MA 10: Focus Session: Higher-Order Magnetic Interactions - Implications in 2D and 3D Magnetism I

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: Wednesday 13:30–16:30 Location: H5

Invited Talk MA 10.1 Wed 13:30 H5

Topological spin crystals stabilized by itinerant frustration — •Yukitoshi Motome — The University of Tokyo, Tokyo, Japan

Topological spin crystals, which are periodic arrays of topological spin textures such as vortices, skyrmions, and hedgehogs, have attracted numerous attention for the potential use of their magnetic, transport, and optical properties for future spintronics and quantum computing. For materializing such unconventional magnetism, it is crucially important to understand the relevant magnetic interactions. Widely known is the Dzyaloshinskii-Moriya interaction, which stabilizes swirling spin textures in competition with ferromagnetic exchange interactions. Here, we theoretically study a different mechanism driven by effective magnetic interactions arising from itinerant nature of electrons. We show that, in addition to the well-known Ruderman-Kittel-Kasuya-Yosida interaction, multiple-spin interactions naturally arise as higher-order contributions from the spin-charge coupling in itinerant magnets. They are intrinsically long-ranged and have characteristic wave numbers specified by the Fermi surfaces, like the Ruderman-Kittel-Kasuya-Yosida interaction. We find that frustration among such long-range multiple-spin interactions, which we call itinerant frustration, can stabilize a variety of topological spin crystals with unique features, even in centrosymmetric systems where the Dzyaloshinskii-Moriya interaction is absent. We discuss our results with recent advances in experiments.

Invited Talk MA 10.2 Wed 14:00 H5

Formation of spin-hedgehog lattices and giant topological transport properties in chiral magnets — •Naoya Kanazawa — University of Tokyo, Tokyo, Japan

The last few years have seen remarkable progress in the discovery of versatile topological spin crystals with different topology, dimensionality and density. In parallel, the crucial role of higher-order magnetic interactions among multiple spins has been gradually recognized. In this talk, we report the formation of three-dimensional topological spin texture, i.e., the lattices of spin hedgehogs in a chiral magnet MnGe and its relatives. Their nature of twisting spins in short periods imply the relevance of such higher-order interactions. We also introduce various giant transport properties, such as topological Hall and thermoelectric effects, which may originate from the effective monopole field and dynamical fluctuations of spin hedgehogs.

This work is done in collaboration with K. Akiba, T. Arima, R. Arita, S. Awaji, C. D. Dewhurst, Y. Fujishiro, M. Ichikawa, K. Ishizaka, H. Ishizuka, F. Kagawa, K. Kakurai, Y. Kawamura, M. Kawasaki, A. Kikkawa, S. Kimura, K. Kindo, T. Koretsune, A. Kitaori, Y. Kozuka, R. Kurihara, A. Matsuo, H. Mitamura, A. Miyake, D. Morikawa, T. Nakajima, A. Nakamura, N. Nagaosa, K. Ohishi, H. M. Rønnow, K. Shibata, T. Shimojima, J. Shiogai, Y. Taguchi, M. Tokunaga, Y. Tokura, A. Tsukazaki, V. Ukleev, J. S. White, X. Z. Yu.

Invited Talk MA 10.3 Wed 14:30 H5

Topological-chiral magnetic interactions driven by emergent orbital magnetism — •Sergii Grytsiuk[1], Jan-Philipp Hanke[1], Markus Hoffmann[1], Juba Bouaziz[1], Olena Gomonay[2], Gustav Bihlmayer[1], Samir Lounis[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

Based on microscopic arguments and a systematic total energy expansion, further validated by electronic structure calculations, we discover a new class of magnetic interactions of chiral nature originating from the so-called topological orbital moment (TOM) of electrons in non-coplanar magnets [1]. The TOMs, $\mathbf{L}^{\mathrm{TO}}$, emerge from the scalar spin chirality of three magnetic moments, $\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_\mathbf{k})$. As a result of a six-spin– or a four-spin interaction, they can interact with each other and interact with the spins of the underlying lattice. In the context of B20-type chiral magnet MnGe, these novel interactions can dominate over the Dzyaloshinskii-Moriya interaction in selecting the chiral ground state, providing possibly a key for solving the open question of the recently observed complex 3D magnetic structures. By providing a mechanism for the physical realization of the Faddeev model with hopfion solutions, topological-chiral interactions might play a key role in triggering the formation of 3D magnetic solitons without the assistance of an external magnetic field.

[1] S. Grytsiuk *et al.*, Nature Commun **11**, 511 (2020).

15 min. break.

