MA 14: Micromagetic Simulation and Electron Theory of Magnetism

Time: Tuesday 9:30–12:00 Location: H23

MA 14.1 Tue 9:30 H23

Notes on the Gilbert equation for dissipative magnetization dynamics — •Manfred Fähnle, Frank Schweiner, and Christian Illg — Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany

The simplest equation of motion for dissipative magnetization dynamics $\vec{M}(\vec{r},t)$ close to the adiabatic limit (timescale ns - ca 100 ps) which describes precession around an effective field and damping (by a local term $\vec{M}\times\alpha\frac{\partial\vec{M}}{\partial t}$ with a constant damping scalar α) is Gilbert's equation. Various types of theories have shown that in general the damping is nonlocal and anisotropic, described by a matrix $\underline{\underline{\alpha}}(\vec{r},\vec{r}';\vec{M}(\vec{r}''))$ which depends on the magnetization configuration $\vec{M}(\vec{r}'')$ at all sites $\vec{r}''$ in the sample. Furthermore, for very fast dynamics an inertial damping term proportional to $\frac{\partial^2\vec{M}}{\partial t^2}$ should be added. The Gilbert equation is a partial differential equation and has to be supplemented by boundary conditions formulated in the most general way by Guslienko and Slavin. The question is discussed whether those boundary conditions have to be applied also for numerical simulations based on Gilbert's equation. A tensorial Green's function is constructed for the solution of the linearized Gilbert equation.

MA 14.2 Tue 9:45 H23

Micromagnetic analysis of nucleation and pinning processes in the intermetallic compound MnBi — Dagmar Goll[1] and •Helmut Kronmüller[2] — [1]Aalen University, Materials Research Institute, Aalen — [2]Max-Planck-Institute for Intelligent Systems, Stuttgart

The low temperature phase (LTP) of the binary intermetallic compound MnBi shows extraordinary magnetic properties in the temperature range up to 600 K. An anisotropy constant of 2.2 MJ/m^3 at 400 K and a large magnetic moment of 3.6 Bohr magnetons of Mn atoms predestinates the low temperature phase (LTP) of MnBi as a high temperature permanent magnet. Depending on the type of microstructure the hysteresis loops are governed either by nucleation or domain wall pinning processes. A micromagnetic analysis of the temperature dependence and of the angular dependence of the coercive field allows a decision whether the nucleation or the pinning mechanism governs the hysteresis loop. In the case of the intermetallic compound MnBi and other supermagnets in general the Stoner-Wohlfarth-Theory has to be expanded with respect to higher anisotropy constants and microstructural effects, as misaligned grains, and the role of grain surfaces with reduced anisotropy constants. Taking care of these effects leads to a quantitative interpretation of recent experimental results obtained for nanocrystalline magnets [1]. Nucleation hardened nanocrystalline magnets with coercive fields up to 2.5 Tesla at 500 K are found to be superior to the pinning hardened multiphase magnets of MnBi. [1] J.B. Yang et al., Appl. Phys. Letters 99, 062505 (2011).

MA 14.3 Tue 10:00 H23

Multiscale study of Bloch points and their dynamics — •Christian Andreas[1,2], Attila Kákay[1], and Riccardo Hertel[2] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, D-52428 Jülich, Germany — [2]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg, CNRS UMR 7504, Strasbourg, France

Compared to domain walls and (anti-) vortices, little is known about the dynamic properties of Bloch points (BPs) [1,2]. BPs are fundamental magnetic structures occurring, e.g., in vortex-type domain walls in nanocylinders [3] or transient when vortex cores switch [4]. They are difficult to treat in micromagnetism because of their maximally inhomogeneous structure and a singularity of the exchange energy density. This violates the basic micromagnetic assumption of smooth variations on atomistic length scales. The problem can be solved by using a Heisenberg model. In order to simulate a BP embedded into a mesoscopic domain structure we developed a multiscale code with a seamless coupling between an atomistic region of interest (ROI) and the magnetization calculated with our finite-element code TetraMag. By moving the ROI we can trace BPs during switching processes. We demonstrate the compatibility of the multiscale model with micromagnetic results and present examples of simulated BP dynamics.
[1] E. Feldtkeller, Z. Angew. Phys. 19, 530 (1965)
[2] W. Döring, J. Appl. Phys. 39, 1006 (1968)
[3] R. Hertel and J. Kirschner, J. Magn. Magn. Mater. 3, L291 (2004)
[4] R. Hertel et al., Phys. Rev. Lett. 11, 117201 (2007)

