

TT 8: Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets I

Time: Monday 9:30–13:00

Location: HSZ 304

TT 8.1 Mon 9:30 HSZ 304

Critical speeding-up near the monopole liquid-gas transition in magnetoelectric spin-ice — ●CHRISTOPH P. GRAMS¹, MARTIN VALLDOR^{1,2}, MARKUS GARST³, and JOACHIM HEMBERGER¹ — ¹II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — ²Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — ³Institut für Theoretische Physik, Universität zu Köln, Cologne, Germany

Competing interactions in the so-called spin-ice compounds stabilize a frustrated ground-state with finite zero-point entropy and, interestingly, emergent magnetic monopole excitations[1]. The properties of these monopoles are at the focus of recent research with particular emphasis on their quantum dynamics. It is predicted[2] that each monopole also possesses an electric dipole moment, which allows to investigate their dynamics via the dielectric function $\epsilon(\nu)$.

In this talk I report on broadband spectroscopic measurements of $\epsilon(\nu)$ in $\text{Dy}_2\text{Ti}_2\text{O}_7$ down to temperatures of 200 mK with a specific focus on the critical endpoint present for a magnetic field along the crystallographic [111] direction[3].

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[1] C. Castelnovo et al., Nature 451 (2008) 42

[2] D. I. Khomskii, Nature Comm. 3 (2012) 1

[3] C. P. Grams et al., arXiv:1307.8287

TT 8.2 Mon 9:45 HSZ 304

Vibrating coil magnetometry in $\text{Dy}_2\text{Ti}_2\text{O}_7$ at milli-Kelvin temperatures — ●CHRISTOPHER DUVINAGE¹, DHARMLINGAM PRABHAKARAN², CHRISTIAN PFLEIDERER¹, and ANDREW T. BOOTHROYD² — ¹Physik-Department, Technische Universität München, D-85748 Garching, Germany — ²Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom

Spin ice attracts great interest as a state in which emergent fractionalized excitations and magnetic-field induced topological forms of order may occur. An important characteristic of the spin ice systems $\text{Dy}_2\text{Ti}_2\text{O}_7$ and $\text{Ho}_2\text{Ti}_2\text{O}_7$, as well as the spin liquid system $\text{Tb}_2\text{Ti}_2\text{O}_7$, is the observation of spin freezing below a few hundred mK [1,2]. We report vibrating coil magnetometry down to mK temperatures of $\text{Dy}_2\text{Ti}_2\text{O}_7$, addressing the evidence for field-induced phase transitions. Of particular interest is the observation of putative magnetisation avalanches in the spin-frozen state which depend sensitively in number and size on the sweep rate of the applied magnetic field. These avalanches have been interpreted in terms of monopole excitations [3].

[1] Krey et al., PRL 108 (2012) 257204

[2] Legl et al., PRL 109 (2012) 047201

[3] Slobinsky et al., PRL 105 (2010) 267205

TT 8.3 Mon 10:00 HSZ 304

Hysteresis and Relaxation Effects in the Spin-Ice Compound $\text{Dy}_2\text{Ti}_2\text{O}_7$ studied by Heat Transport — ●SIMON SCHARFFE, GERHARD KOLLAND, MARTIN HIERTZ, MARTIN VALLDOR, and THOMAS LORENZ — II. Physikalisches Institut, Universität zu Köln, Germany

The magnetic Dy^{3+} ions in the spin ice $\text{Dy}_2\text{Ti}_2\text{O}_7$ form a pyrochlore lattice consisting of corner-sharing tetrahedra. Due to strong crystal field effects an Ising anisotropy arises which aligns the spins along its local easy axis, pointing into or out of a tetrahedra. Possible ground-states at temperatures below 1 K are given by the "ice rule": two spins point into and two out of a tetrahedron. Excited states can be created by flipping one spin and are discussed as magnetic monopoles[1]. We measured the low-temperature thermal conductivity κ and found experimental evidence for heat transport by magnetic monopoles[2,3]. In addition we observe pronounced hysteresis effects which depend on temperature, the magnetic-field direction, the rate of magnetic-field change, and on the direction of the heat current. Moreover the time-dependent relaxation of the heat conductivity is investigated. These data yield information about possible equilibrium states and reveal that in the low-field and low-temperature region extremely slow relaxation processes occur[4].

This work was supported by DFG through SFB 608 and LO 818/2-1.

