AFM interchain coupling leaving room for a possible Bose-Einstein condensation for several T below. The obtained exchange parameters are in agreement with the results for a realistic five-band extended HUBBARD Cu $3d$ O $2p$ model, LSDA+U predictions as well as with inelastic neutron scattering and magnetization data. The single chain frustration rate $\alpha = J_2/|J_1| \approx 0.75$, including all error bars, is definitely smaller than 1. This corresponds to strongly coupled interpenetrating AFM Heisenberg chains in contrast with opposite statements in the literature. A proper account of strong quantum fluctuations and frustration is necessary for a correct assignment of the exchange integrals, which cannot be achieved by a simple renormalization of J_2 from the spin-wave theory.

TT 47.3 Fri 10:00 H 0104

The Physics of Charge Ice in Relation to the Spin Ices — Aroon O'Brien[1,2], •Paul McClarty[1], Frank Pollmann[1], and Roderich Moessner[1] — [1]Max Planck Institute PKS, Dresden, Germany — [2]School of Physics, The University of Sydney, Sydney, Australia

We consider a classical system of charges on the sites of a pyrochlore lattice in the presence of long-range Coulomb interactions. This model, which we call the charge ice model, appeared in the early literature exploring the Verwey transition in magnetite. We revisit this model in the context of recent work on Coulomb phases in condensed matter. In particular, we find many parallels and some subtle differences between the properties of charge ice and those of another model with long-range interactions - the dipolar spin ice model - which has been studied extensively and accounts very well for much of the phenomenology of the spin ice magnets. The Coulomb phase of both models is inherited from their short-range interacting counterparts. We study in detail the degeneracy breaking brought about by the long-range interactions as well as its effects on the thermal properties of the Coulomb phase. Finally, we comment on possible experimental signatures of the Coulomb physics in mixed valence materials.

TT 47.4 Fri 10:15 H 0104

Search for quantum spin ice in $Tb_2Ti_2O_7$ at milli-Kelvin temperatures — S. Legl[1], •C. Krey[1], S.R. Dunsiger[1], C. Pfleiderer[1], H.A. Dabkowska[2], J. Rodriguez[2], and G.M. Luke[2] — [1]Physik Department E21, Technische Universität München, Germany — [2]Department of Physics and Astronomy, McMaster University, Hamilton, Canada

Spin ice attracts great interest as a state in which emergent fractionalized excitations and magnetic-field induced topological forms of order may occur. However, little is known about the importance of quantum fluctuations for the spin ice state. We report a search for so-called quantum spin ice, i.e., a spin ice state driven by quantum fluctuations [1]. Using a vibrating coil magnetometer as combined with a dilution refrigerator [2], we performed comprehensive magnetization measurements in high-quality single crystals of $Tb_2Ti_2O_7$. As an isostructural sibling of the conventional spin ice systems $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$ strong quantum fluctuations are believed to suppress long-range magnetic order in $Tb_2Ti_2O_7$ despite strong antiferromagnetic interactions. We find that $Tb_2Ti_2O_7$ clearly remains paramagnetic down to the lowest temperatures studied without the magnetic field dependence predicted theoretically for quantum spin ice.

[1] Molavian et al., Journal of Physics: Condensed Matter, 21(17):172201 (2009).
[2] Legl et al., Rev. Sci. Instrum. 81, 043911 (2010).

TT 47.5 Fri 10:30 H 0104

Quantum Ice : a Quantum Monte Carlo study — •Olga Sikora[1,2], Owen Benton[1], Nic Shannon[1,2,3], Karlo Penc[4], Frank Pollmann[5], and Peter Fulde[5,6] — [1]H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, UK — [2]Okinawa Institute of Science and Technology, Okinawa, Japan 904-0495 — [3]Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, UK — [4]Research Institute for Solid State Physics and Optics, H-1525 Budapest, Hungary — [5]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [6]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Spin ice systems with fascinating "magnetic monopole" excitations are characterized by macroscopic degeneracy previously discovered in water ice. At very low temperatures we might expect this degeneracy to be lifted by quantum tunneling between different ice configurations.

Here we present the results of large-scale Green's function Monte Carlo simulation of ice-type models which include quantum tunneling. We find compelling evidence of an extended quantum U(1)-liquid ground state with deconfined monopole excitations in both the quantum dimer model [1,2] and the quantum ice model on the diamond lattice [3]. We discuss the fate of "pinch point" singularities seen in neutron scattering experiments on spin ice materials, showing how these are "hollowed out" in the quantum ice model [3,4].

