MA 55: Electron theory and micromagnetism

Time: Friday 9:30–13:15 Location: H38

MA 55.1 Fri 9:30 H38

Ab-initio calculations of the spin wave stiffness constant for permalloy doped with V, Gd, and Pt — •Ondřej Šipr[1], Sergey Mankovsky[2], and Hubert Ebert[2] — [1]Institute of Physics, Czech Academy of Sciences, Praha — [2]Ludwig-Maximilians-Universität München

The modification of the properties of magnetic materials by doping is a promising and intensively studied way to make progress in device technology and spintronics. A very important system in this respect is permalloy $Fe_{20}Ni_{80}$ — not only because of its high magnetic permeability but also because of its transport properties characterized by a high and low electrical conductivity in the majority and minority spin channel, respectively. As the spin dynamics of materials is governed by the spin wave stiffness D or the closely connected exchange stiffness A, we perform *ab-initio* investigation of this quantity for permalloy (Py) doped with V, Gd, and Pt. Our study is based on electronic structure calculations by means of the Korringa-Kohn-Rostoker (KKR) Green's-function method, with disorder treated within the coherent potential approximation (CPA). For Gd as a dopant the open core formalism was employed. The calculated results are in a good agreement with experiment [Lepadatu *et al* PRB **81**, 020413 (2010) and APL **97**, 072507 (2010); Yin *et al* IEEE Magn. Lett. **8**, 3502604 (2016); Hrabec *et al* PRB **93**, 014432 (2016)], correctly reproducing the trends when the chemical type (V, Gd, or Pt) or the concentration (1–10 %) of the dopant are changed.

MA 55.2 Fri 9:45 H38

An extension of the Heisenberg Hamiltonian: temperature dependent and multi-spin exchange parameters from first principles — •Sergiy Mankovsky and Hubert Ebert — Dept. Chemistry, LMU Munich, D-81377 Munich, Germany

We will present an extension of the Heisenberg model by accounting for multi-spin exchange and temperature dependent exchange interactions calculated from first principles based on the electronic structure calculations by means of the Korringa-Kohn-Rostoker (KKR) Green function method. The temperature dependent behaviour of the exchange parameters is obtained accounting for thermal lattice vibrations and spin fluctuations treated by means of the CPA alloy theory within the alloy analogy model [1]. To calculate the multi-spin exchange interactions, we follow the approach reported previously [2], using a higher order expansion of the Green function entering the free energy expression accounting this way for a deviation of magnetic moments from a reference configuration. To demonstrate the impact of these contributions we represent results of calculations for different types of system: pure elemental materials, ordered compounds as well as alloys with chemical disorder.

[1] H. Ebert, S. Mankovsky, et al., Phys. Rev. B **91**, 165132 (2015)
[2] S. Mankovsky, S. Polesya, H. Ebert, arXiv:1810.13175 (2018)

MA 55.3 Fri 10:00 H38

Coupled charge and spin dynamics in a photo-excited doped Mott insulator — •Nikolaj Bittner[1], Denis Golez[1], Hugo Strand[2], Martin Eckstein[3], and Philipp Werner[1] — [1]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [2]Flatiron Institute, Simons Foundation, 162 Fifth Avenue. New York, NY, 10010, USA — [3]Department of Physics, University of Erlangen-Nuernberg, 91058 Erlangen, Germany

Using a nonequilibrium implementation of the extended dynamical mean field theory (EDMFT) we simulate the relaxation of a photo-excited doped Mott insulator. We consider the t-J model and focus on the interplay between the charge- and spin-dynamics in different excitation and doping regimes. The appearance of string states after a weak photo excitation manifests itself in a nontrivial scaling of the relaxation time with the exchange coupling. Moreover, we observe a correlated oscillatory evolution of the kinetic energy and spin-spin correlation function, which is a direct consequence of a strong spin-charge coupling. A strong excitation of the system, on the other hand, suppresses the spin correlations and results in a relaxation that is controlled by hole scattering. Finally, we propose a pump-probe setup, which allows to directly observe oscillations in the optical conductivity originating from string states.

