MA 2: Computational Magnetism I

Time: Monday 9:30–12:45 Location: H 1058

MA 2.1 Mon 9:30 H 1058

Inertial spin waves in non-collinear spin structures — Mikhail Cherkasskii[1], Ritwik Mondal[2], and •Levente Rózsa[3,4] — [1]RWTH Aachen, Aachen, Germany — [2]Indian Institute of Technology (ISM) Dhanbad, Dhanbad, India — [3]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [4]Budapest University of Technology and Economics, Budapest, Hungary

Inertial phenomena emerge in magnetic materials at very short time scales, where the directions of the angular momentum and the magnetic moment become separated. The inertia gives rise to high-frequency excitations which have been observed in ferromagnetic resonance experiments [1]. These excitations form inertial spin-wave bands which have been studied in ferromagnets and collinear antiferromagnets [2].

Here, we discuss the properties of inertial spin waves in non-collinear spin structures. We generalize the linearized inertial Landau-Lifshitz-Gilbert equation used for the calculation of spin-wave modes to arbitrary spin configurations. We apply the method to spin spirals to interpolate between the ferromagnetic and collinear antiferromagnetic limits, and demonstrate the formation of flat bands and non-reciprocal inertial spin-wave dispersion.

[1] K. Neeraj et al., Nat. Phys. 17, 245 (2021). [2] R. Mondal et al., J. Magn. Magn. Mater. 579, 170830 (2023).

MA 2.2 Mon 9:45 H 1058

Atomistic spin dynamics investigation of laser-induced ultrafast magnetization switching in layered ferrimagnets — •José Miguel Lendínez, Silvia Gallego, and Unai Atxitia — Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain

The experimental demonstration of field-free magnetization switching in GdFeCo alloys opened the door to a promising route toward faster and more energy efficient data storage. A recent semi-phenomenological theory has proposed that a fast, laser-induced demagnetization below a threshold value is necessary for switching [1]. Notably, this threshold scales inversely proportional to the number of exchange-coupled nearest neighbours considered in the generic model, which in the simplest case is directly linked to the underlying lattice structure [2].

In this work we use atomistic spin dynamics simulations to investigate the possibility energy efficient laser-induced magnetization switching in generic layered ferrimagnetic alloys. Importantly, the interlayer exchange coupling tunes the dimension of the underlying magnetic model, from bulk 3D alloy for finite values to a 2D alloy for vanishing values. We demonstrate that the larger fluctuations in the 2D system are beneficial for a lower energy switching in comparison to the 3D systems.

[1] F. Jakobs and U. Atxitia, Phys. Rev. Lett. **129** 037203 (2022).
[2] J. A. Velez, R. M. Otxoa, and U. Atxitia, Appl. Phys. Lett. **123**, 112402 (2023).

MA 2.3 Mon 10:00 H 1058

T-symmetric second order optical responses in noncollinear AFMs — •Javier Sivianes[1], Flaviano José Dos Santos[2], and Julen Ibañez-Azpiroz[1,3,4] — [1]Centro de Física de Materiales, UPV, Donostia — [2]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL) — [3]Ikerbasque Foundation, Bilbao, Spain — [4]Donostia International Physics Center (DIPC), Donostia, Spain

There is a growing interest in Mn_5Si_3, a compound that exhibits altermagnet and noncollinear AFM phases [1]. The latter presents a peculiar feature; its atomic positions belong to the centrosymmetric $6/mmm$ point group while its magnetic point group $11'$ lacks inversion symmetry. Notably, this allows for finite second order optical responses to take place such as the shift and injection currents or the nonlinear Hall effect.

In this work we report DFT calculations on the quadratic optical properties of noncollinear Mn_5Si_3, which reach a substantial magnitude comparable to ferroelectric materials. In order to gain insight into the role of the magnetic structure in the nonlinear charge flow, we build a double-exchange tight-binding model. The nonlinear optical signature could be employed to distinguish among the various suggested magnetic structures of the material [1].

