MA 14: Electronic Structure of Magnetism, Computational Magnetism

Time: Tuesday 9:30–12:30 Location: H 0112

MA 14.1 Tue 9:30 H 0112

Spin-orbit coupling effects on spin-dependent inelastic electronic lifetimes in ferromagnets — •Dennis Nenno, Steffen Kaltenborn, and Hans Christian Schneider — Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern

We present results for spin-dependent inelastic electronic lifetimes in the 3d ferromagnets iron, cobalt, and nickel due to carrier-carrier Coulomb interactions including spin-orbit coupling in the band structure and in the wave functions. Including the spin-orbit interaction in the electronic wave functions presents an important step towards the resolution of a long standing discrepancy between theoretical and experimental results for spin-dependent electronic lifetimes. This subject has recently received renewed attention due to its importance for hot-electron spin transport [1]. Our approach is based on density functional theory and an accurately determined dielectric function [2]. With this numerical framework we find that the spin-dependent density of states at the Fermi energy does not, in general, determine the spin dependence of the lifetimes because of the effective spin-flip transitions allowed by the spin mixing [3]. Thus, the majority and minority electron lifetimes computed including spin-orbit coupling for these three 3d ferromagnets do not differ by more than a factor of 2, and agree with experimental results.

[1] M. Battiato, K. Carva, and P. M. Oppeneer, PRB 86, 024404 (2012). [2] S. Kaltenborn and H. C. Schneider, PRB 88, 045124 (2013). [3] S. Kaltenborn and H. C. Schneider, PRB 90, 201104(R) (2014).

MA 14.2 Tue 9:45 H 0112

Systematic derivation of an effective spin-Hamiltonian based on a modified multi-orbital Hubbard model — •Markus Hoffmann and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Theoretical descriptions of magnetic ground states, dynamical or thermodynamical properties of magnetic systems are often achieved through a multi-scale approach: DFT calculations are mapped onto a lattice spin-Hamiltonian whose properties are then evaluated carrying out Monte-Carlo or spin-dynamic simulations. For many bulk materials, the well-known Heisenberg exchange provides a sufficient description of the properties, whereas at surfaces or thin films occasionally so-called higher-order exchange interactions play a significant role. Those interactions are motivated from a single-band Hubbard model of a spin $S = 1/2$ system. However, typical magnetic moments at surfaces are in the order of 2 or 3 μ_B equivalent to $S = 1$ or $S = 3/2$. In this contribution, we present a systematic derivation of effective lattice spin-Hamiltonians based on a rotational invariant multi-orbital Hubbard model including a term ensuring Hund's rule coupling. The model is derived down-folding the degree of freedom into the proper low-energy spin sector using Löwdin's partitioning. Up to fourth order perturbation we found for $S \geq 1$ beyond the conventional Heisenberg term a biquadratic, 3-spin and 4-spin interaction. We show that the so-far not considered 3-spin interaction explains the puzzling energy spectrum of the magnetic states for a single Fe monolayer on Rh(111).

MA 14.3 Tue 10:00 H 0112

Navigation on the energy surface of the noncollinear Alexander-Anderson model using a magnetic force theorem — •Pavel Bessarab[1,2], Valery Uzdin[2,3], and Hannes Jónsson[4,5] — [1]Royal Institute of Technology KTH, Stockholm, Sweden — [2]St. Petersburg State University, St. Petersburg, Russia — [3]St. Petersburg National Research University of Information Technologies, Mechanics and Optics, St. Petersburg, Russia — [4]University of Iceland, Reykjavik, Iceland — [5]Aalto University, Espoo, Finland

Magnetic force theorem is derived within the multiple impurity, noncollinear Alexander-Anderson (NCAA) model - an important tool for efficient calculation of the total energy gradient with respect to orientation of magnetic moments, the magnetic 'forces'. Efficient evaluation of magnetic forces is of great importance for the large scale simulation of spin dynamics, minimization of the energy to identify stable and metastable magnetic states, or, in general, navigation on the energy surface of a magnetic system. NCAA model and magnetic force theorem are applied to calculate minimum energy paths between stable magnetic states of the monolayer Fe clusters on a W(110) surface, revealing complex mechanism of the magnetization reversal. Moreover, a noncollinear magnetic state is identified in a 7 x 7 atomic row Fe island where the magnetic moments are arranged in an antivortex configuration with the central ones pointing out of the (110) plane. The minimum energy path between this antivortex state and the collinear ground state is also calculated and the thermal stability of the antivortex state estimated.