[1] Castelnovo et al., Nature 451 (2008) 42

[2] Kolland et al., Phys. Rev. B, 86 (2012) 060402(R)

[3] Kolland et al., Phys. Rev. B, 88 (2013) 054406

[4] Scharffe et al., J. Phys. Soc. Jpn. Suppl. (in press), arXiv:1311.1139

TT 8.4 Mon 10:15 HSZ 304

Wien Effect on a Lattice — ●VOJTECH KAISER^{1,2}, STEVEN BRAMWELL³, PETER HOLDSWORTH¹, and RODERICH MOESSNER² — ¹ENS Lyon — ²MPI PKS Dresden — ³London Centre for Nanotechnology, UCL

The Second Wien Effect is an increase of conductivity of Coulomb gas in an external field, driven by enhanced dissociation of Coulombically bound pairs. The importance of the Wien effect for spin ice was suggested previously since spin ice maps to a Coulomb gas of magnetic monopoles. We present simulations of lattice Coulomb gas and spin ice. The results confirm Onsager's theory of the Wien effect and reveal additional corrections, while allowing access to microscopic dynamics underlying the increase in the charge carrier density. Main extensions of the original theory involve the Debye screening, field dependent mobility and the character of the association constant. We discuss further corrections specific to spin ice due its emergent topological charge and Dirac string network.

TT 8.5 Mon 10:30 HSZ 304

Magnetic and dielectric Properties of the cubic pyrochlore $\text{Nd}_2\text{Hf}_2\text{O}_7$ — ●J.-H. CHUN¹, P. G. REUVEKAMP¹, R. K. KREMER¹, C. T. LIN¹, R. GLAUM², and A. BRONOVA² — ¹Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — ²Rheinische Friedrich-Wilhelms-Universität, Institut für Anorganische Chemie, D-53121 Bonn, Germany

The magnetic properties of rare-earth (R) pyrochlores (PC) of $\text{R}_2\text{M}_2\text{O}_7$, where M is a 3d or 4d transition metal, have attracted broad attention because geometrical frustration gives rise to unusual magnetic ground states and excitations like spin-ice or magnetic monopoles.[1,2] In contrast the properties and especially the magnetism of the rare-earth PCs with 5d cations are considerably less well investigated. Reasons are the close proximity of the cubic PCs to the fluorite structure and that oxides of the PC family tend to exhibit disorder involving a statistical redistribution of the metal atom cations accompanied by a redistribution of the oxygen vacancy sites. We have prepared polycrystalline samples and single-crystal of $\text{Nd}_2\text{Hf}_2\text{O}_7$ and investigated their structural, magnetic, thermal, lattice and dielectric properties. We report low-temperature magnetic ordering determined by heat capacity and magnetic susceptibility measurements and investigations of the dielectric properties. Measurements of the thermal expansion gave no indication of a structural phase transition down to 5 K.

[1] J. S. Gardner, M. J. P. Gingras, and J. E. Greedan, Rev. Mod. Phys. 82 (2010) 53

[2] A. P. Ramirez, Annu. Rev. Mater. Sci. 24 (1994) 453

TT 8.6 Mon 10:45 HSZ 304

Novel magnetism in the spin-orbit driven Mott insulator Ba_2YIrO_6 — ●TUSHARKANTI DEY¹, ANDREY MALJUK¹, OLGA KATAEVA^{1,2}, FRANK STECKEL¹, DANIEL GRUNER¹, TOBIAS RITSCHEL¹, CHRISTIAN G. F. BLUM¹, ANJA U. B. WOLTER¹, JOCHEN GECK¹, CHRISTIAN HESS^{1,3}, SABINE WURMEHL^{1,4}, and BERND BÜCHNER^{1,4} — ¹Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — ²Kazan Federal University, Kremlevskaya str. 18, 420008, Kazan, Russia — ³Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany — ⁴Institute for Solid State Physics, Dresden Technical University, TU-Dresden, 01062 Dresden, Germany

Single crystals of Ba_2YIrO_6 were synthesized for the first time. The material crystallizes in cubic double perovskite structure. Here the only magnetic ion Ir is expected to be in +5 oxidation state with $5d^4$ electronic configuration. Instead of the expected weak Van Vleck-type magnetism [1], we found Ba_2YIrO_6 is paramagnetic in the temperature range 2-300K. Curie-Weiss fitting (30-300K) of susceptibility data gives a Weiss constant $\theta_{CW}=-15\text{K}$ (AF) but no magnetic ordering is found down to 1.8K. Our study suggests that Ba_2YIrO_6 is a spin-orbit driven

Mott insulator with highly frustrated magnetic interactions originating from the face centered cubic (FCC) lattice formed by the Ir moments. In this presentation, details of crystal growth along with structural, magnetic, thermal and electrical transport measurement results will be discussed.