[1] N. Biniskos. et al., Phys. Rev. B **105**, 104404 (2022).

Funding provided by the European Union's Horizon 2020 research and innovation programme under the European Research Council (ERC) grant agreement No 946629.

MA 2.4 Mon 10:15 H 1058

Spin wave transport in ferromagnetic and antiferromagnetic bilayers — •Moumita Kundu[1], Levente Rozsa[2], and Ulrich Nowak[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Wigner Research Center for Physics, Budapest, Hungary

Spin transport in magnetic insulators is crucial for spin-based multifunctional devices. In our work, we study the transport of spin waves in ferromagnetic(FM) and antiferromagnetic(AFM) insulator bilayers. We focus on uncompensated interfaces that can essentially change the ordering temperatures for both the FM and the AFM[1].

For our investigation, we use atomistic spin dynamic simulations, where magnetic interactions are described using an extended Heisenberg model and we use the stochastic Landau-Lifshitz-Gilbert equation as the equation of motion. It is seen that with both, thermal and monochromatic excitations, the spin wave decays exponentially having a propagation length of several nanometers. The transport of magnons is studied via the magnon accumulation which is defined as the difference in the magnon population leading to diffusion. Additionally, the dispersion relation of such magnons are also calculated for different temperatures. We study the dependence of the propagation of magnons in such heterostructures on damping, anisotropy and exchange coupling at the interface.

[1] V. Brehm, M. Evers, U. Ritzmann, and U. Nowak, PHYSICAL REVIEW B **105**, 104408(2022)

MA 2.5 Mon 10:30 H 1058

Current-induced spin polarization in chiral Tellurium: a first-principles quantum transport study — •Reena Gupta and Andrea Droghetti — School of Physics and CRANN, Trinity College, 2, Dublin, Ireland

Te is a naturally p-doped semiconductor with a chiral structure, where an electrical current causes the conduction electrons to become spin polarized parallel to the transport direction. Here we present a comprehensive theoretical study of this effect by employing density functional theory (DFT) combined with the non-equilibrium Green's functions (NEGF) technique for quantum transport. We suggest that the spin polarization can quantitatively be estimated in terms of two complementary quantities, namely the non-equilibrium magnetic moments and the spin current density. The calculated magnetic moments are directly compared with the values from previous the- oretical studies obtaining overall consistent results. On the other hand, the inspection of the spin current density provides insights of the magnetotransport properties of the material. Specifically, we predict that the resistance along a Te wire changes when an external magnetic field is applied parallel or antiparallel to the charge current direction. The computed magnetoresistance is however quite small. Finally, we show that the description of the current-induced spin polarization in terms of the spin current establishes a straightforward connection with the phenomenon called chiral-induced spin selectivity, recently observed in several nanojunctions.

MA 2.6 Mon 10:45 H 1058

Magnetoelastic effects on sound velocity — Pablo Nieves[1,2], Julian Tranchida[3], Svetoslav Nikolov[4], Alberto Fraile[5], and •Dominik Legut[1] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czechia — [2]University of Oviedo, Oviedo, Spain — [3]CEA, DES/IRESNE/DEC, France — [4]Sandia National Laboratories, Alberque, NM, USA — [5]Bangor University, Bangor, Wales, UK

In this work, we leverage atomistic spin-lattice simulations to examine how magnetic interactions impact the propagation of sound waves through a ferromagnetic material. To achieve this, we characterize the sound wave velocity in BCC iron, a prototypical ferromagnetic material, using three different approaches that are based on the oscillations of kinetic energy, finite-displacement derived forces, and corrections to the elastic constants, respectively. Successfully applying these meth-

ods within the spin-lattice framework, we find good agreement with the Simon effect including high-order terms. In analogy to experiments, morphic coefficients associated with the transverse and longitudinal waves propagating along the [001] direction are extracted from fits to the fractional change in sound velocity data. The present efforts represent an advancement in magnetoelastic modeling capabilities which can promote the design of future magnetoacoustic devices [1].

