MA 54: Electron Theory of Magnetism and Micromagnetic Simulations

Time: Friday 9:30–13:00 Location: H34

Invited Talk MA 54.1 Fri 9:30 H34

Itinerant Magnetism in the Parent Iron-Based Superconductors: hidden frustration, nematic transitions, and spin-orbit coupling — •Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany

The pnictides have captured the imagination of the condensed matter community mainly on account of their high Tc's exceeding 50K. However, underpinning this is an equally fascinating topic, namely their magnetic properties, which have been studied in exquisite detail for a range of compounds unusually broad for an itinerant magnet.

This talk will cover rich phase diagram as function of doping, pressure, displaying e.g. separate magnetic and nematic critical points. It showcases important topics such as the interplay of orbital, nematic and magnetic order on account of the orbital character of the Fermi pockets involved. Experimental signatures of these phenomena will be also discussed.

15 min. break

MA 54.2 Fri 10:15 H34

The Gilbert damping in random ferromagnetic alloys from the LMTO method — •Ilja Turek[1], Josef Kudrnovsky[2], and Vaclav Drchal[2] — [1]Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno, Czech Republic — [2]Institute of Physics, Acad. Sci. Czech Rep., Prague, Czech Republic

We present an *ab initio* theory of the Gilbert damping tensor for spin-polarized random alloys within the relativistic tight-binding LMTO method and the coherent potential approximation (CPA) [1]. The formulation employs the atomic-sphere approximation which leads to effective nonlocal torque operators entering the LMTO torque-correlation formula. In contrast to traditional local torque operators [2, 3], the nonlocal torques are nonrandom and spin-independent; the CPA-vertex corrections are indispensable for an exact equivalence of both torques. The developed theory has been applied to random ferromagnetic alloys of $3d$ elements (Fe, Co, Ni), to pure iron with a model atomic-level disorder (simulating the effect of a finite temperature), and to stoichiometric FePt alloys with a varying degree of the $L1_0$ atomic long-range order. [1] I. Turek et al., arXiv: 1510.03571 (2015). [2] H. Ebert et el., Phys. Rev. Lett. 107, 066603 (2011). [3] A. Sakuma, J. Phys. Soc. Japan 81, 084701 (2012).

MA 54.3 Fri 10:30 H34

Influence of spin-orbit coupling on the magnetic dipole term T_z in XMCD sum rules — •Ondrej Sipr[1], Hubert Ebert[2], and Jan Minar[2,3] — [1]Institute of Physics ASCR, Prague — [2]Ludwig-Maximilians-Universität, München — [3]University of West Bohemia, Pilsen

Sum rules are a powerful tool for interpreting x-ray magnetic circular dichroism (XMCD) spectra: they give access to $m_{\rm spin}$ and $m_{\rm orb}$ separately. However, these rules provide $m_{\rm spin}$ only in a combination as $m_{\rm spin} + 7T_z$, where T_z is the expectation value of the intra-atomic dipole operator ("magnetic dipole term"). While T_z can be usually neglected in the bulk, it can be large for surfaces, monolayers and clusters where, additionally, a considerable anisotropy of T_z is expected.

Interpretation of T_z often relies on an approximate expression for T_z valid if spin-orbit coupling (SOC) can be neglected. In that case, moreover, T_z depends on the direction of magnetization in a specific way, allowing for its elimination from XMCD experiment by doing measurements at the magic angle. Therefore, it is desirable to check whether the effect of SOC on T_z can or cannot be neglected.

We calculated T_z for Co monolayers and adatoms on noble metals (Cu, Ag, Au, Pd, Pt). We found that the effect of SOC on T_z can be neglected for monolayers but not for adatoms. Simple intuition or the magic-angle-based elimination of T_z from XMCD data thus cannot be used for adatoms or clusters which, at the same time, are systems where T_z is very important.

MA 54.4 Fri 10:45 H34

Implementation of the Relativistic DLM scheme within the SPR-KKR method: Finite temperature magnetic properties of metals and alloys. — •Sergiy Mankovsky and Hubert Ebert — Dept. Chemie, Universität München, D-81377 München, Deutschland

The relativistic disordered local moment (RDLM) method [1,2] has been implemented within the fully relativistic spin polarized KKR band structure method. Corresponding electronic structure calculations within this approach, that account self-consistently for temperature induced magnetic disorder, allows to go beyond the rigid spin approximation. This important step may be crucial in particular for itinerant electron magnetic materials and gives access to a more reliable investigation of various temperature dependent magnetic properties (e.g. average magnetization, magnetic anisotropy or transport properties). To illustrate the capability of this approach, calculations have been performed both for pure materials as well as for compounds. The results are compared with those obtained by other methods and with the experimental data.