MA 55.4 Fri 10:15 H38

Hybridization-switching induced Mott transition in magnetic ABO_3 perovskites — •Atanu Paul[1], Anamitra Mukherjee[2], Indra Dasgupta[1], Arun Paramekanti[3], and Tanusri Saha-Dasgupta[4,5] — [1]School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata, India — [2]School of Physical Sciences, National Institute of Science Education and Research, Jatni, India — [3]Department of Physics, University of Toronto, Ontario, Canada — [4]Department of Condensed Matter Physics and Materials Science, S.N. Bose National Centre for Basic Sciences, Kolkata, India — [5]School of Mathematical & Computational Sciences, Indian Association for the Cultivation of Science, Kolkata, India

We propose the concept of "hybridization-switching induced Mott transition" which is relevant to a broad class of magnetic ABO_3 perovskite materials including $BiNiO_3$ and $PbCrO_3$ which feature extended 6*s* orbitals on the A-site cation (Bi or Pb), and A-O covalency induced ligand hole. Using *ab initio* electronic structure and model Hamiltonian calculations, we show that such systems exhibit a breathing phonon driven A-site to oxygen hybridization-wave instability which conspires with strong correlations on the magnetic B-site transition metal ion (Ni or Cr) to induce an antiferromagnetic Mott insulator. These Mott insulators with active A-site orbitals are shown to undergo a pressure induced antiferromagnetic insulator to ferromagnetic metal transition accompanied by a colossal volume collapse due to ligand hybridization switching.

MA 55.5 Fri 10:30 H38

Ferromagnetism in alternating Hubbard ladder — •Kaouther Essalah[1], Ali Benali[1], Anas Abdelwahab[2], Eric Jeckelmann[2], and Richard Scalettar[3] — [1]University of Tunis El-Manar, Tunis, Tunisia — [2]Leibniz University, Hannover, Germany — [3]University of California, Davis, USA

We are using Density Matrix Renormalization Group (DMRG) method to study spin correlations in chains with many variants of alternating number of legs. The system is described using the half-filled Hubbard model. We are calculating excitation gaps, charge and spin densities as well as correlation functions. We compare our results to those of the well known geometries of even and odd number of leg ladders.

MA 55.6 Fri 10:45 H38

Broken symmetry states of magnetic molecular complexes — •Yaroslav Pavlyukh, Wolfgang Huebner, and Georgios Lefkidis — Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67653 Kaiserslautern, Germany

The broken-symmetry (BS) approach is broadly used to extract the magnetic properties of many-body systems from a DFT calculation. However, there is an ambiguity in the nature of the underlying electronic states and the corresponding spin densities: the spin density from DFT is not a well-defined property and the Kohn-Sham determinants need not be eigenfunctions of the square of the total spin ($\hat{\mathbf{S}}^2$).

Here we propose a procedure, in which the detailed analysis of a redundant number of electronic many-body excitations gives insight into the intrinsic magnetic properties of the system. We perform highly correlated multi-determinant calculations on two prominent synthesized and characterized metallacrown molecules with frustrated antiferromagnetic order driven by the superexchange mechanism, i.e., $\{CuCu_4\}$ and $\{CuFe_4\}$ [1]. For those we unambiguously show that the BS states are not eigenstates of $\hat{\mathbf{S}}^2$ and, in addition, theoretically compute several magnetic (exchange coupling J [2]) and relativistic properties (g-tensors), which we find to be in close agreement with experiment.

[1] Y. Pavlyukh, E. Rentschler, H. J. Elmers, W. Hübner, and G. Lefkidis, Phys. Rev. B **97**, 214408 (2018)
[2] W. Hübner, Y. Pavlyukh, G. Lefkidis, and J. Berakdar, Phys. Rev. B **96**, 184432 (2017)

MA 55.7 Fri 11:00 H38

Spin excitations in magnetic nanostructures with spin-orbit coupling from first-principles time-dependent DFT+U — •Manuel dos Santos Dias, Sascha Brinker, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

Time-dependent density functional theory has been very successful in describing spin excitations and spin fluctuations of surface-supported magnetic adatoms and dimers [1,2]. However, orbital correlation effects are poorly described by the adiabatic local spin density approximation. We combined our linear-response theory of magnetic nanostructures with spin-orbit coupling in real-space [3] with a parameter-free Hubbard-U-like kernel [4]. Magnetic adatoms on Cu(111) and Pt(111) serve as a benchmark to explore whether orbital polarization impacts dynamical quantities such as spin pumping or spin relaxation. Dimers and trimers are used to study the interplay between orbital correlation and delocalization, and to show the scalability of this approach.
This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] J. I. Azpiroz *et al.*, J. Phys.: Condens. Matter **30**, 343002 (2018)
[2] F. S. M. Guimarães *et al.*, Phys. Rev. B **96**, 144401 (2017)
[3] M. dos Santos Dias *et al.*, Phys. Rev. B **91**, 075405 (2015)
[4] N. Tancogne-Dejean *et al.*, Phys. Rev. B **96**, 245133 (2017)