1. P. Nieves, J. Tranchida, S. Nikolov, A. Fraile, and D. Legut, Phys. Rev. B 105, 134430 (2022).

15 min. break

MA 2.7 Mon 11:15 H 1058

Are Magnons Just The Van Der Waals Interaction In Disguise? — •Robert Lawrence — School of Physics, Engineering and Technology, University of York, Heslington, North Yorks. YO10 5DD, UK

For systems without significant magnetism (such as non-magnetic, carbon-based molecules) it is well-known that correctly capturing the properties of the system – such as the interlayer spacing of graphite – requires considering the dynamical correlations, such as the van der Waals interactions. These dynamical correlations lead to quantised electric dipole waves throughout the system [1]. In magnetic systems magnetic correlations are also possible, in addition to the electric dipole-induced electric dipole interactions.

In this talk, we present our work extending semi-empirical van der Waals models to include both the magnetic and electric parts simultaneously, and demonstrate how this can naturally lead to the emergence of the Heisenberg model of magnetism. Finally, we discuss how this model leads to the ability to predict long-range magnetic coupling (and hence parameterise magnons) in a more computationally efficient manner than finite displacements on large supercells.

[1] A. Ambrosetti, N. Ferri, R.A. Distasio Jr. , A. Tkatchenko, Wavelike charge density fluctuations and van der Waals interactions at the nanoscale, *Science*, 351, 6278, 2016

MA 2.8 Mon 11:30 H 1058

Unravelling local spin-model parameters based on non-collinear magnetic states — Bendegúz Nyári[1,2] and •László Szunyogh[2,1] — [1]HUN-REN-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Budapest Hungary — [2]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary

The theory of local spin-interactions as calculated from non-collinear magnetic states via multiple scattering Green's function technique will be described. Two alternative formalisms is implemented to perform calculations for specific spin-configurations of a Cr trimer deposited on a Au(111) surface. The two calculations provide with the same two-spin rotation energies, however, the local interaction parameters turn out to be remarkably different. The ambiguity between these results occurs due to longitudinal contributions to the interactions and can perfectly be eliminated in terms of projections to the transversal subspace in the local coordinate system. Moreover, a global spin model containing isotropic two-spin and four-spin interactions is used to calculate the two-spin rotation energies and a reasonable agreement is found between the results obtained from the global and local models. An analytic formulation based on a Green's function expansion technique also clearly identifies the higher-order global multispin interactions as the source of the tensorial local spin-model parameters as suggested earlier [1,2].

[1] M. dos Santos Dias et al., Phys. Rev. B 103, L140408 (2021).
[2] M. dos Santos Dias et al., Phys. Rev. B 105, 026402 (2022).

MA 2.9 Mon 11:45 H 1058

Bi-directionally coupled simulation of magnetization dynamics and elastodynamics — •Peter Flauger[1], Matthias Küss[2], Michael Karl Steinbauer[1], Bernhard Emhofer[1], Matthias Volz[3], Hubert Krenner[3], Manfred Albrecht[2], and Claas Abert[1] — [1]University of Vienna — [2]University of Augsburg — [3]University of Münster

The interaction of surface acoustic waves (SAWs) with spin waves (SWs) in magnetic thin films via the magnetoelastic effect allows e.g. for the excitation of SW modes with prolonged propagation distances [1] or magnetic field sensors [2] and is thus of current scientific interest. In this work, we present a self-consistent solver for coupled magnetization dynamics and linear elasticity simulations based on the finite-differences method as an extension to the python library magnum.np [3]. This solver is then used to investigate the excitation of spin waves in magnetic thin films by SAWs. The observed non-reciprocity of the excitation with respect to the propagation direction and the power loss of the SAW are compared to experimental results on Ni films on a $LiTaO_3$ substrate [4].

[1] C. Chen *et al.*, Appl. Phys. Lett. **110**, 072401 (2017).
[2] A. Kittmann *et al.*, Sci. Rep. **8**, 278 (2018).
[3] F. Bruckner *et al.*, Sci Rep. **13**, 12054 (2023).
[4] M. Küß *et al.*, Phys. Rev. Appl. **15**, 034046 (2021).

