MA 14: Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions

Time: Tuesday 9:30–12:00 Location: H47

Invited Talk MA 14.1 Tue 9:30 H47

Overriding universality of ferromagnetic phase transitions through nano-scale materials design — •Andreas Berger — CIC nanoGUNE BRTA, E-20018 San Sebastian, Spain

In recent years, significant interest has developed in magnetic thin films, in which the exchange coupling strength is ferromagnetic everywhere, but locally varying by means of nano-scale materials design. This interest is associated with the fact that such designed materials profiles translate into strongly varying magnetization states down to the 1-2 nm length scale, which is somewhat surprising, given that ferromagnetism is a collective phenomenon [1]. Correspondingly, such exchange-graded magnetic materials have shown themselves to be a very efficient way of modifying magnetic properties of otherwise rather conventional materials [1]. The most impressive result is hereby the possibility to tune critical exponents, in particular the magnetization onset exponent β in an extremely wide parameter range, which represents a unique way to override the universality usually associated with phase transitions of ferromagnets [2]. The same approach also enabled a complete separation of the temperature dependent onset of ferromagnetism at the Curie temperature from the onset of hysteresis, even in anisotropic materials [3], and it allowed for an enhancement of magnetocaloric properties [4]. Thus, exchange-graded materials are an extremely promising way to design the thermal evolution of magnetic properties and adapt it to device requirements. [1] Phys. Rev. B 98, 064404 (2018); [2] Phys. Rev. Lett. 127, 147201 (2021); [3] Phys. Rev. Appl. 16, 034038 (2021); [4] J. Phys. D 54, 304003 (2021).

MA 14.2 Tue 10:00 H47

Poisson-Dirichlet distributions and weakly first-order spin-nematic phase transitions — •Nils Caci[1], Peter Mühlbacher[2], Daniel Ueltschi[2], and Stefan Wessel[1] — [1]RWTH Aachen University, Aachen, Germany — [2]University of Warwick, Coventry, United Kingdom

Weakly first-order transitions, i.e. discontinuous phase transitions with very large correlation lengths, have become a vivid subject in condensed matter research and beyond in recent years. Therefore, establishing quantum systems in which weakly first order phase transitions can be robustly demonstrated is of great interest. We present a quantitative characterization of generic weakly first-order thermal phase transitions out of planar spin-nematic states in three-dimensional spin-one quantum magnets, based on calculations using Poisson-Dirichlet distributions (PD) within a universal loop model formulation, combined with large-scale quantum Monte Carlo calculations. In contrast to earlier claims, the thermal melting of the nematic state is not continuous, instead we identify a weakly first-order transition. Furthermore, we obtain exact results for the order parameter distribution and cumulant ratios at the melting transition. Our findings establish the thermal melting of planar spin-nematic states as a generic platform for quantitative approaches to weakly first-order phase transitions in quantum systems with a continuous SU(2) internal symmetry.

MA 14.3 Tue 10:15 H47

Derivation of Spin Hamiltonian by Algebraic Methods — •Hiroshi Katsumoto[1], Fabian Lux[1,2], Yuriy Mokrousov[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

Complex magnetism is known to emerge from competing Heisenberg interactions and higher-order spin interactions [1]. In addition, previously unknown interactions such as the Chiral-Chiral interaction due to topological orbital magnetism turn also out to be essential to explain the magnetic properties [2]. However, a method for uniquely deriving spin Hamiltonians that captures the spin interactions of a given system has not yet been established. In this presentation, we give rigorous spin Hamiltonians for isotropic spin interactions for a given total localized spin S and the number of magnetic sites. The derivation of the spin Hamiltonian is based on the algebraic structure that the spin operators follow for arbitrary spin magnitude. By organizing the algebraic structure obeyed by the general spin operators, we discuss the construction of the exact spin Hamiltonian and the higher-order terms of interactions, especially for the cases $S = 1/2$ and 1.

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[1] M. Hoffmann *et al.*, Phy. Rev. B **101**, 024418 (2020).

[2] S. Grytsiuk *et al.*, Nat. Commun. **11**, 511 (2020).