[1] G. Khaliullin, Phys. Rev. Lett. 111 (2013) 197201

TT 8.7 Mon 11:00 HSZ 304

Spiral order in Li_2IrO_3 — ●STEPHAN RACHEL¹, JOHANNES REUTHER², and RONNY THOMALE³ — ¹Institut für Theoretische Physik, TU Dresden — ²California Institute of Technology — ³Institut für Theoretische Physik, Universität Würzburg

Iridates are amongst the most interesting complex oxide materials. The non-interacting band structure of the honeycomb Iridates has been claimed to feature the quantum spin Hall effect due to large spin orbit coupling. The true materials exhibit considerable Coulomb interactions leading to different types of magnetic order (e.g., zig-zag or spiral order). Here we show how one can obtain such magnetic phases by considering the strong-coupling limit of a topological Hubbard model. In particular, we find an incommensurate phase with spiral order which is consistent with the recent experimental findings for Li_2IrO_3 .

15 min. break.

TT 8.8 Mon 11:30 HSZ 304

Theoretical investigation of isoelectronic Li doping in sodium iridate $(\text{Na}_{1-x}\text{Li}_x)_2\text{IrO}_3$ — ●MICHAELA ALTMAYER¹, S. MANNI², S. K. CHOI³, I. I. MAZIN⁴, R. COLDEA³, HARALD O. JESCHKE¹, ROSER VALENTI¹, and P. GEGENWART² — ¹Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — ²I. Physikalisches Institut, Georg-August-Universität Göttingen, D-37077, Göttingen, Germany — ³Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom — ⁴Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

In the recent years honeycomb iridates have been intensively debated as promising candidates for the realization of the Heisenberg-Kitaev-model. Due to the different magnetic ground states of Na_2IrO_3 and Li_2IrO_3 (zigzag for the former and possibly incommensurate for the latter), it is interesting to investigate the series $(\text{Na}_{1-x}\text{Li}_x)_2\text{IrO}_3$. Synthesis of the Li doped Na_2IrO_3 was successful at least up to 20% Li, but there are indications of phase separation at higher concentrations. We investigated the $(\text{Na}_{1-x}\text{Li}_x)_2\text{IrO}_3$ series by full relaxation within density functional theory (DFT). At each doping level, we investigated all possible Na/Li distributions in a supercell containing four formula units and found the substitution of Na by Li in the honeycomb plane Ir_2Na to be most stable for small dopings in the area $0 < x \leq 0.25$. Total energies yield a tendency for phase separation above a doping level of $x = 0.25$ in agreement with experiment.

TT 8.9 Mon 11:45 HSZ 304

Band structure and optical properties of $\text{Na}_3\text{Ir}_3\text{O}_8$ — ●ALEXANDER YARESKO — MPI FKF, Stuttgart, Germany

$\text{Na}_4\text{Ir}_3\text{O}_8$ attracted much attention due to its fascinating magnetic properties. It is a weak Mott insulator in which magnetic Ir^{4+} ions form a frustrated non-centrosymmetric hyper-kagome lattice. Because of geometrical frustrations Ir spins do not order down to lowest temperature but instead remain in a 3D spin-liquid state. Recently, monocrystals of another hyper-kagome Ir compound $\text{Na}_3\text{Ir}_3\text{O}_8$ have been synthesized, In contrast to $\text{Na}_4\text{Ir}_3\text{O}_8$, $\text{Na}_3\text{Ir}_3\text{O}_8$ is a semi-metal with a low carrier density and weak paramagnetism of valence electrons. If spin-orbit interaction (SOI) is neglected, LDA calculations for $\text{Na}_3\text{Ir}_3\text{O}_8$ give an insulating solution despite of noninteger $\text{Ir}^{4.33+}$ valence. SOI, however, closes the band gap and $\text{Na}_3\text{Ir}_3\text{O}_8$ becomes a compensated metal. In this presentation it is shown that the gap appears because of formation of quasi-molecular orbitals on Ir triangles which become partially delocalized due to SOI. The semi-metallic band structure together with the lack of inversion symmetry lead to unusual optical properties which seem to suggest anomalously strong electron-phonon coupling.

