MA 5: Spin Structures and Magnetic Phase Transitions I

Time: Monday 9:30–12:45 Location: EB 202

MA 5.1 Mon 9:30 EB 202

Exploring and Tuning Magnetic Order in Rare-Earth Tritellurides — •Thom Ottenbros[1], Claudius Mueller[1,2], Shiming Lei[3,5], Ratnadwip Shingha[4,5], Leslie Schoop[5], Nigel Hussey[1,6], and Steffen Wiedmann[1] — [1]HFML-FELIX, Radboud University, Nijmegen, The Netherlands — [2]UT, Enschede, The Netherlands — [3]HKUST, Hong Kong — [4]IITG, Guwahati, India — [5]Princeton University, New Jersey, USA — [6]HH Wills, Bristol, UK

In recent years, a new class of layered antiferromagnetic (AFM) materials has appeared that consist of alternating stacks of localized, magnetically ordered and itinerant, non-magnetic electrons, giving rise to rich phase diagrams in which spin and charge degrees of freedom play a central role. In the rare-earth tritelluride RTe3 family, this interplay between the spin and charge interactions is particularly complex, with the itinerant 5p Te electrons undergoing a charge density wave transition at elevated temperatures.

In this work, we present thermal expansion (TE) and high-field magnetostriction (MS) studies on GdTe3, the ideal candidate material to investigate the cascade of AFM ordered phases due to the relatively high transition temperatures with a suspected striped AFM spin structure. We present MS data along different high-symmetry orientations and demonstrate that out-of-plane uniaxial strain alters the magnetic phase diagram. Finally, from analysis of the quantum oscillations in the MS, we find evidence for a strain-induced Fermi surface reconstruction. Our results demonstrate the remarkable complexity and tunability of the ordered magnetic states and spin structures in GdTe3.

MA 5.2 Mon 9:45 EB 202

Generalization of Dzyaloshinskii-Moriya interaction to any beyond Heisenberg spin model — •Hiroshi Katsumoto[1], Yuriy Mokrousov[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

In the past decade, it has become clear that the competition between Heisenberg and higher-order exchange interactions can promote very complex magnetic structures. While higher-order terms among isotropic exchange interactions are known to stem not only from the number of sites but also from the spin magnitude [1], Moriya derived the Dyzaloshinskii-Moriya interaction (DMI), which has emerged as a key mechanism to stabilize chiral magnetism, only for spin-1/2 systems. Starting from a fermionic model and applying perturbation theory to the first order in the spin-orbit coupling, we generalized Moriya's work and derived an expression that generates the DMI sequentially for any higher-order exchange interaction. The application of this expression to particular spin models provides consistently all recently suggested DMIs extended to higher-order exchange interactions [2].

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[1] M. Hoffmann *et al.*, PRB **101**, 024418 (2020).

[2] A. Lászlóffy *et al.*, PRB **99**, 184430 (2019); S. Brinker *et al.*, NJP **21**, 083015 (2019); S. Grytsiuk *et al.*, Nat. Commun. **11**, 511 (2020); S. Mankovsky *et al.*, PRB **101**, 174401 (2020).

MA 5.3 Mon 10:00 EB 202

Generalization of Lieb's Theorem to a Class of Non-Bipartite Lattice Structures — •Fabio Pablo Miguel Méndez Córdoba[1,2,3], Joseph Tindall[4], Dieter Jaksch[2,5], and Frank Schlawin[2,3,6] — [1]Departamento de Física, Universidad de Los Andes, A.A. 4976, Bogotá, Colombia — [2]Universität Hamburg, Luruper Chaussee 149, Gebäude 69, D-22761 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, Hamburg D-22761, Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010 — [5]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, UK — [6]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

Lieb's theorem is of fundamental importance for our understanding of correlated magnetic systems. It predicts the ground state magnetization and magnetic order for interacting itinerant electrons by establishing the connection between the magnetic properties of the Hubbard and Heisenberg models. However, Lieb's theorem is valid only for bipartite lattices. In this work, we extend the theorem to a class of non-bipartite lattices by reinterpreting the lattice structure as a collection of disconnected bipartite subsystems. This extension allows for accurately predicting the emergent magnetic structure, which the corresponding Heisenberg model misses.

MA 5.4 Mon 10:15 EB 202

Thermal phase transitions of a spin-1/2 Ising-Heisenberg model on the extended Lieb lattice in a magnetic field — •Jozef Strecka and David Sivy — Faculty of Science, P. J. Safarik University, Kosice, Slovakia

The spin-1/2 Ising-Heisenberg model on the extended Lieb lattice can be rigorously mapped in presence of the external magnetic field to an effective spin-1/2 Ising square lattice with temperature-dependent interaction and field. It is shown that an effective field may vanish along a phase boundary between a quantum monomer-dimer phase and a classical ferrimagnetic phase, which allows an exact determination of thermal phase transitions between these two phases even in presence of non-zero magnetic field. Similar thermal phase transitions can be additionally found between a quantum antiferromagnetic phase and a disordered paramagnetic phase of the model. It is demonstrated that the line of discontinuous phase transitions terminates at the Ising critical point corresponding to a continuous phase transition. The aforementioned exact results for discontinuous and continuous thermal phase transitions in a magnetic field are corroborated by classical Monte Carlo simulations.