MA 14.4 Tue 10:30 H47

***Ab initio* approach to compute magnetic Gibbs free energies and phase transitions using magnetically constrained supercells** — •Eduardo Mendive Tapia[1,2,3], Nicolas Essing[1], Rudolf Zeller[1], Stefan Blügel[1], Jörg Neugebauer[2], and Tilmann Hickel[2] — [1]Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [3]Universitat de Barcelona, D-08028 Barcelona, Spain

We present a first-principles approach for the computation of the magnetic Gibbs free energy of materials using magnetically constrained supercell calculations [1]. Our approach, based on an adiabatic approximation for the local moment orientations [2], describes magnetic phase transitions and how electronic and magnetovolume mechanisms generate a discontinuous (first-order) character. Results obtained for bcc Fe and the triangular antiferromagnetic state of Mn$_3$AN (A = Ga, Ni) [3] will be presented and used to explain their negative volume expansion and the first-order nature observed experimentally. The performance of two different density functional theory codes, the Vienna Ab Initio Simulation package (VASP) and the linear-scaling KKR-nano code suitable for thousands of atoms (https://jukkr.fz-juelich.de), will be shown.

[1] E. Mendive-Tapia, J. Neugebauer, T. Hickel, Phys. Rev. B **105**, 064425 (2022).

[2] B. Gyorffy *et al.*, J. Phys. F: Met. Phys. **15** 1337 (1985).

[3] D. Boldrin *et al.*, Phys. Rev. X **8** 041035 (2018).

MA 14.5 Tue 10:45 H47

spin-reorientation in CuCr2S4 from muSR — •elaheh sadrollahi[1], jochen litterst[2], lilian prodan[3,4], vladimir tsurkan[3,4], and alois loidl[3] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Germany — [2]Institut für Physik der kondensierten Materie, Technische Universität Braunschweig, Germany — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [4]Institute of Applied Physics, MD 2028, Chisinau, Republic of Moldova

Muon Spin Relaxation and Rotation (muSR) experiments have been performed on the thio spinel CuCr2S4 for further clarifying the long-standing controversy regarding its electronic and magnetic states [1,2]. Long regarded as ferromagnet (Tc=378 K) with magnetic moments residing only on Cr, CuCr2S4 is nowadays considered a ferrimagnetic with small magnetic moments on the Cu sites [3]. In addition to the transition at Tc, our muSR data reveal transitions around 50 K and 100 K with changes in spontaneous rotation signals and in relaxation behaviour. There is a close resemblance between these muSR results with those found for Fe1-xCuxCr2S4 with high Cu concentrations [4]. We interpret the transitions with spin re-orientations and will discuss the Jahn-Teller effect as a possible reason.[1] F. K. Lotgering et al., J. Phys. Chem. Solids 30, 799 (1969) and Solid State Commun. 2, 55 (1964). [2] J. B. Goodenough, Solid State Commun. 5, 577 (1967) and J. Phys. Chem. Solids 30, 261 (1969).[3] A. Kimura et al., Phys. Rev. B 63,224420 (2001).[4] E. Sadrollahi, Doctoral Thesis (2018): https://publikationsserver.tubraunschweig.de/receive/dbbs_mods_00066058.

MA 14.6 Tue 11:00 H47

identification of a new hidden-order phase in the magnetic phase diagram of Ce$_3$Pd$_{20}$Si$_6$ — •F. Mazza[1], P. Y. Portnichenko[2], P. Steffens[3], M. Boehm[3], E. S. Choi[4], M. Nikolo[5], S. Paschen[1], and D. S. Inosov[2] — [1]TU Wien, Austria — [2]TU Dresden, Germany — [3]ILL, Grenoble, France — [4]Florida State University, Tallahassee, USA — [5]St. Louis University, USA

Magnetically hidden order is a hypernym for electronic ordering phenomena whose microscopic symmetry cannot be revealed with conventional neutron or x-ray diffraction. In a handful of f-electron systems, the ordering of odd-rank multipoles leads to order parameters with a vanishing neutron cross-section. Among them, Ce$_3$Pd$_{20}$Si$_6$ is known for its unique phase diagram exhibiting two distinct multipolar-ordered ground states (phases II and II′), separated by a field-driven quantum phase transition. Using torque magnetometry at subkelvin temperatures, here we find another phase transition at higher fields above 12 T, which appears only for low-symmetry magnetic field directions. While the order parameter remains unknown, this discovery renders $Ce_3Pd_{20}Si_6$ the first known material with two metamultipolar phase transitions. They are both clearly manifested in the magnetic-field dependence of the field-induced (111) Bragg intensities measured with neutron scattering for $\mathbf{B} \parallel [11\bar{2}]$. Furthermore, the magnetic excitation spectrum suggests that the new phase II″ may have a different propagation vector in the vicinity of $\mathbf{Q} = (010)$, revealed by the minimum in the dispersion representing the Goldstone mode of this hidden-order phase.

