MA 14: Focus Session: Higher-Order Magnetic Interactions - Implications in 2D and 3D Magnetism II

Materials in which the magnetic moments order or cooperate in unusual ways underpin a plethora of physical phenomena, from strong magnetoelectric effects to topological quasiparticles, thus holding great promise for future spintronic and quantum computing applications. Magnetic interactions are the fundamental quantities that explain the complex magnetic phase diagrams and exotic excitation spectra of these intriguing materials. Recent theoretical and experimental developments have led to a realization of a pivotal role played by higher-order magnetic interactions in stabilizing intricate magnetic structures. The 4-spin 3-site interaction stabilizes an up-up-down-down state, which can become chiral. Theoretically, novel 4-spin chiral interactions and even 6-spin (chiral-chiral) couplings might explain the emergence of complex short-period 3D magnetic structures, and could open a path to the discovery of materials hosting 3D topological magnetization textures, such as magnetic hopfions. Experimentally, 4-spin interactions are conjectured to play a central role in skyrmions lattice formation in frustrated centrosymmetric materials. This area of research will make a strong impact in the field of magnetism in the upcoming years.

Organizers: Samir Lounis (University of Duisburg-Essen and Forschungszentrum Jülich), Manuel dos Santos Dias and Stefan Blügel (Forschungszentrum Jülich), Jonathan White (Paul Scherrer Institut)

Time: Thursday 13:30–15:15 Location: H5

Invited Talk MA 14.1 Thu 13:30 H5

The role of itinerant electrons and higher order magnetic interactions among fluctuating local moments in metallic magnets — •Julie Staunton — University of Warwick, Coventry CV4 7AL, U.K.

When external stimuli or varying temperature alter its magnetic properties, a metal's complex electronic fluid, with its emergent magnetic 'local moments', transforms. The itinerant electrons, coupled to these more localised spin degrees of freedom, have a profound effect on structure, electronic transport, and so on. The ab initio Density Functional Theory-based Disordered Local Moment method successfully describes this physics. It can locate and characterise magnetic phase transitions and calculate temperature and field-dependent magnetic properties. It will be shown how the theory provides a Gibbs free energy function of local moment order parameters with two central objects - local moment correlation functions in the paramagnetic state and local internal magnetic fields as functions of magnetic order. The potentially most stable magnetic phases and dominant 'exchange' interactions between pairs of local moments or effective 'spins' are identifiable from the first. Higher order magnetic interactions are extracted from the second and depend on how the electronic structure evolves with the state and extent of magnetic order. The approach will be illustrated by applications to the magnetic order and its link to the Fermi surfaces of rare earth metals and their compounds, permanent magnetic properties and the rich magnetic-strain phase diagrams and associated caloric effects of some transition metal antiferromagnets.

MA 14.2 Thu 14:00 H5

Short period magnetization texture of B20-MnGe explained by thermally fluctuating local moments — •Eduardo Mendive Tapia[1,2], Manuel dos Santos Dias[1], Sergii Grytsiuk[1], Julie Staunton[3], Stefan Blügel[1], and Samir Lounis[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [3]University of Warwick, CV4 7AL, Conventry, UK

B20-type compounds, such as MnSi and FeGe, host helimagnetic and skyrmion phases at the mesoscale, which are canonically explained by the combination of ferromagnetic isotropic interactions with weaker chiral Dzyaloshinskii-Moriya ones. Mysteriously, MnGe evades this paradigm as it displays a noncollinear magnetic state at a much shorter nanometer scale [1]. Using a Disordered Local Moment theory within the KKR method [2,3], here we show that the length scale and volume-dependent magnetic properties of MnGe stem from purely isotropic exchange interactions generally obtained in the paramagnetic state. Our approach is validated by comparing MnGe with the canonical B20-helimagnet FeGe. The free energy of MnGe is calculated, from which we show how triple-q magnetic states can stabilize by adding higher-order interactions. –Work funded by the DAAD and EU Horizon 2020 via ERC-consolidator Grant No. 681405-DYNASORE.

[1] Fujishiro et al., Nat. Commun. **10**, 1059 (2019)
[2] Gyorffy et al., J. of Phys. F: Metal Phys. **15**, 1337 (1985)
[3] Jülich KKR codes (https://jukkr.fz-juelich.de)

MA 14.3 Thu 14:15 H5

Symmetry analysis of multi-spin interactions — •Levente Rózsa — University of Konstanz, Konstanz, Germany

Two-spin interactions including the isotropic exchange and Dzyaloshinsky-Moriya (DM) interactions or the magnetocrystalline anisotropy play a fundamental role in the formation of non-collinear spin structures. Going beyond the two-spin approximation enables the stabilization of, e.g., the zero-field nanoskyrmion lattice attributed to four-spin isotropic interactions [1]. A four-spin generalization of the DM interaction has also been proposed recently [2,3,4].