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MA 5.5 Mon 10:30 EB 202

Investigation of the first-order antiferromagnetic phase transition of $SrMn_2P_2$ and $CaMn_2P_2$ by thermal-expansion measurements with controlled force — •Sven Graus, N. S. Sangeetha, Teslin R. Thomas, Maximilian van de Loo, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

$SrMn_2P_2$ and $CaMn_2P_2$ adopt a trigonal layered structure with Mn-atoms on a corrugated honeycomb lattice and show insulating behavior. $CaMn_2P_2$ has an antiferromagnetic transition at $T_N = 70$ K of strong first-order character and $SrMn_2P_2$ exhibits a weak first-order antiferromagnetic transition at the Néel temperature $T_N = 53$ K [1]. These first-order antiferromagnetic transitions are unique among the class of Mn-based 122-compounds and their mechanism remains to be explained. It is possibly related to structural changes. We perform high-resolution thermal-expansion measurements by capacitance dilatometry around these phase transitions. In these dilatometry measurements a controlled force in a specific crystallographic direction is applied, varying from $\sim$0.5 N up to several N. This presents a highly sensitive approach to investigate possible lattice distortions or changes of elastic moduli.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] Sangeetha et al., PNAS **118**, e2108724118 (2021).

MA 5.6 Mon 10:45 EB 202

The role of quantum fluctuations for the spin-flop transition in hematite — •Tobias Dannegger and Ulrich Nowak — Fachbereich Physik, Universität Konstanz

Hematite is a canted antiferromagnet with promising properties for spintronics applications such as long range spin transport. At higher temperatures, its equilibrium properties and phase transitions are well described by a semiclassical spin model, but towards low temperatures, qualitative differences between the predictions of a classical model and experimental results arise [1]. Here, we explore how quantum effects can account for those differences using mean-field calculations and exact diagonalisation of the quantum Heisenberg Hamiltonian. Based on an ab initio parametrised model, we compute low-temperature spin-flop fields and compare them to classical calculations and measurements on a hematite single-crystal.

[1] T. Dannegger et al., *Phys. Rev. B* **107**, 184426 (2023).

15 min. break

MA 5.7 Mon 11:15 EB 202

Kosterlitz-Thouless transition in the finite 2DXY model with 4-fold anisotropy — •David Venus — McMaster University, Hamilton, Canada

The RG equations for the infinite 2DXY model with 4-fold anisotropy under geometric scaling, are linearized about their fixed point, and then solved exactly for a finite system by integration up to a system size L. The solution demonstrates that the finite anisotropic 2DXY system: a) does not exhibit a non-universal 2nd-order transition observed in the infinite system; b) is characterized by a product of the anisotropy and $\ln L$; c) with small anisotropy flows past the critical point and exhibits a KT transition; d) with large anisotropy flows to an Ising transition.

The solution near the critical point validates a perturbative approach in small 4-fold anisotropy appropriate, for instance, for ferromagnetic films. This gives quantitative results for the coupling, vortex fugacity and effective 4-fold anisotropy across the entire finite-size transition. In particular, the coupling has a universal point of inflection where vortex-antivortex pairs unbind, as opposed to the "universal jump" seen in the infinite, isotropic system.

MA 5.8 Mon 11:30 EB 202

The zoo of states in the 2D Hubbard model — •Robin Scholle, Pietro Bonetti, Demetrio Vilardi, and Walter Metzner — MPI for Solid State Research, Stuttgart, Germany

We use real-space Hartree-Fock theory to unbiasedly construct a phase diagram of the 2D Hubbard model in temperature and doping. We are able to detect various spin- and charge order patterns including Néel, stripe and spiral order. I will give a short summary of the method followed by a presentation of our current results and a possible outlook for further applications.

MA 5.9 Mon 11:45 EB 202

Magnetic phase transitions in $TbFeO_3$ — •Johanna Jochum[1], Michal Stekiel[2], Alexander Engelhardt[3], Astrid Schneidewind[2], and Christian Pfleiderer[1,3] — [1]Heinz Maier-Leibnitz Zentrum, Technische Universität München, 85748 Garching — [2]JCNS-MLZ, Forschungszentrum Jülich GmbH, Outstation Garching, 85748 Garching — [3]Physik Department, Technische Universität München, 85748 Garching

Rarearth (RE) orthoferrite have been studied widely due to their multiferroic properties [1] on the one hand and on the other hand owing to a series of magnetic transitions, which follow from the interaction between the magnetic sublattices of the Fe and RE atoms [2]. The latter manifests in partial ordering and spin reorientation transitions of these sublattices. $TbFeO_3$ in particular, shows two spin-reorientation transitions. In the high temperature phase (HT) only the Fe sublattice is magnetically ordered. At the first transition, the Fe sublattice polarizes the Tb ions leading to a rotation of the spins of both system towards the crystallographic b axis (IT). At 3K the Tb sublattice orders antiferromagnetically, and the Fe sublattice returns to its high temperature state (LT) [3]. We have studied these spin-reorientation transitions in $TbFeO_3$ as a function of magnetic field using neutron diffraction. The data suggest that the transition from HT to the IT is suppressed as the magnetic field isincrease, leading to strong fluctuations that extend to temperatures beyond the zero field transition.

