MA 38: Electron Theory of Magnetism and Correlations

Time: Friday 9:30–11:15 Location: H43

MA 38.1 Fri 9:30 H43

Magnetic torque and DMI-like spin-lattice-coupling parameters from first principles — •S. Mankovsky[1], H. Lange[1], S. Polesya[1], M. Weissenhofer[2], U. Nowak[2], and H. Ebert[1] — [1]Dept. Chemistry, LMU Munich, D-81377 Munich, Germany — [2]Fachbereich Physik, Uni. Konstanz, 78457 Konstanz, Germany

Magneto-elastic couplings can play a crucial role both for ground state magnetic properties of materials giving rise to modified forms of the magnetic ground state accompanied by a spontaneous lattice deformation, as well as for spin-lattice dynamics, e.g. having a leading role for Gilbert damping in insulators.

As the magneto-elastic properties are fully determined by the electronic structure, the corresponding spin-lattice coupling (SLC) parameters can be calculated at a first-principles level. Aiming at that, we start with the phenomenological atomistic spin-lattice Hamiltonian which can be seen as an extension of the standard Heisenberg spin Hamiltonian. Focusing on the SOC-driven SLC effects, we discuss the torque on the magnetic moment as well as the modification of the Dzyaloshinskii-Moriya interaction (DMI) induced by an atomic displacement, giving access to corresponding SLC parameters. The expressions for these SLC parameters have been worked out based on the fully-relativistic KKR Green functions formalism. Corresponding calculations have been done for different two-dimensional and three-dimensional systems. Their properties as well as possible impact on the magnetic structure are discussed in comparison with the ordinary MCA and DMI parameters.

MA 38.2 Fri 9:45 H43

Angular momentum transfer via relativistic spin-lattice coupling from first principles — •Hannah Lange[1], Sergiy Mankovsky[1], Svitlana Polesya[1], Markus Weissenhofer[2], Ulrich Nowak[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, Butenandtstr. 11, 81377 Munich — [2]Dept. Physics, Uni Konstanz, 78457 Konstanz

The transfer and control of angular momentum is a key aspect for spintronic applications. Only recently, it was shown that it is possible to transfer angular momentum from the spin system to the lattice on ultrashort time scales [1]. Hence, combined molecular-spin dynamics simulations using first-principles parameters might give access to the central aspects of the underlying mechanisms.

To contribute to the understanding of angular momentum transfer between spin and lattice degrees of freedom we present a scheme to calculate fully-relativistic spin-lattice coupling parameters from first-principles. By treating changes in the spin configuration and atomic positions at the same level, closed expressions for the atomic spin-lattice coupling parameters can be derived in a coherent manner up to any order. Analyzing the properties of these parameters, in particular their dependence on spin-orbit coupling, we find that even in bcc Fe the leading term for the angular momentum exchange between the spin system and the lattice is a Dzyaloshiskii-Moriya-type interaction, which is due to the symmetry breaking distortion of the lattice.

[1] Tauchert et al. Nature 602, 73 (2022).

MA 38.3 Fri 10:00 H43

Double-Exchange Enhanced Magnetic Blue-Shift of Mott Gaps — •Mohsen Hafez-Torbati[1], Davide Bossini[2], Frithjof B. Anders[1], and Goetz S. Uhrig[1] — [1]Technical University of Dortmund, Dortmund, Germany — [2]University of Konstanz, Konstanz, Germany

Strong correlations in Mott insulators induce a substantial charge excitation energy known as the Mott gap. We study how the Mott gap is affected by long-range antiferromagnetic ordering upon reducing the temperature below the Néel temperature. Our finding is that the Mott gap is increased by the magnetic ordering: a magnetic blue-shift (MBS) occurs. We unveil the origin of the MBS of the Mott gap by analyzing the Hubbard model and the Hubbard-Kondo model and clarify the subtle differences. We show that in the Hubbard model the MBS is determined by the magnetic exchange coupling. In the Hubbard-Kondo model an additional contribution proportional to the hopping is induced by the double-exchange mechanism. We describe the magnetic contribution to the band gap blue-shift observed in the optical conductivity of α-MnTe and pinpoint a hopping contribution of 64% and a magnetic exchange contribution of 36%. A MBS with the energy scale of the hopping and the exchange interaction bears the potential to enable spin-to-charge conversion on extreme time scales, highly promising for spintronic and magnonic applications.

