MA 43: 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 and Stefan Blügel (Forschungszentrum Jülich), Jonathan White (Paul Scherrer Institut)

Time: Thursday 9:30–13:00 Location: HSZ 04

Invited Talk MA 43.1 Thu 9:30 HSZ 04

Magnetic vortices, skyrmions, and hedgehogs stabilized by long-range multiple-spin interactions — •Yukitoshi Motome — The University of Tokyo, Tokyo, Japan

Topological magnetic 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 relativistic Dzyaloshinskii-Moriya interaction, which stabilizes swirling spin textures in competition with ferromagnetic exchange interactions. Here, we theoretically study another interactions working for more than two spins simultaneously. We show that such multiple-spin interactions naturally arise in itinerant magnets as higher-order contributions from the spin-charge coupling. They are intrinsically long-ranged with characteristic wave numbers specified by the Fermi surfaces, like the Ruderman-Kittel-Kasuya-Yosida interaction. We find that such long-range multiple-spin interactions can stabilize a variety of topological magnetic textures with unique features, even in centrosymmetric systems where the Dzyaloshinskii-Moriya interaction is absent: vortex crystals with chiral stripes, skyrmion crystals with a high topological number, unusual skyrmions in Rashba metals, and magnetic hedgehog lattices. We discuss our results with recent advances in experiments.

Invited Talk MA 43.2 Thu 10:00 HSZ 04

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 implies 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 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 43.3 Thu 10:30 HSZ 04

Topological-chiral magnetic interactions driven by emergent orbital magnetism — •S. Grytsiuk[1], J.-P. Hanke[1], M. Hoffmann[1], J. Bouaziz[1], O. Gomonay[2], G. Bihlmayer[1], S. Lounis[1], Y. Mokrousov[1,2], and S. 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 noncoplanar magnets [1]. The TOMs, $\mathbf{L}^{\mathrm{TO}}$, emerge from the scalar spin chirality of three magnetic moments, $\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S_k})$. 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 Comm., accepted (2019); ArXiv:1904.02369

MA 43.4 Thu 11:00 HSZ 04

The chiral biquadratic pair interaction — •Sascha Brinker, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

The Dzyaloshinskii-Moriya interaction being chiral and driven by relativistic effects, leads to the stabilization of highly-noncollinear spin textures such as skyrmions, which thanks to their topological nature are promising building blocks for magnetic data storage and processing elements. Here, we reveal and study a new chiral pair interaction, $\vec{C}_{ij} \cdot (\vec{S}_i \times \vec{S}_j)(\vec{S}_i \cdot \vec{S}_j)$, which is the biquadratic equivalent of the Dzyaloshinskii-Moriya interaction. First, we derive this interaction and its guiding principles from a microscopic model, and we connect the atomistic form to the micromagnetic one. Second, we study its properties in the simplest prototypical systems, magnetic $3d$ transition metal dimers deposited on surfaces, resorting to systematic first-principles calculations. Lastly, we discuss its importance and implications not only for magnetic dimers but also for extended systems, namely one-dimensional spin spirals and complex two-dimensional magnetic structures, such as a nanoskyrmion lattice found in an Fe monolayer on Ir(111).

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S. Brinker *et al.*, New J. Phys. **21**, 083015 (2019)

15 min. break.

Invited Talk MA 43.5 Thu 11:30 HSZ 04

How to understand the physics of complex spin structures — •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 43.6 Thu 12:00 HSZ 04

Discovery of a triple-Q state in an ultrathin transition-metal film — Jonas Spethmann[1], Sebastian Meyer[2], Kirsten von Bergmann[1], Soumyajyoti Haldar[2], Jonas Sassmannshausen[1], •Stefan Heinze[2], Roland Wiesendanger[1], and André Kubetzka[1] — [1]Department of Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098 Kiel, Germany