[1] Y. Ke, et al., Sci. Rep. 6, 19775 (2016) [2] R. L. White, JAP 40, 1061 (1969) [3] A. K. Ovsianikov et al., JMMM 563 170025 (2022)

MA 5.10 Mon 12:00 EB 202

Origin of the antiparallel spin coupling of a $Nd_3Fe_3Sb_7$ single crystal. — •Sabrina Palazzese[1,4], F. Pabst[3], Sh. Yamamoto[1], K. Kummer[2], D. Gorbunov[1], S. Chattopadhyay[1], T. Herrmannsdoerfer[1], M. Richter[5], R. Ray[5], M. Ruck[3], E. Weschke[6], O. Prokhnenko[6], B. Lake[6], and J. Wosnitza[1,4] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden — [2]European Synchrotron Radiation Facility (ESRF) — [3]Fakultät für Chemie und Lebensmittelchemie, TU Dresden — [4]Institut für Festkörper- und Materialphysik, TU Dresden — [5]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) — [6]Helmholtz-Zentrum Berlin (HZB)

We investigated $Nd_3Fe_3Sb_7$ using SQUID magnetometry and X-ray magnetic circular dichroism. Previous studies on polycrystalline samples show that $Nd_3Fe_3Sb_7$ exhibits a rather complex magnetism [1]. We found an unusual antiparallel coupling between the magnetic moments of Nd $4f$ and Fe $3d$ along the c-axis. This is also observed in the isostructural compound $Pr_3Fe_3Sb_7$, as demonstrated by neutron diffraction [2], but the origin of this behavior has not been further elucidated. The compound shows ferrimagnetic ordering below the spin-reorientation transition and planar magnetic anisotropy above it. DFT calculations indicate an induced magnetic moment in the Sb atoms. We attribute the antiparallel coupling to a potential superexchange interaction mediated by the Sb atoms.

[1] N. Nasir, *et al.*, *Intermetallics* **18**, 2361 (2010).
[2] F. Pabst, *et al.*, *Adv. Mat.* **35**, 2207945 (2023).

MA 5.11 Mon 12:15 EB 202

On the valence of chalcogen spinels — •Vinícius Estevo Silva Frehse, Aleksander Sukhanov, Elaheh Sadrollahi, and Marein Rahn — IFMP, Dresden, Germany

The valence characteristics in the metallic ferromagnetic spinels CuCr2X4 (X = S, Se, Te) has long been subject to debate. At the heart of this controversy lies the ambiguity between two scenarios, proposed by F. K. Lotgering and J. B. Goodenough: According to Lotgering, monovalent non-magnetic Cu ions (3d10) exist next to mixed-valent (3+/4+) Cr with a reduced magnetic moment. Conversely, in the Goodenough model, Cu is divalent (3d9), with an anti-parallel spin-polarization that partially compensates the Cr3+ magnetism. In the light of potentially competing or almost degenerate valence distributions on a frustrated lattice, it would be of great interest to clarify the order parameter and mechanism of a pronounced low-temperature phase transition that has recently been observed by local and bulk magnetic probes (μSR, NMR and Mössbauer spectroscopy). Surprisingly, we find that magnetic neutron powder diffraction is not sensitive to this transition. A review of past and present experimental evidence provides some constraints on the unusual scenarios that could reconcile this apparent contradiction.

MA 5.12 Mon 12:30 EB 202

The role of magnetoelastic coupling in $GdRu_2Si_2$ and uniaxial pressure effects on the skyrmion-lattice phase — •Lukas Gries[1], Daniel Mayoh[2], George Wood[2], Geetha Balakrishnan[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Physics, University of Warwick, United Kingdom

The centrosymmetric tetragonal antiferromagnet $GdRu_2Si_2$ displays a rich phase diagram including the square magnetic skyrmion lattice phase. Here, we present high-resolution capacitance dilatometry and magnetisation studies on single crystals in external magnetic fields up to 15 T. Our data show significant magneto-elastic coupling as proven by pronounced anomalies in thermal expansion and magnetostriction at the phase boundaries. The clear signatures of the phase boundaries allow us to discover new phases, thereby expanding and complementing the magnetic phase diagram. We qualitatively and quantitatively determine the uniaxial pressure dependencies of the phase boundaries. In particular the skyrmion-lattice phase is enlarged and stabilised in field and temperature by uniaxial pressure applied along the crystallographic c axis.