MA 15: Computational Magnetism 2

Time: Tuesday 9:30–11:30 Location: H48

MA 15.1 Tue 9:30 H48

An *ab initio* study of temperature effects on the optical and magneto-optical properties of ferromagnetic BCC Fe — •Kisung Kang, David G. Cahill, and André Schleife — Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

This work investigates the temperature-dependent optical properties of ferromagnetic BCC Fe in terms of electron, lattice, and magnetic temperatures. With the supercell approach, lattice and magnetic temperature is portrayed by the perturbed atomic and magnetic structures at finite temperature. In imaginary optical conductivity spectra at finite temperature, a large signal at low energy range is induced by phonon and magnon-assisted intraband transitions. We identify that this surging signal originates from the change of the dipole transition matrix elements. Magnetic temperature provokes a unique spectral change which is a redshift of the peak near 2.8 eV in the imaginary optical conductivity spectrum. From band unfolding analysis, it turns out that thermal demagnetization induces the reduction of exchange splitting in the electronic band structure, leading to the electron excitation with a smaller energy transition and explaining the peak redshifting. **Illinois MRSEC NSF DMR-1720633 Kisung Kang's present address: The NOMAD laboratory, Fritz-Haber-Institut der Max-Placnk-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

MA 15.2 Tue 9:45 H48

An ab-initio parameterised spin model of hematite — •Tobias Dannegger[1], András Deák[2], Shubhankar Das[3], E. F. Galindez Ruales[3], Eunchong Baek[3], Mathias Klăui[3], László Szunyogh[2,4], and Ulrich Nowak[1] — [1]Department of Physics, University of Konstanz — [2]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics — [3]Institute of Physics, Johannes Gutenberg University Mainz — [4]MTA-BME Condensed Matter Research Group, Budapest University of Technology and Economics

The canted antiferromagnetic insulator hematite, known for motivating the theory of the Dzyaloshinskii–Moriya interaction [1, 2] as well as the first description of the Morin transition [3], is of interest in modern antiferromagnetic spintronics because of its long-distance spin transport properties [4]. We present an ab-initio parameterised atomistic spin model of hematite that accurately reproduces its magnetic properties and phase transitions, and shows how dipole-dipole interactions play an important role in determining the transition between the antiferromagnetic and weak ferromagnetic phase. We compare our model's predictions with extensive experimental measurements on a hematite single crystal and find good quantitative agreement across a wide range of temperatures.

[1] I. Dzyaloshinskii, *J. Phys. Chem. Solids* **50**, 241 (1958).
[2] T. Moriya, *Phys. Rev.* **120**, 91 (1960).
[3] F. J. Morin, *Phys. Rev.* **78**, 819 (1950).
[4] R. Lebrun et al., *Nature* **561**, 222 (2018).

MA 15.3 Tue 10:00 H48

The pyrochlore $s = 1/2$ Heisenberg antiferromagnet at finite temperature — •Robin Schäfer[1], Imre Hagymási[1,2], Roderich Moessner[1], and David Luitz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Strongly Correlated Systems *Lendület* Research Group, Budapest, Hungary

We use state-of-the-art computational methods to investigate a frustrated three-dimensional quantum spin liquid candidate, the pyrochlore $s = 1/2$ antiferromagnet at finite temperature.

Using a systematic cluster expansion based on tetrahedra, including clusters up to 25 lattice sites with nontrivial hexagonal and octagonal loops, we gain access to various thermodynamic properties in the thermodynamic limit at finite temperature. We found a pronounced maximum in the specific heat at $T = 0.57J$ that is stable across finite size clusters and converged in the series expansion. At $T \approx 0.25J$ (the limit of convergence of our method), the residual entropy per spin is $0.47k_B \log(2)$, which is relatively large compared to other frustrated models at this temperature.

The generality of this algorithm allows us to investigate realistic compounds: Using recent experimental data on the dipolar-octopolar pyrochlore $Ce_2Zr_2O_7$, we were able to determine possible regions for the exchange parameters which give an accurate description of the high temperature regime.

MA 15.4 Tue 10:15 H48

Stabilisation of external-magnetic-field-induced magnetisation switching with respect to thermal fluctuations — •Grzegor J. Kwiatkowski[1], Mohammad H. A. Badarneh[1], and Pavel F. Bessarab[1,2] — [1]Science Institute of the University of Iceland, Reykjavík, Iceland — [2]Department of Physics and Electrical Engineering, Linnaeus University, Kalmar, Sweden

As magnetic memory devices are the cornerstone of data storage, rapid global growth of information transfer creates a pressing need for faster and more energy-efficient memory devices. One of the important directions of research is focused on optimizing the magnetization switching protocols [1,2] showing that both the amplitude of the external pulse as well as the switching time can be significantly reduced in comparison to currently used ones. Before those ideas are implemented one needs to test reliability of the designed optimal pulses when thermal fluctuations are present.

We present the effect of thermal fluctuations on the success rate of magnetization switching induced by an optimized external magnetic field pulse [1]. Furthermore, using perturbation theory and direct numerical simulations we systematically study how to increase the probability of switching by modifying the external pulse depending on the system parameters, temperature and chosen switching time.