[1] O. Sikora et al., Phys. Rev. Lett. 103, 247001 (2009)
[2] O. Sikora et al., Phys. Rev. B 84, 115129 (2011)
[3] N. Shannon et al., arXiv:1105.4196
[4] O. Benton et al., in preparation.

TT 47.6 Fri 10:45 H 0104

Thermal Transport in the Spin-Ice compound $Dy_2Ti_2O_7$ — •Gerhard Kolland, Oliver Breunig, Simon Scharffe, Johanna Frielingsdorf, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

The magnetic Dy sites in $Dy_2Ti_2O_7$ form a pyrochlore lattice consisting of corner-sharing tetrahedra. A strong crystal field results in an Ising anisotropy of the magnetic moments of the Dy sites, which align along their local easy axis in the [111]-direction, pointing into or out of the tetrahedra. As a consequence, the spin system is geometrically frustrated. Possible ground-states at temperatures below 1 K are given by the "ice-rule": two spins point into and two out of a tetrahedron. This behaviour is analogous to the hydrogen displacement in water ice, revealing a residual entropy for $T \to 0$. Excited states can be created by flipping one spin – leading to the configurations of "1-in/3-out" and "3-in/1-out". In zero magnetic field, these excitations can easily propagate and are discussed as magnetic monopoles [1]. We measured the thermal conductivity down to 300 mK for external magnetic fields up to 8 T. The thermal conductivity is strongly field dependent and anisotropic with respect to the field direction. To investigate the influence of the magnetic excitations on the heat transport we compare our data to the thermal conductivity of $Dy_{2-x}Y_xTi_2O_7$ with $x = 1, 2$.

Work supported by the DFG through SFB 608.

[1] Castelnovo et. al. (2008). Nature, **451**(7174), 42-5

TT 47.7 Fri 11:00 H 0104

Spin transport in the XXZ chain at finite temperature and momentum — •Robin Steinigeweg[1] and Wolfram Brenig[2] — [1]J. Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia — [2]Institute for Theoretical Physics, Technical University Braunschweig, Mendelssohnstr. 3, D-38106 Braunschweig, Germany

We investigate the role of momentum for the transport of magnetization in the spin-1/2 Heisenberg chain above the isotropic point at finite temperature and momentum. Using numerical and analytical approaches, we analyze the autocorrelations of density and current and observe a finite region of the Brillouin zone with diffusive dynamics below a cut-off momentum, and a diffusion constant independent of momentum and time, which scales inversely with anisotropy. Lowering the temperature over a wide range, starting from infinity, the diffusion constant is found to increase strongly while the cut-off momentum for diffusion decreases. Above the cut-off momentum diffusion breaks down completely.

15 min. break.

TT 47.8 Fri 11:30 H 0104

Emergent critical phase in 2D frustrated Heisenberg model — •Peter Philipp Orth[1], Premala Chandra[2], Piers Coleman[2], and Jörg Schmalian[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

It is well-known that a discrete Ising ($\mathbb{Z}_2$) order parameter emerges in the frustrated square lattice J_1-J_2-Heisenberg model, which may be broken at finite temperature. We ask whether a different discrete symmetry $\mathbb{Z}_q$ with $q > 2$ may be found in other frustrated Heisenberg models, giving rise to a different finite temperature phase transition. Indeed, we identify an emergent $\mathbb{Z}_6$ symmetry at low temperatures in a frustrated Heisenberg model on a 2D lattice that contains both the sites of the triangular and its dual honeycomb lattice. Our analysis combines a spin-wave expansion, susceptible to short-distance physics, with renormalization group arguments of the corresponding long-wavelength non-linear sigma model. Our results are even more appealing since the $\mathbb{Z}_6$ clock model has a rich finite temperature phase diagram with two distinct Berezinskii-Kosterlitz-Thouless (BKT) phase transitions separated by a massless critical phase. We also discuss possible realizations of this system using cold-atoms in optical lattices.

TT 47.9 Fri 11:45 H 0104

Unconventional phase transition in the classical triangular-lattice Heisenberg antiferromagnet in applied magnetic field — •Luis Seabra[1], Tsutomu Momoi[2], Philippe Sindzingre[3], and Nic Shannon[4] — [1]Max-Planck-Institut für Physik komplexer System, Dresden, Germany — [2]Condensed Matter Theory Laboratory, RIKEN, Wako, Japan — [3]LPTMC, Université P. et M. Curie, Paris, France — [4]H. H. Wills Physics Laboratory, University of Bristol, U. K.