MA 2.10 Mon 12:00 H 1058

Relativistic magnetic interactions from non-orthogonal basis sets — •Gabriel Martínez-Carracedo[1], László Rózsa[2], Amador García-Fuente[1], László Szunyogh[3], Ferrer Jaime[1], László Udvardi[3], and Bendegúz Nyári[3] — [1]Departamento de Física, Universidad de Oviedo, 33007 Oviedo, Spain — [2]Department of Physics of Complex Systems, Eötvös Loránd University, 1117 Budapest, Hungary — [3]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Mûegyetem rkp. 3., H-1111 Budapest, Hungary

We introduce a method using density functional theory to determine magnetic exchange interactions and on-site anisotropy tensors in extended Heisenberg spin models. Our approach, based on the Liechtenstein-Katsnelson-Antropov-Gubanov torque formalism, involves energy variations during infinitesimal rotations. Using a non-orthogonal basis set of pseudo-atomic orbitals in the Kohn-Sham Hamiltonian expansion, we demonstrate the method's accuracy and flexibility by computing tensors for magnetic nanostructures and two-dimensional magnets and results align well with the Korringa-Kohn-Rostoker Green's function method.

MA 2.11 Mon 12:15 H 1058

Quantum effects on unconventional pinch-point singularities in pyrochlore materials — •Lasse Gresista[1,2], Simon Trebst[1], and Yasir Iqbal[2] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Department of Physics and Quantum Centre of Excellence for Diamond and Emergent Materials (QuCenDiEM), Indian Institute of Technology Madras, India

The discovery of emergent gauge theories in condensed matter systems is associated with novel phenomena such as fractionalization and topological excitations. A prime example are spin ice compounds, which are materials hosting a ground state described by an emergent U(1) gauge theory, featuring monopole excitations arising from the fractionalization of microscopic spin degrees of freedom. Remarkably, signatures of the gauge structure are visible in neutron scattering measurements as *pinch-point* singularities. Recently, classical spin liquids on the pyrochlore lattice have been proposed with a higher-rank gauge structure, where instead of a conventional gauge field the low-energy physics is described by fluctuations of a tensor field with a continuous gauge freedom. The corresponding classical correlations show variations of the conventional pinch-point singularities, such as *pinch-lines* or *multi-fold* pinch-points. Here, we investigate the effect of quantum fluctuations on these signatures using a pseudo-fermion functional renormalization group approach. We observe a significant modification of the signal drastically different from the simple broadening due to thermal fluctuations, highliting the importantance of quantum fluctuations in possible material realizations and interpretation of experimental observations.

MA 2.12 Mon 12:30 H 1058

Magnetodynamics in molecular dynamics simulations using the thermal Stoner-Wohlfarth model — •Deniz Mostarac, Andrey Kuznetzov, Pedro A. Sanchez, Dieter Süss, and Sofia Kantorovich — University of Vienna, Vienna, Austria

In this contribution we present a state-of-the-art, hybrid approach, based on an extension of the generalized Stoner-Wohlfarth model to capture thermal activation in magnetic colloids. With this approach we can simulate internal magnetization dynamics of magnetic colloids, including both Brownian and Néel relaxation mechanisms, in large scale, long time scale bulk simulations. The model is qualified against classical systems (solid superparamagnet and a dilute ferrofluid) that are well understood theoretically to demonstrate the range of applicability and the scaleability of the model. Finally, a case study of a suspension of magnetic filaments with superparamagnetic colloids is presented, that highlights that long-range dipolar interactions in quasi-

infinite colloidal systems, particularly ones where the translational and rotational degrees of freedom between the colloids are coupled,[1,2] necessitates the use of a sophisticated model incorporating magnetodynamics explicitly and accurately. [1] Mostarac, D., et al. Nanoscale (2020). [2] Mostarac, D., et al. Macromolecules (2022).