MA 14.7 Tue 11:15 H47

Magnetic and thermodynamic properties of van-der-Waals $\mathbf{CuCrP_2S_6}$ — •Kranthi Kumar Bestha[1,2], Laura Teresa Corredor Bohorquez[1], Vilmos Kocsis[1], Sebastian Selter[1], Saicharan Aswartham[1], Bernd Buechner[1,2], and Anja U. B. Wolter[1] — [1]Institute for Solid State Research, Leibniz IFW Dresden, 01069, Dresden, Germany — [2]Institute of Solid State and Materials Physics and Wuerzburg-Dresden Cluster of Excellence ct.qmat, Technical University Dresden, 01062 Dresden, Germany

Two-dimensional van-der-Waals materials with intrinsic multiferroic properties are advantageous over 3D multiferroic materials for next generation nanoscale magnetic and electric devices. $CuCrP_2S_6$ is a quasi-2D vdW multiferroic candidate with magnetic and ferroelectric polarization arising from Cr and Cu sublattices, respectively. $CuCrP_2S_6$ exhibits intralayer ferromagnetic and interlayer antiferromagnetic interactions. $M(T)$ and $Cp(T)$ on single crystal $CuCrP_2S_6$ reveal antiferromagnetic ordering at T_N=31.5 K. Our magnetic data reveal predominant ferromagnetic interactions below the ordering temperature and short-range ferromagnetic correlations above T_N. Magnetic fields applied in the ab-plane exhibit a spin-flop transition at a relatively small magnetic field of 4.3 kOe with weak anisotropy in the ab-plane. For a clear understanding of the magnetic anisotropy of this material, in-plane and out-of-plane angular-dependent dc magnetic studies were performed. Different symmetries are observed for both the in- and out-of-plane angular-dependent data. Our results are summarized in H-T phase diagrams for different main directions.

MA 14.8 Tue 11:30 H47

Probing magneto-elastic coupling in the quasi-2D van der Waals ferromagnet $\mathbf{Cr_2Ge_2Te_6}$ — •Laura T. Corredor[1], Bastian Rubrecht[1,2], Takahiro Sakurai[3], Hitoshi Ohta[4], Alexey Alfonsov[1], Sebastian Selter[1], Saicharan Aswartham[1], Vladislav Kataev[1], Anja U. B. Wolter[1], and Bernd Büchner[5] — [1]Institute for Solid State Research, Leibniz IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [3]Research Facility Center for Science and Technology, Kobe University, Kobe 657-8501, Japan — [4]Molecular Photoscience Research Center, Kobe University, Nada, Kobe 657-8501 Japan — [5]Institute of Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

The first 2D uniaxial ferromagnetic semiconductor $Cr_2Ge_2Te_6$ -with a layered structure-is promising for exciting new applications such as ultra-compact spintronics or magnonic devices, which need 2D long-range magnetic order as crucial feature. Since magnetocrystalline anisotropy is essential for the stabilization of magnetic order in 2D spin systems, the possibility to control it via a tunable external parameter- such as pressure or strain- can provide useful hints for the engineering of magneto-electric heterostructures with strained architectures. With this motivation, magnetization and ferromagnetic resonance (FMR) experiments under hydrostatic pressure on $Cr_2Ge_2Te_6$ single crystals were performed. Insights on the magneto-elastic coupling and magnetic interactions with the increase of pressure are discussed.

MA 14.9 Tue 11:45 H47

Spin structure of Frenkel excitons on $\mathbf{Cu^{2+}}$-ions in the antiferromagnet $\mathbf{CuB_2O_4}$ revealed by magneto-absorption spectroscopy — •Dennis Kudlacik[1], Natalia E. Kopteva[1], Dimitri R. Yakovlev[1], Mikhail V. Eremin[3], Alexey R. Nurmukhametov[3], Manfred Bayer[1], and Roman V. Pisarev[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]St. Petersburg, Russia — [3]Kazan, Russia

Frenkel excitons in magnetic insulators have attracted considerable interest in recent years as they allow the migration or transmission of a localized excitation. We have investigated this property which is reflected in the Davydov splitting of the exciton in the antiferromagnet copper metaborate, CuB_2O_4 [1]. This magnetic insulator consists of two weakly interacting sublattices of Cu^{2+} ions. Below the Neel temperature of $T_N = 21$ K its magnetic structure is dominated by the antiferromagnetic order of the 4b sublattice which comprises 4 Cu^{2+} ions twice degenerate in spin resulting in the formation of 8 collective charge-spin Frenkel-Davydov excitations. From a comparison of the experimental data with the results of the theoretical model we define the parameters of Frenkel exciton states, determine the electron-energy transfer between antiferromagnetically coupled copper spins as well as the anisotropic Cu^{2+} g-factors of ground and excited states.

[1] N. E. Kopteva et al., Phys. Rev. B 105, 024421 (2022).