Multi-spin interactions are conventionally derived based on a perturbative expansion [2,4], which becomes cumbersome if many spins or higher orders of the spin-orbit coupling are involved. Here we present a systematic way of constructing multi-spin interaction terms based on a symmetry analysis. In the case of four spins, besides the isotropic and DM interactions, we identify symmetric second-order and fourth-order anisotropies, as well as a DM-like asymmetric anisotropy term. It is discussed how these coupling terms transform under point group operations, analogously to the Moriya rules; how they can be fitted based on the energies of specific spin configurations; and which types of non-collinear structures emerge based on these interactions.

[1] S. Heinze et al., Nat. Phys. 7, 713 (2011).
[2] S. Brinker et al., New J. Phys. 21, 083015 (2019).
[3] A. Lászlóffy, L. Rózsa et al., Phys. Rev. B 99, 184430 (2019).
[4] S. Grytsiuk et al., Nat. Commun. 11, 511 (2020).

MA 14.4 Thu 14:30 H5

Spontaneous atomic-scale hexagonal spin lattices driven by higher-order exchange interactions — •Mara Gutzeit[1], André Kubetzka[2], Soumyajyoti Haldar[1], Henning Pralow[1], Roland Wiesendanger[2], Stefan Heinze[1], and Kirsten von Bergmann[2] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstraße 15, 24098 Kiel, Germany — [2]Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Higher-order exchange interactions (HOI) beyond the pair-wise Heisenberg exchange can be the origin of a variety of complex magnetic structures such as conical spin spirals [1], multi-Q states [2,3], or nanoskyrmion lattices [4]. Here, using spin-polarized scanning tunneling microscopy we explore uniaxial spin states as well as two-dimensionally modulated spin structures in ultrathin Fe/Rh films on the Ir(111) surface. Density functional theory calculations elucidate how HOI stabilize spontaneous atomic-scale hexagonal spin lattices exhibiting only a small deviation from collinearity in these systems which are characterized by a weak Dzyaloshinskii-Moriya interaction. We demonstrate that a subtle interplay of HOI is responsible for the transition between different magnetic ground states.

[1] Yoshida *et al.* PRL **108**, 087205 (2012)
[2] Krönlein *et al.* PRL **120**, 207202 (2018)

[3] Spethmann *et al.* PRL **124**, 227203 (2020)
[4] Heinze *et al.* Nat. Phys. **7**, 713 (2011)

MA 14.5 Thu 14:45 H5

Dzyaloshinskii-Moriya Interaction revisited — •Hiroshi Katsumoto and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In recent years, the Dzyaloshinskii-Moriya interaction (DMI) has received enormous attention. New materials, new physical issues, and new measurement methods have led to new questions. *E.g.*, recent theoretical studies have proposed higher-order interaction terms for this DMI [1]. Introduced by Dzyaloshinskii [2] on the basis of phenomenological and group-theoretical arguments in combination with classical axial vectors and substantiated by Moriya [3] for the first time microscopically based on the quantum mechanical spin-orbit interaction, in systems where the inversion symmetry is locally broken, the DMI affects the magnetic properties. We reiterate the cause of weak ferromagnetism in centrosymmetric materials and investigate the relationship between the Lifshitz invariant associated with macroscopic chiral symmetry breaking and microscopic DMI. We will discuss how to uniquely write down the interaction term in the spin Hamiltonian from the irreducible representation depending on the size of the spin.

We acknowledge funding from the DARPA TEE program through grant MIPR (#HR0011831554) from DOI, and Deutsche Forschungsgemeinschaft (DFG) through SPP-2137 and SFB-1238 (project C1).

[1] S. Brinker, *et al.*, New J. Phys. **21**, 083015 (2019).
[2] I.E. Dzialoshinskii, Sov. Phys. JETP **5**, 1259 (1957).
[3] T. Moriya, Phys. Rev. **120**, 91 (1960).

MA 14.6 Thu 15:00 H5

Chiral multi-site interactions in prototypical magnetic systems — •Sascha Brinker[1], Manuel dos Santos Dias[1], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Atomistic spin models can successfully explain the properties of magnetic materials once the relevant magnetic interactions are identified. Recently, new types of chiral interactions that generalize the Dzyaloshinskii-Moriya interaction have been proposed [1,2,3,4]. Here, we present a systematic construction of a generalized spin model containing isotropic and chiral multi-site interactions, motivated by a microscopic model, and their symmetry properties are established. We show that the chiral interactions arise solely from the spin-orbit interaction and that the multi-site interactions do not have to follow Moriya's rules, unlike the Dzyaloshinskii-Moriya interaction [1,4]. We then report on density functional theory calculations for prototypical magnetic systems, finite magnetic nanostructures on heavy metal substrates and two-dimensional systems with inversion symmetry.

[1] S. Brinker, M. dos Santos Dias and S. Lounis, New J Phys **21**, 083015 (2019); [2] A. Lászlóffy *et al.*, Phys Rev B **99**, 184430 (2019); [3] S. Grytsiuk *et al.*, Nat Commun **11**, 511 (2020); [4] S. Brinker, M. dos Santos Dias and S. Lounis, Phys Rev Research **2**, 033240 (2020)

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