15 min. break

MA 55.8 Fri 11:30 H38

Critical temperature and effective magnetic moment of experimentally known magnetic Heusler alloys from first principles — •Roman Kováčik[1], Phivos Mavropoulos[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, National and Kapodistrian University of Athens, GR-15784 Zografou, Greece

We present systematic calculations of the critical temperature (Curie or Néel) and the effective magnetic moment of a large number (∼150) of experimentally known magnetic Heusler alloys. The method of calculation comprises three steps: (i) calculation of the ground-state electronic structure within density functional theory (local spin density approximation and generalized gradient approximation) employing the Korringa-Kohn-Rostoker Green function method [1], (ii) extraction of exchange parameters to fit the Heisenberg model [2], and (iii) Monte Carlo simulation based on the Heisenberg model. We analyze the critical temperature dependence on various parameters defining the alloys and address the effect of the longitudinal spin fluctuations on selected alloys. The effective magnetic moment reflecting the degree of short range order above the critical temperature is obtained by fitting the magnetic susceptibility to the Curie-Weiss law and compared to available experimental data. Support from JARA-HPC (jara0182) and the EU CoE MaX (grant no. 676598) is gratefully acknowledged.
[1] H. Ebert *et al.*, Rep. Prog. Phys. 74, 096501 (2011), also see: www.judft.de. [2] A. I. Liechtenstein *et al.*, JMMM 67, 65 (1987).

MA 55.9 Fri 11:45 H38

Spin-model study of magnetism in graphene-based systems — László Oroszlány[1,2], Jaime Ferrer[3], András Deák[4,5], László Udvardi[4,5], and •László Szunyogh[4,5] — [1]Eötvös Loránd University, Budapest, Hungary — [2]MTA-BME Lendület Topology and Correlation Research Group, Budapest, Hungary — [3]Universidad de Oviedo & CINN, Oviedo, Spain — [4]Budapest University of Technology and Economics, Budapest, Hungary — [5]MTA-BME Condensed Matter Research Group, Budapest, Hungary

We briefly present the implementation of the method by Lichtenstein *et al.* [1] for evaluating isotropic exchange interactions from density functional theory based on the SIESTA code. We demonstrate that in case of simple metallic ferromagnets the Heisenberg interactions obtained from well–established computational methods are well reproduced. We then study magnetic correlations in single-side flourinated graphene (C2F) and in zig-zag graphene ribbons representing *sp* magnetism. Similar to Ref. [2], our calculated exchange interactions support a Néel type of magnetic ground state for C2F. For the graphene ribbons we calculate a stiffness constant over 3000 meVÅ^2, even larger than in Ref. [3], and find a transition between 1D and 2D long-range behavior depending on the thickness of the ribbon.
[1] A. I. Lichtenstein *et al.*, J. Magn. Magn. Mater. **67**, 65 (1987)
[2] A.N. Rudenko *et al.*, Phys. Rev. B **88**, 081405(R) (2013)
[3] O. V. Yazyev and M. I. Katsnelson, Phys. Rev. Lett. **100**, 047209 (2008)

MA 55.10 Fri 12:00 H38

Extending Liechtenstein's method to strong spin-orbit coupled systems — •Louis Ponet[1,2] and Sergey Artyukhin[1] — [1]Istituto Italiano di Tecnologia, Genova, Italia — [2]Scuola Normale Superiore di Pisa, Pisa, Italia

Localized magnetism in transition metal compounds has been very successfully modeled using a variation on the classical Heisenberg model. Calculating the model parameters, so-called magnetic exchange constants, from first-principles has been a notoriously difficult task, usually involving the comparison of total energies from numerous supercell ab-initio calculations. For simple compounds with small magnetic unit cells this approach is feasible and indeed has produced accurate results. A computationally more efficient Green's function-based method developed by Liechtenstein et al., and later adapted for use with Wannier functions by Rudenko et al., remedies this by calculating the exchange coefficients from a single DFT calculation. However this method was only formulated in the situation where there is low-strength atomic SOC present in the material. The crucial assumption is that the spins can rotate without perturbing other degrees of freedom. This picture breaks down when the localized spins are situated on atoms with strong spin-orbit coupling, such as the 5d-transition metal ions. This is because the low-energy degrees of freedom entangle spins and orbitals (describing the charge distribution). This leads to strongly anisotropic magnetic interactions, not contained in the Heisenberg model, leading to new physical phenomena as discussed by Jackeli et al. Here we explore the extension of the Liechtenstein method to this situation.