MA 14.4 Tue 10:15 H23

Multiple-q states in classical triangular-lattice Heisenberg antiferromagnet with frustrated interactions — •Andrey Leonov and Maxim Mostovoy — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

In geometrically frustrated magnets with the triangular lattice, the interplay of nearest-(J1) and next-nearest neighbor (J2) interactions can destabilize the homogeneous magnetic structure and induce diverse incommensurate multiple-q states. Within the basic J1-J2 exchange Hamiltonian with the Zeeman term, the single-q state is the ground state, whereas the double-q (2Q) and the triple-q (3Q) states are only metastable solutions [1]. In this contribution we show that additional magnetic couplings can render the 2Q and 3Q states into thermodynamically stable phases. We also show that at low temperatures the 3Q state in the frustrated triangular antiferromagnet is similar to the skyrmion crystal lattice recently observed in non-centrosymmetric magnets (e.g. MnSi and FeGe), but has a higher degree of degeneracy and the number of Goldstone modes. [1] T. Okubo et al., Phys. Rev. Lett. 108, 017206 (2012); [2] A. Leonov, Ph.D thesis, Dresden University of Technology, Dresden (2012).

MA 14.5 Tue 10:30 H23

Low temperature magnetic phase of bulk MnSi: An *ab initio* study — •Giovanna Lani, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The magnetic phase diagram of bulk MnSi has been the object of several experimental and theoretical studies over the years, recently receiving renewed interest, due to the debated nature of its magnetic order around the Curie temperature upon the application of a small magnetic field. On the other hand, it is well established from neutron scattering experiments, that at low temperature MnSi exhibits helical spin spiral order along the ⟨111⟩ direction. Employing density functional theory calculations based on the full-potential linearized augmented plane wave method as implemented in the `FLEUR` code [1], we carry out a comprehensive study of the exchange interactions in this system and present here our preliminary results. Working in the adiabatic approximation, we evaluate the Heisenberg exchange parameters (J_{ij}) and compare their behavior with the one expected by the RKKY interaction for ferromagnets. The J_{ij} coefficients are then employed to calculate the energy of spin spirals with different wave vectors. Finally we estimate the Curie temperature via mean field approximation and Monte Carlo calculations and compare it with previous calculations and available measurements.
[1] www.flapw.de

MA 14.6 Tue 10:45 H23

Magnetic phase transitions of ferromagnetic and antiferromagnetic alloys from first principles — •Konstantin Tillmanns, Phivos Mavropoulos, and Stefan Blügel — Peter Grünberg Institut and Institute forAdvanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We investigate a wide spectrum of ordered and disordered magnetic alloys concerning their magnetization, half metallicity and Curie/Néel temperature using an *ab initio* approach. We employ the Korringa-Kohn-Rostoker (KKR) Green function method [1] for the electronic structure and the method of infinitesimal rotations [2] for the exchange coupling parameters. These are derived both from the ground state and from the disordered local moment (DLM) state [3] and utilized in a Heisenberg model whose thermodynamical properties are studied by Monte Carlo simulations. By this we locate the magnetic phase transition. We furthermore focus on a comparison of the critical temperatures calculated by the different theoretical approaches (ground-state and DLM starting points) with experimental data.
[1] N. Papanikolaou, R. Zeller, and P.H. Dederichs, J. Phys. Condens. Matter **14**, 2799 (2002); H. Ebert, D. Ködderitzsch and J. Minár, Rep. Prog. Phys. **74**, 096501 (2011); see also `http://www.kkr-gf.org`.
[2] A.I. Liechtenstein et. al., J. Magn. Magn. Mater. **67**, 65 (1987).
[3] H. Akai and P.H. Dederichs, Phys. Rev. B **47**, 8739 (1993).