The classical Heisenberg antiferromagnet on a two-dimensional triangular lattice is a paradigmatic problem in frustrated magnetism. Its "120 degree" classical ground state gives rise to three distinct low-temperature phases under the combined effect of magnetic field and thermal fluctuations. However, many of the details of the magnetic phase diagram remain surprisingly obscure. We address this problem using modern Monte Carlo simulation techniques. At low to intermediate values of magnetic field, we find evidence for a continuous three-state Potts phase transition from the paramagnet into the one-third magnetisation plateau. We also find evidence for conventional Kosterlitz-Thouless transitions from the magnetisation plateau into the canted "Y-state", and into the 2:1 canted phase. However, at higher fields, the phase transition from the paramagnet into the 2:1 canted phase, while continuous, does not appear to fall into any conventional universality class, being instead described by continuously varying exponents. We argue that this deserves further study as an interesting example of a finite-temperature phase transition with compound order-parameter symmetry.

TT 47.10 Fri 12:00 H 0104

Magnetic properties of the Kitaev-Heisenberg model and effects of spin vacancies — Fabien Trousselet, Giniyat Khaliullin, and •Peter Horsch — Max-Planck-Institut f. Festkörperforschung, Heisenbergstr.1, D-70619 Stuttgart

We study the ground state properties of the Kitaev-Heisenberg model in a magnetic field and explore the evolution of spin correlations in the presence of non-magnetic vacancies [1]. This model may be relevant for layered iridates A2IrO3 (A=Na or Li) [2]. By means of exact diagonalizations, the phase diagram without vacancies is determined as a function of the magnetic field and the ratio between Kitaev and Heisenberg interactions. We show that in the (antiferromagnetic) stripe ordered phase the static susceptibility and its anisotropy can be described by a spin canting mechanism, accounting as well for the transition to the polarized phase when including quantum fluctuations perturbatively.

Effects of spin vacancies depend sensitively on the type of the ground state. In the liquid phase, the magnetization pattern and its spatial anisotropy around a single vacancy in a small field is determined. In the stripe phase, the combination of a vacancy and a small field breaks the six-fold symmetry of the model and stabilizes a particular stripe pattern. Similar symmetry-breaking effects occur even at zero field due to interaction effects between vacancies. This selection mechanism and intrinsic randomness of vacancy positions may lead to spin-glass behavior.

[1] F. Trousselet, G. Khaliullin and P. Horsch, PRB 84, 054409 (2011).
[2] Y. Singh and P. Gegenwart, PRB 82, 064412 (2010);

TT 47.11 Fri 12:15 H 0104

Critical scales in anisotropic spin systems from the functional renormalization group — •Stefan Göttel[1,2], Sabine Andergassen[1,2], Dirk Schuricht[1,2], Carsten Honerkamp[2,3], and Stefan Wessel[3,4] — [1]Institute for Theory of Statistical Physics, RWTH Aachen — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Theoretical Solid State Physics, RWTH Aachen — [4]JARA-High-Performance Computing

We apply a recently developed functional renormalization group scheme [Reuther *et. al*, Phys. Rev. B **81**, 144410 (2010)] for quantum spin systems to the spin-1/2 antiferromagnetic XXZ model on a two-dimensional square lattice. Based on an auxiliary fermion representation we derive flow equations which allow a resummation of the perturbation series in the spin-spin interactions. This way, the spin susceptibilities are calculated for different values of the anisotropy parameter, confirming the phase transition between planar and axial ordering at the isotropic point. As recently proposed in [Reuther *et. al*, Phys. Rev. B **84**, 100406(R) (2011)], we extract critical temperatures from the flow. In the Ising limit these results coincide with the Onsager solution, but violate the Mermin-Wagner theorem at the isotropic point and a satisfactory description of the behavior in the vicinity of the phase transition is not possible. A quantitative comparison with quantum Monte-Carlo shows major differences. We trace this problem back to an incorrectly generated selfenergy and discuss potential improvements.

TT 47.12 Fri 12:30 H 0104

Vacancies in non-collinear antiferromagnets — •Alexander Wollny[1], Lars Fritz[2], and Matthias Vojta[1] — [1]Institut für theoretische Physik, Technische Universität Dresden, 01062 Dresden — [2]Institut für theoretische Physik, Universität zu Köln, 50937 Köln

We study dilute magnetic impurities and vacancies in two-dimensional frustrated magnets with non-collinear order. Taking the triangular-lattice Heisenberg model as an example, we use quasiclassical methods to determine the impurity contributions to the magnetization and susceptibility. Most importantly, each impurity moment is *not* quantized, but receives non-universal screening corrections due to local relief of frustration. At finite temperatures, where bulk long-range order is absent, this implies an impurity-induced magnetic response of Curie form, with a prefactor corresponding to a *fractional* moment per impurity. We also discuss the behavior in an applied magnetic field, where we find a singular linear-response limit for overcompensated impurities.