Invited Talk MA 10.4 Wed 15:15 H5

Complex spin structures in thin transition metals films and their oxides — •Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Germany

The term "magnetism" subsumes a plethora of interactions originating from various physical mechanisms. Their competition often results in highly complex spin structures, such that the specific origin is masked and can only be unraveled by combining experiment and theory. For example, for an Fe monolayer on Rh(111) an up-up-down-down (↑↑↓↓) spin structure was predicted by DFT [1] which was only later understood to originate from the previously unconsidered four-spin–three-site beyond-Heisenberg interaction [2]. We could indeed confirm this ↑↑↓↓ spin structure experimentally by spin-polarized STM. Three orientational domains were observed, the field-dependent behavior of which is surprisingly complex, potentially due to uncompensated spins at domain boundaries. Furthermore, in a recent survey of submonolayer transition metal oxides on Ir and Pt(001) we observed highly complex spin structures which appears to be driven by a Dzyaloshinskii-Moriya-enhanced Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [3]. However, the orientation of the Dzyaloshinskii-Moriya vector and the observation of a long-wavelength spin rotation have not yet been adequately explained [4].

[1] A. Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)
[2] A. Krönlein *et al.*, Phys. Rev. Lett. **120**, 207202 (2018)
[3] M. Schmitt *et al.*, Nature Comm. **10**, 2610 (2019)

[4] M. Schmitt *et al.*, Phys. Rev. B **100**, 054431 (2019)

MA 10.5 Wed 15:45 H5

Two-dimensional atomic-scale spin textures in Fe monolayers — André Kubetzka, Roland Wiesendanger, and •Kirsten von Bergmann — Department of Physics, University of Hamburg, Germany

Higher-order interactions can induce two-dimensionally modulated magnetic ground states at zero magnetic field, and spin-polarized scanning tunneling microscopy (SP-STM) is a powerful tool to characterize such spin structures down to the atomic scale [1-3].

Using SP-STM we have recently observed several different square or hexagonal magnetic ground states in Fe monolayers in contact with Rh and Ir layers. The details of the resulting states with magnetic periods on the order of one nanometer depend critically on the stacking of the Fe layer and the number of adjacent Rh or Ir layers [1,4-7].

[1] S. Heinze *et al.*, Nature Phys. **7**, 713 (2011).
[2] Y. Yoshida *et al.*, Phys. Rev. Lett. **108**, 087205 (2012).
[3] J. Spethmann *et al.*, Phys. Rev. Lett. **124**, 227203 (2020).
[4] K. von Bergmann *et al.*, Nano Lett. **15**, 3280 (2015).
[5] N. Romming *et al.*, Phys. Rev. Lett. **120**, 207201 (2018).
[6] A. Kubetzka *et al.*, Phys. Rev. Materials **4**, 081401(R) (2020).
[7] M. Gutzeit *et al.*, (in preparation).

MA 10.6 Wed 16:00 H5

Three- and four-spin interactions from first-principles: calculations and properties — •Sergiy Mankovsky, Svitlana Polesya, and Hubert Ebert — Dept. Chemistry, LMU Munich, Butenandtstrasse 11, D-81377 Munich, Germany

We discuss an extension of the Heisenberg Hamiltonian by accounting for the contributions of higher order interactions calculated on a first-principles level, that can play a crucial role for the stabilization of various types of non-collinear magnetic structure, as for example skyrmions. All calculations are performed by making use of the fully relativistic Korringa-Kohn-Rostoker (KKR) Green function method. We focus on the three-spin and four-spin interaction parameters concerning their calculation and properties. In particular, we discuss their controversial interpretation and the origin of the three-spin chiral interaction (TCI) represented by an expression worked out recently (Phys. Rev. B, **101**, 174401 (2020)). An interpretation of the TCI is suggested, showing explicitly its dependence on the relativistic spin-orbit coupling and on the topological orbital susceptibility (TOS). This is based on an expression for the TOS that is worked out on the same footing as the expression for the TCI. Using first-principles calculations we demonstrate in addition numerically the common topological properties of the TCI and TOS.

MA 10.7 Wed 16:15 H5

Role of higher-order exchange interactions for skyrmion stability — •Souvik Paul[1,2], Soumyajyoti Haldar[2], Stephan von Malottki[2], and Stefan Heinze[2] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany — [2]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel, Germany

Magnetic skyrmions have recently become a research focus as they show promise for future magnetic memory and logic devices. One key obstacle for applications is the stability of skyrmionic bits against thermal fluctuations. The importance of Heisenberg exchange interaction, Dzyaloshinskii-Moriya interaction, magnetocrystalline anisotropy and dipole-dipole interactions in skyrmion stability has been reported. However, due to their origin from a fourth-order perturbation theory, non-Heisenberg higher-order exchange interactions (HOI) − the biquadratic, the three-site-four-spin and the four-site-four-spin interaction − have so far been neglected. Using *ab-initio* parametrized atomistic spin dynamics simulations in ultrathin films, we demonstrate that the HOI play an important role for skyrmion stability. We find that the effect of the first two HOI, to a large extent, can be included in the effective Heisenberg exchange constants. However, the four-site four spin interaction behaves qualitatively in a different way and has a large contribution on the energy barrier stabilizing skyrmions and antiskyrmions against annihilation. Our study opens up a new avenue for increasing the stability of topological spin structures.