[1] J. B. Staunton et al., Phys. Rev. B **74**, 144411 (2006)
[2] A. Deak et al., Phys. Rev. B **89**, 224401 (2014)

MA 54.5 Fri 11:00 H34

A detailed view on the effect of the spin-orbit coupling on the magnetocrystalline anisotropy: case study of FePt — •Saleem Ayaz Khan[1], Peter Blaha[2], Hubert Ebert[3], Jan Minar[1,3], and Ondrej Sipr[1,4] — [1]University of West Bohemia, Pilsen — [2]Technische Universität Wien — [3]Ludwig-Maximilians-Universität München — [4]Institute of Physics ASCR, Prague

To obtain magnetocrystalline anisotropy (MCA) energy via ab-initio calculations, the spin orbit coupling (SOC) has to be accounted for. This can be done either fully by solving the relativistic Dirac equation or pertubatively via the second variation approach. To assess whether employing one or the other method has got a significant impact on the calculated magnetocrystalline anisotropy is not trivial: different ways of dealing with the SOC are implemented in different codes which rely on different methods and as the MCA energy is very sensitive to various technical parameters, a very careful examination of various convergence parameters has to be performed to get a meaningful comparison. Our study of the MCA of bulk FePt focuses on comparison of results of the Wien2k FLAPW code, where the SOC is implemented via the second variation approach, and of the SPRKKR code, where the Dirac equation is solved using a full-potential KKR Green function method.

15 min. break

MA 54.6 Fri 11:30 H34

Chiral bobbers new type of stable particle like states in chiral magnets — Filipp N. Rybakov[1], Alexander B. Borisov[1], Stefan Blügel[2], and •Nikolai S. Kiselev[2] — [1]M. N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg 620990, Russia — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present a recently discovered new type of a thermodynamically stable magnetic quasi-particle, which appears at interfaces, and surfaces of isotropic chiral magnets [1]. Because of the essential chirality of such a state and its localization close to the surface with the finite penetration depth, like a fishing bobber at a water surface, we use term chiral bobber (ChB) to refer to this object. The ChB is a soliton solution of micromagnetic equations localized in all three dimensions. It constitutes a new class of particles the hybrid particles composed of a smooth magnetization field and a magnetic singularity (Bloch point). Both contribute to three-dimensional torque fields and interesting dynamical and electron transport properties. Such new particle like state exhibits high thermal stability and thereby can be considered as promising object for fundamental research and practical applications in spintronic devices. We provide arguments that such a state can be found in different Si or Ge based B20-type alloys.

[1] F.N. Rybakov, A.B. Borisov, S. Blügel, & N.S.Kiselev, New type of stable particle like states in chiral magnets. Phys. Rev. Lett. 115, 117201 (2015).

MA 54.7 Fri 11:45 H34

Skyrmionic magnetization switching in nanorods — •Michalis Charilaou[1], Hans-Benjamin Braun[2], and Jörg Friedrich

Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]School of Physics, University College Dublin, Ireland

Magnetization switching mechanisms in nanorods, i.e., cylindrical nanowires, have been investigated in great detail, experimentally, theoretically, and computationally, because of their promising potential for technological implementation in data-storage devices. Depending on the shape, dimension, and anisotropic properties of a nanowire, possible reversal mechanisms are quasi-coherent rotation, domain-wall nucleation, and curling, all of which can transform the magnetization continuously from one state to another. In this work, we will show via micromagnetic simulations that in nanorods the magnetization switches by forming two skyrmion lines of opposite chirality, which begin at the wire ends via curling and propagate towards the center. During the propagation of the skyrmion lines, the transformation of the magnetic structure is continuous, but for a full reversal topological point defects, such as Bloch points, need to be created such that the switching becomes irreversible.

MA 54.8 Fri 12:00 H34

Domain walls in square magnetic nanowires - velocity of the Bloch point as a function of temperature — •Kristof M. Lebecki and Dominik Legut — IT4Innovations Centre, VŠB Technical University of Ostrava, Czech Republic

We simulate a magnetic head-to-head domain wall (DW) in an elongated nanowire with a square cross section. Material parameters of the sample resemble permalloy. Cross-section size is selected in such a way that there is a Bloch point in the middle of the DW. The DW has a vortex structure, either right-handed or left-handed - in accordance to the external magnetic field (applied along the wire).