MA 55.11 Fri 12:15 H38

Micromagnetic Study of Magnetization States in FeGe Nanospheres — •Swapneel Amit Pathak and Riccardo Hertel — Université de Strasbourg et CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, 67000 Strasbourg, France

Magnetic structures in nanoscale ferromagnets are known to depend strongly on the particle size and shape, with recent attention being drawn towards three-dimensional nanomagnets [1]. However, in the case of chiral magnets, with pronounced Dzyaloshinskii-Moriya interaction, three-dimensional finite-size effects remain largely unexplored. Most of the studies on these materials pertain to thin-film geometries or disk shapes [2]. In this work, we employ micromagnetic finite-element simulations to investigate magnetic structures unfolding in FeGe particles of spherical shape. We find a variety of chiral equilibrium states as a function of the diameter and the external applied field. The structures can be categorized as helical states, merons, skyrmions, and chiral bobbers in different variants. The results, summarized in a phase diagram, show that specific magnetic structures can be stabilized depending on the particle size. For example, chiral bobbers can occur at much smaller dimension ($r \geq 50nm$) as compared to skyrmions ($r \geq 70nm$). The study furthers the understanding of these complex spin structures, which have recently been proposed as candidates for fundamental units of information in spintronics applications [3].
[1] A. Fernandez-Pacheco *et al.*, Nat. Comm., **8**, 15756 (2017)
[2] M. Beg em *et al.*, Sci. Rep., **5**, 17137 (2015)
[3] F. Zheng *et al.*, Nat. Nano., **13**, pp. 451-455 (2018)

MA 55.12 Fri 12:30 H38

Micromagnetic simulations for static and dynamic characterization of a linear chain of 20 magnetite nanoparticles — •Thomas Feggeler[1], Benjamin Zingsem[1,2], Alexandra Terwey[1], Michael Winklhofer[3], Ralf Meckenstock[1], Michael Farle[1], Heiko Wende[1], and Katharina Ollefs[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [2]Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]School of Mathematics and Science, University of Oldenburg, 26129 Oldenburg, Germany

We simulated the angular dependent Ferromagnetic Resonance (FMR) of a chain of 20 cubic magnetite nanoparticles (30 nm x 30 nm x 30 nm, truncated edges), resembling a particle chain within a bacterium Magnetospirillium Gryphiswaldense (strain MSR-1, wild-type). A simulated external magnetic field has been rotated 180 degrees in-plane around the chain, varying the field strength from 450 mT to 50 mT at each angle. In the simulated angle dependent Ferromagnetic Resonance spectrum multiple angular dependent resonance lines are visible, indicating an angular dependent anisotropy with a periodicity of 180 degrees, which is in good agreement to the experimental FMR measurements on such a sample. By the help of the simulation it is possible to identify the parts of the particle chain, in which each resonant eigenstate is localized. Partial financial support by DFG Project: OL513/1-1 is acknowledged.

MA 55.13 Fri 12:45 H38

Calculation of micromagnetic parameters from atomistic simulations in presence of crystal defects — •Matteo Rinaldi, Matous Mrovec, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The purpose of this work is to elucidate the relationship between the microstructure and the magnetic properties of electrical steels (Fe-Si) using scale-bridging computational techniques that combine atomistic simulations with mesoscopic micromagnetic framework. The relevant parameters for the micromagnetic model (build up from the Landau-Lifshitz-Gilbert and the Landau-Lifshitz-Bloch equations) will be calculated with atomistic techniques such as density functional theory(DFT) and tight-binding(TB) models. The parameters analyzed are the spin-wave stiffness constant and the prefactors in the expression for the magnetocrystalline anisotropy. For the calculation of these quantities some of the available methods will be tested in both frameworks (TB and DFT). This combination enables simulations of extended defects (such as dislocations, grain and phase boundaries, interfaces) that are crucial for the microstructure and the study of their influence on the micromagnetic parameters. The micromagnetic calculations will be subsequently employed and compared with experimental data.

MA 55.14 Fri 13:00 H38

Novel magnetic states in nano clusters — •Robert Baldock and Nicola Marzari — Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We predict that very small clusters of ferromagnetic spins may exhibit stable magnetic states with fractional overall magnetisation in two and three dimensions. These ultra small systems, which are dominated by finite size effects, do not conform to mean field models of the magnetization. Instead, exotic magnetisation field temperature phase diagrams are observed, where discrete fractional magnetisations are stabilised at finite fields and temperatures.

We study these systems using advanced free energy methods, including nested sampling, which enable us to directly obtain magnetisation-temperature free energy surfaces, from which the magnetisation field temperature phase diagrams can be computed directly.