MA 14.7 Tue 11:00 H23

Magnetic systems at elevated temperatures by relativistic disordered local moments theory — •Danny Böttcher[1,2] and Jürgen Henk[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

The mismatch of experimentally and theoretically observed, temperature-dependent magnetic properties, in particular the magnetic moment and the Curie temperature, requires improvements in first-principles calculations. The magnetism of ferromagnets at elevated temperatures is described within a relativistic disordered local moments theory. The fluctuation strength of the local magnetic moments at a given temperature is obtained from first-principles calculations, taking into account the temperature-dependent distribution function of the local moment directions and spin-orbit coupling. We introduce to the approach and apply it to bulk Fe, Co, and Ni. Agreement of the magnetization versus temperature dependence with our Monte-Carlo method is found in the entire temperature range of $0 < T < T_c$.

MA 14.8 Tue 11:15 H23

Localization of magnetocrystalline anisotropy energy: Answering the Unanswerable — •Ondrej Sipr[1], Sven Bornemann[2], Hubert Ebert[2], and Jan Minar[2] — [1]Institute of Physics ASCR, Cukrovarnicka 10, Prague, Czech Republic — [2]Department Chemie, Ludwig-Maximilians-Universitat Munchen, Munchen, Germany

Magnetocrystalline anisotropy is one the of the key properties that determine the practical applicability of various systems containing magnetic atoms and clusters. Calculating it from first principles is a great challenge both numerically and fundamentally. However, to get a full picture, one needs not only to calculate the magnetocrystalline anisotropy energy (MAE) as accurately as possible but also to understand intuitively which factors effect it in various ways. For ad-atoms and films, one of the hotly debated issues in this context is what is the role of the substrate or, in other words, whether the MAE comes from only the magnetic ad-atoms or whether there is also a sizable contribution from the substrate.

In principle, the question about the localization of the MAE cannot be answered because energy is not an extensive quantity. However, by a carefull choice of model systems where the spin-orbit coupling and the exchange field are selectively switched on and off, one can still get a well-defined insight into how different atoms contribute to the "non-localizable" MAE. We illustrate this approach by inspecting the MAE for Co ad-atoms and monolayers on Pd, Pt, Cu, Ag, and Au (111) surfaces calculated under various schemes.

MA 14.9 Tue 11:30 H23

Construction of transition matrix elements for the scattering of crystal electrons at magnons — •Michael Haag, Christian Illg, and Manfred Fähnle — Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany

The scattering of crystal electrons at magnons in itinerant magnets is very important for the fields of spintronics and magnonics, and therefore an ab-initio treatment of these processes is highly desirable. The transition matrix elements for these scattering events are constructed in a second quantization formalism for crystal electron states which are represented by linear-muffin-tin-orbital basis functions. The exchange parameter appearing in these matrix elements is related to the exchange-correlation potential matrix of the spin-density functional theory. A comparison with the theory of electron-phonon scattering in magnets is made.

MA 14.10 Tue 11:45 H23

A comparison of magnetic and non-magnetic Compton profiles for locally dynamic correlated electrons of Fe, Ni and Cr. — •Liviu Chioncel[1], Diana Benea[2], Jan Minar[3], Hubert Ebert[3], Christoph Hugenschmidt[4,5], Hubert Ceeh[4], Michael Leitner[6], and Peter Boeni[4] — [1]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [2]Faculty of Physics, Babes-Bolyai University, Ro-400084 Cluj-Napoca, Romania — [3]Chemistry Department, University Munich, D-81377 München, Germany — [4]Technische Universität München, Physik Department E21, D-85748 Garching, Germany — [5]FRM II, Technische Universität München, D-85747 Garching, Germany — [6]Technische Universität München, Physik Department E13, D-85748 Garching, Germany

The total and magnetically resolved Compton profiles are analyzed within the combined Density Functional and Dynamical Mean Field Theory (DMFT) for the transition metal elements Fe, Ni and Cr. A relative good agreement between the measured and computed Magnetic Compton profiles of Fe and Ni is obtained with the standard Local Density or the Generalized Gradient correction, while larger discrepancies are seen for the total Compton profile. Including many-body correlations captured by DMFT the computed Magnetic Compton profile is further improved, while no significant improvement is seen for the total Compton profile. We are lead to the conjecture that MCP encodes local correlations, while a correct theoretical description of the total CP may require the presence of non-local interactions.