MA 38.4 Fri 10:15 H43

A Theory for Colors of Strongly Correlated Electronic Systems — •Swagata Acharya[1], Cedric Weber[2], Dimitar Pashov[2], Mark van Schilfgaarde[3], Alexander I Lichtenstein[4], and Mikhail I Katsnelson[1] — [1]Radboud University, Nijmegen, The Netherlands — [2]King's College London, London, UK — [3]National Renewable Energy Laboratory, Colorado, US — [4]Institute of Theoretical Physics, University of Hamburg, Germany

Many strongly correlated transition metal insulators are colored, even though they have large fundamental band gaps and no quasi-particle excitations in the visible range. We pick two archetypal cases as examples: NiO with green color and MnF2 with pink color. We show that a perturbative theory based on low-order extensions of the GW approximation is able to explain the color in NiO, and indeed well describe the dielectric response over the entire frequency spectrum, while the same theory is unable to explain why MnF2 is pink. We show its color originates from higher order spin-flip transitions that modify the optical response. This phenomenon is not captured by low-order perturbation theory, but is contained in dynamical mean-field theory (DMFT), which has a dynamical spin-flip vertex that contributes to the charge susceptibility. Within our combined self-consistent GW-BSE approximation and DMFT approach we can describe the peaks in subgap charge susceptibilities in both NiO and MnF2 . As a secondary outcome of this work, we establish that the one-particle properties of paramagnetic NiO and MnF2 are both well described by an adequate single Slater-determinant theory and do not require a dynamical vertex.

MA 38.5 Fri 10:30 H43

Electron-plasmon and electron-magnon scattering in ferromagnets from first principles by combining *GW* and *GT* self-energies — Dmitrii Nabok, •Stefan Blügel, and Christoph Friedrich — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

This work combines two powerful self-energy techniques: The well-known *GW* method and a self-energy recently developed by us [1] that describes the renormalization caused by the scattering of electrons with magnons and Stoner excitations. This *GT* self-energy, which is fully **k** dependent and contains infinitely many spin-flip ladder diagrams, was shown to have a profound impact on the electronic band structure of Fe, Co, and Ni. For example, it predicted a band anomaly in iron that was later confirmed experimentally. In the present work [2], we refine the method by combining *GT* with the *GW* self-energy. The resulting *GWT* spectral functions exhibit strong lifetime effects and emergent dispersion anomalies. They are in a better agreement with experimental spectra than those obtained with *GW* or *GT* alone, even showing partial improvements over local-spin-density approximation dynamical mean-field theory. The shape of the iron band anomaly improves, too. We acknowledge the Center of Excellence MaX Materials Science at the Exascale (EU H2020-INFRAEDI-2018) for financial support.

[1] M.C.T.D. Müller, S. Blügel, and C. Friedrich, Phys. Rev. B **100**, 045130 (2019)

[2] D. Nabok, S. Blügel, and C. Friedrich, Npj Comput. Mater. **7**, 178 (2021)

MA 38.6 Fri 10:45 H43

Effective exchange interaction in non-collinear states from electronic structure theory — •Simon Streib[1], Ramon Cardias[2], Manuel Pereiro[1], Anders Bergman[1], Erik Sjöqvist[1], Cyrille Barreteau[3], Anna Delin[2], Olle Eriksson[1,4], and Danny Thonig[4,1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, Sweden — [3]SPEC, CEA, CNRS, Université Paris-Saclay, France — [4]School of Science and Technology, Örebro University, Sweden

The determination of exchange parameters in non-collinear magnetic configurations directly from the electronic structure has been a challenge since the initial development of the Lichtenstein-Katsnelson-

Antropov-Gubanov (LKAG) formalism for collinear configurations. Usually, the isotropic exchange interaction between two magnetic moments is only taken into account to bilinear order (Heisenberg exchange). We introduce instead a generalized isotropic two-spin exchange interaction, which takes all orders into account, and from which we derive an effective exchange interaction. We demonstrate how in an arbitrary non-collinear configuration this effective exchange interaction can be extracted from the energy curvature tensor, which describes the local energy curvature with respect to the directions of two magnetic moments. We apply our formalism to examples from tight-binding electronic structure and demonstrate strong fluctuations of the effective exchange interaction during spin dynamics simulations [1].

[1] S. Streib et al., arXiv:2203.11759.

MA 38.7 Fri 11:00 H43

Electric-field control of the exchange interactions — •Svitlana Polesya[1], Sergiy Mankovsky[1], Eszter Simon[1], Alberto Marmodoro[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, Butenandtstrasse 11, D-81377 Munich, Germany — [2]Inst. of Physics, Czech Academy of Sciences, Cukrovarnicka 10, 162 00 Praha 6, Czech Republic

The impact of an applied electric field on the exchange coupling parameters has been investigated based on first-principles electronic structure calculations by means of the KKR Green function method. The calculations have been performed for a Fe monolayer (ML) and for deposited Fe films on different substrates, i.e., metallic (Pt) and semiconducting (GaAs). We analyze the origin of the field-induced change of the exchange interactions J_{ij} and the features of their field-dependent behavior specific for the studied systems. In particular, rather pronounced changes of J_{ij} have been found for the Fe/Pt(111) system due to the localized electronic states at the Fe/Pt interface. In the case of Fe/GaAs(001) films we discuss also the dependence of the field-induced modification of J_{ij} on the thickness of the Fe film. For all studied systems, a strong impact of surface relaxation is found both for the ground-state exchange parameters as well as for their field induced modification.