[1] Kwiatkowski, G. J. et al. Phys. Rev. Lett., 126(17), 177206
[2] Badarneh, M. H. A. et al. F. Nanosyst.: Phys. Chem. Math., 11(3), 294-300

MA 15.5 Tue 10:30 H48

Energy-efficient control of magnetization reversal in nanoparticles — •Mohamamd Badarneh[1], Grzegorz Kwiatkowski[1], and Pavel Bessarab[1,2] — [1]Science Institute of the University of Iceland, 107 Reykjavik, Iceland — [2]Department of Physics and Electrical Engineering, Linnaeus University, Kalmar, Sweden

Control of magnetization switching is of critical importance for the development of novel technologies based on magnetic materials. Here we identify by means of optimal control theory energy-efficient protocols for magnetization switching in nanoparticles with uniaxial and biaxial anisotropy [1]. Optimal control paths minimizing the energy cost of magnetization reversal are calculated as functions of the switching time and materials properties, and used to derive energy-efficient switching pulses of external magnetic field. Hard-axis anisotropy reduces the minimum energy cost of magnetization switching due to activation of the internal torque in the desired switching direction. Analytical estimates quantifying this effect are obtained based on the perturbation theory. The optimal switching time providing a tradeoff between fast switching and energy efficiency is obtained. The energy cost of switching and the energy barrier between the stable states can be tuned independently in a biaxial nanomagnet. This provides a solution for the dilemma between energy-efficient writability and good thermal stability of magnetic memory elements. This work was funded by the Icelandic Research Fund (Grant No. 217813-052).

[1] G.J. Kwiatkowski et al., Phys. Rev. Lett. 126, 177206 (2021).

MA 15.6 Tue 10:45 H48

Exchange striction from first principles: how electron-phonon coupling modifies magnetic exchange — •Ryota Ono and Sergey Artyukhin — Italian Institute of Technology, Via Morego, 30, 16163 Genoa, Italy

Electron-phonon coupling refers to interactions between electrons and lattice distortions. We investigate how such coupling affects interactions between spins in solids. Ionic displacements from equilibrium positions modify overlap integrals between magnetic ions and ligands and thus modulate magnetic exchange. By extracting the self-consistent potential in the first-order in ionic displacements within the Born-Oppenheimer approximation, we obtain a general formula of the change in the one-electron Hamiltonian (electron-phonon coupling). The realistic electron-phonon coupling parameters entering a model Hamiltonian are accessible thorough the constrained density functional perturbation theory [1]. Using the obtained parameters, we

construct a multiband Hubbard-like model. Finally, realistic magnetic interactions are obtained through Anderson's superexchange theory.

[1] Y. Nomura and R. Arita, Phys. Rev. B 92, 245108 (2015)

MA 15.7 Tue 11:00 H48

First principles theory of electron-magnon scattering and the spin polarized electron energy loss spectroscopy — •Sebastian Paischer[1], Pawel Buczek[2], Mikhail Katsnelson[3], and Arthur Ernst[1] — [1]JKU Linz — [2]HAW Hamburg — [3]Radboud University Nijmegen

Magnetic solids constitute a very important class of materials as they are extensively used in everyday life and are essential to many new technologies currently under development. In spite of their high relevance, some of the basic properties, like the interaction between electronic and magnetic degrees of freedom still remain a mystery. It leads to spin dependent lifetimes of electronic states and inelastic electron transport to name but a few. In our current study we investigate the impact of magnetic excitations on the electronic spectrum of solids as well as the scattering of high energy electrons with magnetic materials to formulate an ab initio theory for the spin polarized electron energy loss spectroscopy (SPEELS). Our approach is formulated in the framework of the formally exact many body GW theory. The novelty in our approach is that quantities from linear response time dependent density functional theory (LRTDDFT) calculations will be used to approximate an effective interaction between electrons and magnons. As our LRTDDFT calculations are based upon the Korringa-Kohn-Rostocker method, bulk systems as well as complex geometries can be accounted for. In this presentation, we sketch the theoretical basis of the electron-magnon scattering as well as the SPEELS theory and show several results.

MA 15.8 Tue 11:15 H48

The Complex Magnetic Structure and Giant Topological Hall Conductivity in Kagome Metal $YnMn_6Sn_6$ — •Hao Wang[1], Stefan Blügel[1], and Yuriy Mokrousov[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany.

The discovery of topological Kagome magnets attracts enormous research interest in recent years. The typical band structure of a Kagome lattice includes a flat band and a Dirac point. The high localized electrons induced strong many-body interactions in the flat bands and the linear dispersion of the Dirac point could lead to many intriguing physical phenomena, such as the quantum anomalous Hall effects, superconductivity, and the non-Fermi liquid behavior. Furthermore, the relationship between the complex noncolinear magnetic structures and band topology of the Kagome magnets also deserves further exploration. In this work, using first-principles calculation and spin Hamiltonian analysis, we investigated the complex magnetic structures, phase transition, and topological Hall conductivity of the Kagome metal YMn6Sn6. We confirm that the ground state of this material is a double flat-spiral structure, and we demonstrate the important role of thermal fluctuation in the origin of the giant Hall conductivity. This work provides a platform to understand the complex magnetic structure and topological properties of Kagome magnets for future spintronic devices.