TT 8.10 Mon 12:00 HSZ 304

Magnetism in spin models for depleted honeycomb-lattice iridates: Spin-glass order towards percolation — ●MATTHIAS VOJTA and ERIC C. ANDRADE — Technische Universität Dresden, 01062 Dresden, Germany

Iridates are characterized by a fascinating interplay of spin-orbit and electron-electron interactions. The honeycomb-lattice materials

A_2IrO_3 (A=Na,Li) have been proposed to realize pseudospin-1/2 Mott insulating states with strongly anisotropic exchange interactions, described by the Heisenberg-Kitaev model, but other scenarios involving longer-range exchange interactions or more delocalized electrons have been put forward as well.

Here we study the influence of non-magnetic doping, i.e., depleted moments, on the magnetic properties of experimentally relevant variants of the Heisenberg-Kitaev and Heisenberg J_1 - J_2 - J_3 models. We generically find that the zigzag order of the clean system is replaced, upon doping, by a spin-glass state with short-ranged zigzag correlations. We determine the spin-glass temperature as function of the doping level and argue that this quantity allows to experimentally distinguish the different proposed spin models when the doping is driven across the site percolation threshold of the honeycomb lattice.

TT 8.11 Mon 12:15 HSZ 304

Analysis of the electronic and magnetic properties of honeycomb and triangular lattice iridates — ●YING LI¹, HARALD O. JESCHKE¹, IGOR I. MAZIN², and ROSER VALENTI¹ — ¹Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — ²Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

Honeycomb lattice iridates have been recently discussed as a possible realization of the Heisenberg-Kitaev model in which the electronic structure is dominated by the spin-orbit (SO) interaction. This picture is still under debate. We present calculations on the electronic structure and optical conductivity of Na_2IrO_3 within the density functional theory (DFT) method. Our results show that the measured insulator gap and optical conductivity can be reproduced by GGA+SO+U with a magnetic zigzag configuration. Besides, we analyze the optical conductivity on different directions and the contribution due to different states. Further, we also discuss the electronic structure and underlying microscopic model of a few triangular lattice iridates and compare their properties with the behavior of the honeycomb iridates.

TT 8.12 Mon 12:30 HSZ 304

Spin-orbit physics of $j=1/2$ Mott insulators on the triangular lattice — ●MICHAEL BECKER¹, MARIA HERMANN¹, BELA BAUER², MARKUS GARST¹, and SIMON TREBST¹ — ¹Cologne University, Cologne, Germany — ²Microsoft Research Station Q, Santa Barbara, USA

We investigate the Heisenberg-Kitaev model on the triangular lattice which is thought to capture the essential physics of the spin-orbital entanglement in a broad class of effective $j = 1/2$ Mott insulators such as certain Iridate compounds – one potential candidate material being the recently synthesized $\text{Ba}_3\text{IrTi}_2\text{O}_9$. While first results have recently been reported for the classical limit of this model, our focus is on its quantum version. Using a combination of numerical techniques, such as exact diagonalization and the density matrix renormalization group, which we complement with various analytical approaches, we can identify its entire phase diagram. The most interesting features of this phase diagram resemble what has already been found in the classical limit – a \mathbb{Z}_2 vortex lattice phase in the vicinity of the Heisenberg limit and a “nematic” phase around the antiferromagnetic Kitaev point.

TT 8.13 Mon 12:45 HSZ 304

Discriminating antiferromagnetic signatures in ultracold fermions by tunable geometric frustration — CHIA-CHEN CHANG¹, RICHARD T. SCALETTAR¹, ●ELENA V. GORELIK², and NILS BLÜMER² — ¹Department of Physics, University of California, Davis, USA — ²Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Recently, it has become possible to tune optical lattices continuously between square and triangular geometries. We compute thermodynamics and spin correlations in the corresponding Hubbard model using determinant quantum Monte Carlo and show that the frustration effects induced by the variable hopping terms can be clearly separated from concomitant bandwidth changes by a proper rescaling of the interaction. An enhancement of the double occupancy by geometric frustration signals the destruction of nontrivial antiferromagnetic correlations at weak coupling and entropy $s \lesssim \ln(2)$ (and restores Pomeranchuk cooling at strong frustration), paving the way to the long-sought experimental detection of antiferromagnetism in ultracold fermions on optical lattices.

[1] C.-C. Chang, R. T. Scalettar, E. V. Gorelik, and N. Blümer, Phys. Rev. B **88** (2013) 195121.