MA 14.4 Tue 10:15 H 0112

Non-harmonic quantum dynamics of single spin systems — •Mario Krizanac, David Altwein, Elena Vedmedenko, and Roland Wiesendanger — Institute of Applied Physics and Interdisciplinary Nanoscience Center Hamburg , Germany

The time evolution of single quantum spins became accessible to the experimental observation in the last years [J. Phys. D:Appl. Phys.44(2011)]. Therefore, it was our motivation to study the dynamics of single quantum spin systems with uniaxial anisotropy in an external magnetic Bz-field from a theoretical perspective within the Schroedinger formalism. It has been found that the spin dynamics shows a very complicated non-harmonic periodicity. The period depends on the ratio of the external magnetic Bz-field and the uniaxial anisotropy in Sz direction. We observed two cases, the first one of very high periodicity and a second one of low periodicity. The conditions for these cases can be formulated in the form of a simple equation, which can be easily generalized to describe these conditions for single quantum spin systems of any size.

Atomic magnetism revealed by spin-resolved scanning tunnelling spectroscopy [J. Phys. D: Appl. Phys.44(2011)] Jens Wiebe, Lihui Zhou and Roland Wiesendanger Institute of Applied Physics, Hamburg University, Jungiusstrasse 11, D-20355 Hamburg, Germany

MA 14.5 Tue 10:30 H 0112

Real-time dynamics of a classical spin exchange coupled to a Fermi sea — •Mohammad Sayad and Michael Potthoff — I. Institut für Theoretische Physik , University of Hamburg, Germany

Using a numerical time-step propagation technique, we study the real-time dynamics of a single classical spin locally coupled via an antiferromagnetic exchange J to a system of non-interacting electrons. The dynamics is initiated by suddenly switching a local magnetic field B. In the regime of weak J and B, linear-response theory and the separation of time scales can be employed to derive the Landau-Lifshitz-Gilbert equation. We show, however, that this theory must break down and that the Gilbert damping becomes ill-defined in the case of one-dimensional systems. The reversal time of the spin is systematically calculated in the entire parameter regime. For strong J we find an incomplete relaxation on a short time scale followed by a slow drift towards saturation. Retardation effects and deviations from adiabatic spin dynamics are discussed for systems with a single and with two classical spins.

15 min. break

MA 14.6 Tue 11:00 H 0112

Finite temperature and magnetic field transport in 1D quantum magnets — •Xenophon Zotos — Physics Department - University of Crete — Crete Center for Quantum Complexity and Nanotechnology — FORTH - IESL

I'll present recent exact results on the finite temperature and magnetic field magneto-thermal transport in the one dimensional spin-1/2 Heisenberg model obtained using the Bethe ansatz (BA) method. In particular, I'll discuss the behavior of spin Drude weight as a function of magnetic field down to low temperatures. These new results are based on a previous analysis by the author of the spin Drude weight in zero magnetic field.

Furthermore, I'll discuss the thermodynamics, thermal transport and dynamics (ESR), of the spin S=1 easy-plane quasi-one dimensional quantum magnet NiCl2-4SC(NH2)2 (DTN). The analysis is based on an effective spin-1/2 anisotropic (s= 1/2) Heisenberg model description that is put on a firm basis by comparing the thermodynamics of the S=1 model, obtained using TMRG, with exact BA specific heat and magnetisation results for the s=1/2 Heisenberg model. For the

thermal conductivity in a magnetic field, Ill compare numerical data on the S=1 model obtained using exact diagonalization techniques to exact results using the BA method. For the ESR data, using a recently developed BA technique, I'll show that the extremely sharp line observed in experiments, is due to a singular excitation to a single excited state.

MA 14.7 Tue 11:15 H 0112

Multi-scale modelling of magnetization dynamics — •Andrea De Lucia, Mathias Kläui, and Bejnamin Krüger — Institut für Physik, Johannes Gutenberg Universität, Mainz

A Multi-scale Magnetization Dynamics Simulation scheme was developed and applied to systems with special spin structures and properties. The MicroMagnum simulator was used as starting point and expanded to include a Multi-scale approach. The software selectively simulates different regions of a ferromagnetic sample employing the most suitable discretization and model according to the properties of each region. Simulating magnetization dynamics in a Multi-scale environment allows one to rapidly evaluate the Landau-Lifshitz-Gilbert equation in a mesoscopic sample with nanoscopic accuracy where needed. Possible application of this software include Skyrmion Dynamics, Domain Wall motion and Spin Wave generation.

MA 14.8 Tue 11:30 H 0112

Effective models for exchange bias systems based on atomistic spin dynamics simulations — •Irina Stockem, Stefan Muschack, and Christian Schröder — Bielefeld Institute for Applied Materials Research, University of Applied Sciences Bielefeld, Wilhelm-Bertelsmann-Str. 10, 33602 Bielefeld, Germany

The exchange bias anisotropy was observed at stacked ferromagnetic and antiferromagnetic layers by Meiklejohn and Bean in the 1950^{th} [1]. The exchange bias leads to an asymmetric shift of the hysteresis loop, which is fixed during the fabrication process in conventional systems. In novel systems, like Co/Cr_2O_3, this shift can be switched [2]. Although the discovery of the exchange bias is more than half a century ago a comprehensive theoretical model is still missing. Many simplified and analytical solvable models exist but these are not applicable to real exchange biased structures. In order to obtain a better understanding of the dominating factors of exchange bias systems we have developed effective models and investigated these by spin dynamics simulations [3]. We compare our results to existing models and to atomistic spin dynamics simulations of a three dimensional Co/Cr_2O_3 model system.