Higher-order exchange interactions have been proposed based on the Hubbard model [1-3]. These terms can stabilize intriguing magnetic ground states due to a superposition of spin spirals. A prominent example is the triple-Q state predicted for a Mn monolayer on Cu(111) [4]. Here, we experimentally verify the existence of two – previously predicted but so far unobserved – magnetic ground states in a Mn monolayer on the Re(0001) surface using spin-polarized scanning tunneling microscopy. For fcc stacking of Mn the row-wise antiferromagnetic state occurs, while for hcp-Mn a superposition of three row-wise antiferromagnetic states, the triple-Q state, appears. Density functional theory calculations elucidate the subtle interplay of different magnetic interactions to form these spin structures and provide insight into the role played by relativistic effects.

[1] M. Takahashi, J. Phys. C Solid State Phys. **10**, 1289 (1977)
[2] A. H. MacDonald *et al.*, Phys. Rev. B **37**, 9753 (1988)
[3] M. Hoffmann and S. Blügel, arXiv:1803.01315 (2018)
[4] P. Kurz *et al.*, Phys. Rev. Lett. **86**, 1106 (2001).

MA 43.7 Thu 12:15 HSZ 04

Isotropic four-spin interactions in magnetic trimers — •Andras Laszloffy[1,2], Bendeguz Nyari[2], and Laszlo Szunyogh[2] — [1]Wigner Research Center for Physics, Budapest, Hungary — [2]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary

Recently a rapidly growing interest emerged in investigating the role of higher order spin interactions, both the SU(2) invariant and the chiral ones. In this contribution we study the effect of four-spin interactions along selective paths in the spin-configuration space of magnetic trimers. In order to calculate the SU(2) invariant four-spin interactions we use a Green's function perturbation scheme, where the spinless part of the Hamiltonian defines the unperturbed system, while the spin-dependent part of the Hamiltonian is treated as perturbation. Two-spin and four-spin interactions can then be obtained in second and fourth order perturbation of the Green's function. We demonstrate how the four-spin interactions enter the spin-model parameters obtained from the method of infinitesimal rotations leading to spurious tensorial two-spin interactions. The theory can be straightforwardly implemented in the Korringa-Kohn-Rostoker Green's function technique and in terms of this method we perform calculations for Cr and Mn trimers deposited on heavy metal surfaces. Comparing the energy obtained from the spin model with direct calculations of the band energy proves that the inclusion of the four-spin interactions significantly increases the accuracy of the spin-model description of the magnetic clusters under consideration.

MA 43.8 Thu 12:30 HSZ 04

First-principles multispin interactions and their impact on magnetic properties — •Sergiy Mankovsky, Svitlana Polesya, Alberto Marmodoro, Eszter Simon, and Hubert Ebert — Dept. Chemistry, LMU Munich, Butenandtstrasse 11, D-81377 Munich, Germany

We discuss the impact of interatomic exchange interactions on magnetic properties beyond the classical Heisenberg model. These extensions include the Dzyaloshinskii-Moriya interaction (DMI), biquadratic (chiral and non-chiral), three-spin and four spin interaction, which can be calculated from first principles on the basis of the fully relativistic Korringa-Kohn-Rostoker (KKR) Green function method. In particular, the role of the non-chiral biquadratic interactions will be discussed in connection to the spin-wave stiffness and critical temperature of magnetic materials. We will discuss also the impact of the higher-order chiral exchange interactions on the formation of skyrmion magnetic structures which is often attributed to the effect of the DMI competing with the isotropic exchange and external magnetic fields. We will discuss also the possibility of an external electric field to tune the exchange interactions with an emphasis on the DMI, and accordingly discuss its impact on the Skyrmion formation.

MA 43.9 Thu 12:45 HSZ 04

Role of higher-order exchange interactions for skyrmion stability — •Souvik Paul, Soumyajyoti Haldar, Stephan von Malottki, and Stefan Heinze — 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 for 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 to increase the stability of topological spin structures.