We focus our attention on temperature effects. For that we have implemented the Landau-Lifshitz-Bloch equation in the OOMMF simulation program. Landau-Lifshitz-Bloch equation leads to new effects, for instance magnetization can be locally squeezed. This is especially pronounced in the vicinity of the Bloch point. We consider the influence of temperature on the DW movement, especially the behavior of the Bloch point as a function of temperature. Also, we evaluate the role of the DW helicity. This helps us to test the recent suggestion that Bloch-point mobility drops down with the increase of temperature.

MA 54.9 Fri 12:15 H34

Mechanisms of skyrmion nucleation and annihilation in thin films of chiral magnets — •Pavel Bessarab[1], Gideon Müller[2], Filipp Rybakov[3], Nikolai Kiselev[2], Stefan Blügel[2], Lars Bergqvist[1], and Anna Delin[1] — [1]KTH Royal Institute of Technology, Kista, Sweden — [2]Forschungszentrum Jülich, Jülich, Germany — [3]Institute of Metal Physics, Ekaterinburg, Russia

Theoretical calculations of minimum energy paths (MEPs) for skyrmion nucleation and annihilation in thin films of chiral magnets are presented. MEPs which provide information about the microscopic mechanism and energy barrier of magnetic transitions are identified using a recently developed geodesic nudged elastic band (GNEB) method [1]. The GNEB calculations revealed two mechanisms of the skyrmion annihilation. In ultra-thin films, the MEP corresponds to a radial collapse of the skyrmion. In thicker films, a singularity forms at the film surface and propagates through the film. A maximum is found in the energy barrier for the skyrmion annihilation as a function of film thickness corresponding to a crossover between the two mechanisms. This analysis provides a deeper understanding of skyrmion formation and stability and helps develop ways to control magnetic skyrmions in real nanostructures.

[1] P.F. Bessarab, V.M. Uzdin, H. Jónsson, *Comput. Phys. Commun.* **196**, 335 (2015).

MA 54.10 Fri 12:30 H34

Micromagnetic MuMax3 simulations for different magnetic structures: Coupled layers and core-shell nanotubes — •Thomas Feggeler[1], Ralf Meckenstock[1], Detlef Spoddig[1], Irene Iglesias[2], and Michael Farle[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Institute of Physics and Technology, Immanuel Kant Baltic Federal University, 236004, Nevskogo 14, Kaliningrad, Russia

Simulations of FMR spectra (X-band) of a cobalt stripe ($\sim 1.9\ \mu$m $\cdot \sim 0.5\ \mu$m, thickness: ~ 30 nm) deposited on a permalloy disc (diameter: $\sim 2\ \mu$m, thickness: ~ 30 nm) were performed. Coupling modes due to the exchange interaction between the differently shaped materials are visualized. The simulations were done in support of scanning transmission X-ray microscope measurements with a lateral resolution of 100 nm.

For magnetization measurements on biphase microwires consisting of different core/shell material combinations with a glass coating between the central wire and the outer tube (diameter core: $\sim 20\ \mu$m, diameter core + glass coating: $\sim 30\ \mu$m, total diameter: up to 40 μm, length: ~ 4.5 mm), hysteresis simulations rescaled to nanometer size (diameter core: 20 nm, outer diameter: 40 nm, length: 800 nm) were done. Simulations provide a good match to the experiment and confirm a two-step reversal process with different domain wall nucleation fields for the central wire and the outer tube.

MA 54.11 Fri 12:45 H34

Calculation of GMR effects in granular systems — •Daniel Kappe[1,2], Lisa Teich[2], Christian Schröder[2], and Andreas Hütten[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Bielefeld Institute for Applied Materials Research, University of Applied Sciences Bielefeld, Germany

A macroscopic, semiclassical model was implemented to calculate GMR effects systems which are composed of a non-magnetic matrix and magnetic nanoparticles. There are a couple of publications, which propose models to describe granular systems [1,2]. Those approaches average over all grains and thus do not address the magnetic configuration of the small magnetic particles and clusters of particles. The presented model uses Finite Elements calculations and inputs from micromagnetic simulations [3] to address this issue.

[1] Zhang, Shufeng, and Peter M. Levy. "Conductivity and magnetoresistance in magnetic granular films." Journal of applied physics 73.10 (1993): 5315-5319.

[2] Xing, Lei, and Yia-Chung Chang. "Theory of giant magnetoresistance in magnetic granular systems." Physical Review B 48.6 (1993): 4156.

[3] Teich, Lisa, and Christian Schröder. "Hybrid Molecular and Spin Dynamics Simulations for Ensembles of Magnetic Nanoparticles for Magnetoresistive Systems." Sensors 15.11 (2015): 28826-28841.