[1] W. H. Meiklejohn and C. P. Bean, Phys. Rev. **105**, 904 (1957).
[2] Y. Shiratsuchi et al., Appl. Phys. Lett. **100**, 262413 (2012).
[3] L. Engelhardt and C. Schröder, in Molecular Cluster Magnets, World Scientific Publishers, Singapore (2011).

MA 14.9 Tue 11:45 H 0112

Simulation of coercivities and magnetization reversal mechanisms in fourfold ferromagnetic systems of different dimensions and orientations — •Tomasz Blachowicz[1] and Andrea Ehrmann[2] — [1]Silesian University of Technology, Institute of Physics, Poland — [2]Niederrhein University of Applied Sciences, Faculty of Textile and Clothing Technology, Germany

The stability of magnetic states during magnetization reversal, especially at remanence, belongs to the important issues in examination of magnetic nanosamples. Our presentation gives an overview of different fourfold magnetic wire systems, simulated by Magpar. Wire lengths have been chosen from 30 nm to 70 nm, while the single wires have length-to-diameter ratios between 3 and 11. Simulations have been carried out for angular in-plane directions of the externally applied field from 0° (parallel to one pair of wires) to 45°. Depending on system dimensions and external field angle, different magnetization reversal mechanisms could be observed as well as changes between stable and instable magnetic states [1].

Intermediate states at vanishing external field, reached by minor loops starting at steps in the hysteresis loop, are of special interest for application in novel data storage media systems. The presentation shows different possibilities to create such states and examines their stability by comparing hysteresis loops, special distribution of magnetization, and exchange energy as function of the externally applied field for a number of sample dimensions and external field angles.

[1] T. Blachowicz, A. Ehrmann, J. Appl. Phys. 113, 013901 (2013)

MA 14.10 Tue 12:00 H 0112

Micromagnetic analysis of nucleation and pinning processes in supermagnets — Dagmar Goll[1], Therese Dragon[2], Matthias Katter[3], and •Helmut Kronmueller[2] — [1]Aalen University, Materials Research Institute (IMFAA), Aalen — [2]Max Planck Institute for Intelligent Systems — [3]Vacuumschmelze GmbH & Co. KG, Hanau

The large discrepancy between theoretical predictions and realized magnetic properties of hysteresis loops of high-quality permanent magnets, known as Brown-paradox, has been the matter of discussions over decades of years. In particular whether the leading hardening mechanism is due to a nucleation mechanism or to domain wall pinning has been the topic of many publications with contrary statements. Here the existence of single or multi-domain grains plays a central role. This contribution presents the following basic results which allow a distinction between the two types of hardening mechanisms: 1. Coercive field H_c as a function of maximum applied magnetic field. 2. Change of domain patterns as a function of applied magnetic field. 3. Angular dependence of H_c. 4. Temperature dependence of H_c. Experimental results obtained for nanocrystalline systems of FePt and MnBi and sintered Nd-Fe-B based permanent magnets are compared with micromagnetic analytical results. It is shown that for high-quality permanent magnets the dominant hardening mechanism corresponds to the nucleation process.

MA 14.11 Tue 12:15 H 0112

Nonlinear frequency-dependent effects in the dc magnetization of uniaxial magnetic nanoparticles in superimposed strong alternating current and direct current fields — •William Coffey[1], Nijun Wei[1], Sergey Titov[1], Yuri Kalmykov[2], and Declan Byrne[1] — [1]Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland — [2]Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique, F-66860, Perpignan, France

The dc component of the magnetization of noninteracting fine magnetic particles possessing simple uniaxial anisotropy and subjected to strong ac and dc bias magnetic fields is calculated via the magnetic Langevin equation. In the presence of an ac driving field, the dc component of the magnetization of uniaxial particles alters drastically leading to new nonlinear effects; in particular, it becomes frequency-dependent. In axial symmetry, where the strong ac field is parallel to the easy axis of a particle, two distinct dispersion regions in the dc magnetization at low and mid-frequencies emerge, corresponding to longitudinal overbarrier and intrawell relaxation modes. Such frequency-dependent behavior allows one to estimate the magnetization reversal time via the half-width of the low-frequency dispersion band. Otherwise, by applying the strong ac field at an angle to the easy axis of a particle so breaking the axial symmetry, a third high-frequency nonlinear resonant dispersion in the dc component of the magnetization appears accompanied by parametric resonance behavior due to excitation of transverse modes with frequencies close to the precession frequency.