# MA 38: Electron Theory of Magnetism and Correlations

Time: Wednesday 9:30–12:15 Location: HSZ 403

MA 38.1 Wed 9:30 HSZ 403

**Large coercivity fields and magnetic anisotropy in $Li_2Sr[(Li_{1-x}Fe_x)N]_2$** — •Tanita Johanna Ballé[1], Peter Höhn[2], and Anton Jesche[1] — [1]EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

$Li_2(Li_{1-x}Fe_x)N$ is the material with the highest known coercivity field with a value of more than 11 T and shows huge magnetic anisotropy. These properties are attributed to an orbital contribution to the magnetic moment of iron that is unquenched due to the perfect linear, twofold coordination of iron between nitrogen [1]. $Li_2Sr[(Li_{1-x}Fe_x)N]_2$ provides a similar geometry. In order to evaluate the necessity as well as sufficiency of the linear, twofold coordination for the high coercivity field and anisotropy to emerge, we investigated single crystals of $Li_2Sr[(Li_{1-x}Fe_x)N]_2$ with $x = 0.41$. A thorough structural characterization was carried out by means of powder and single crystal X-Ray diffraction as well as chemical analysis. Isothermal and temperature dependent magnetization measurements were performed in the range of $T = 2$ K - 300 K and applied fields of up to $\mu_0 H = 7$ T. A coercivity field of almost 7 T at 2 K and a high magnetic anisotropy were indeed observed. Furthermore we found an enhanced magnetic moment and magnetic susceptibility in this material that indicate a significant orbital contribution to the magnetic moment of iron. [1] A. Jesche *et al.*, Nat. Commun. **5**:3333. doi: 10.1038/ncomms4333 (2014)

MA 38.2 Wed 9:45 HSZ 403

**Bilinear and higher order exchange couplings in condensed matter physics by multiple-parameter perturbation theory** — •Danny Thonig[1], Pavel Bessarab[2], Lars Bergqvist[2], Manuel Pereiro[1], Anna Delin[2], and Olle Eriksson[1] — [1]Department of Physics and Astronomy, University Uppsala, Sweden — [2]Department of Materials and Nano Physics, KTH, 16440 Kista, Sweden

A profound concept in theoretical modelling is epitomised by the mapping of total energy variations on effective Hamiltonians. For instance, bilinear couplings describe well the interaction between atomistic magnetic moments (Heisenberg model) or lattice vibrations (force constant matrix)[1]. Nevertheless, these models are inconsistent at finite temperature and call for a full description.

We will present our multiple-parameter perturbation approach based on first principles method and its realisation in the real-space Slater-Koster parametrised Tight Binding method. Thermal, chemical or occupational disorder are considered as average in real space.

The current method will be applied to bulk Stoner magnets. Zero temperature bilinear coupling parameters are well reproduced, but finite temperature gives significant changes in the magnitude and long-range character. We will present new types of couplings, e.g. bilinear spin-lattice or orbital moment coupling, and a generalisation for higher-orders. Our results give a fundamental new insight into coupling mechanism in condensed matter physics.

[1] V. Vitek and D. J. Srolovitz, "Atomistic Simulation of Materials: Beyond Pair Potentials" Plenum Press, New York (1989)

MA 38.3 Wed 10:00 HSZ 403

**The frozen magnon method beyond the long-wave approximation** — •Adam Jakobsson — Luleå University of Technology, Luleå, Sweden

The magnetic force theorem provides convenient ways to study exchange interactions in magnetic systems since it gives access to total energy differences between different magnetic states from non-self-consistent density functional theory calculations. This enables the efficient mapping of the total energy of the system as a function of the directions of the atomic moments in a Heisenberg model. However, it is well known that short range interactions in itinerant magnetic systems are poorly described with the conventional use of the theorem. In order to overcome this deficiency, numerous strategies have been developed over the years. We propose a two-step procedure and show that only by adding pre-converged constraining fields to non-self-consistent spin-spiral total energy calculations we obtain results that match self-consistent calculations. With this procedure, we can now do frozen magnon calculations which go beyond the long-wave approximation and thus properly describe the energy landscape of itinerant magnets. As a consequence only the exchange parameters from the non-self-consistent two-step procedure are in quantitative agreement with self-consistently derived exchange parameters. We exemplify this for three different systems: bcc Fe, fcc Ni and FeCo.

MA 38.4 Wed 10:15 HSZ 403

**Staircase of crystal phases of hard-core bosons on the kagome lattice** — •Daniel Huerga[1], Sylvain Capponi[2], Jorge Dukelsky[3], and Gerardo Ortiz[4] — [1]Institut fur Physik Theorique III, Stuttgart, Germany — [2]Laboratoire de Physique Theorique CNRS, Toulouse, France — [3]Instituto de Estructura de la Materia CSIC, Madrid, Spain — [4]Physics Department Indiana University, Bloomington IN, USA

We study the quantum phase diagram of a system of hard-core bosons on the kagome lattice with nearest-neighbor repulsive interactions, for arbitrary densities, by means of the hierarchical mean-field theory and exact diagonalization techniques. This system is isomorphic to the spin S=1/2 XXZ model in presence of an external magnetic field, a paradigmatic example of frustrated quantum magnetism. In the non-frustrated regime, we find two crystal phases at densities 1/3 and 2/3 that melt into a superfluid phase when increasing the hopping amplitude, in semiquantitative agreement with quantum Monte Carlo computations. In the frustrated regime and away from half-filling, we find a series of plateaux with densities commensurate with powers of 1/3. The broader density plateaux (at densities 1/3 and 2/3) are remnants of the classical degeneracy in the Ising limit. For densities near half-filling, this staircase of crystal phases melts into a superfluid, which displays finite chiral currents when computed with clusters having an odd number of sites. Both the staircase of crystal phases and the superfluid phase prevail in the noninteracting limit, suggesting that the lowest dispersionless single-particle band may be at the root of this phenomenon.

MA 38.5 Wed 10:30 HSZ 403

**Ab-initio calculations of QMOKE in bcc Fe, Drude term modelling** — •Ondřej Stejskal[1], Robin Silber[1,2], Jaroslav Hamrle[3], Martin Veis[3], and Jaromír Pištora[1] — [1]VSB-Technical University of Ostrava, Czech Republic — [2]CSMD, Physics Department, Bielefeld University, Germany — [3]Charles University, Prague, Czech Republic

The part of the magnetooptic Kerr effect (MOKE) that is even in magnetization is called the quadratic MOKE (QMOKE). Permittivity tensor fully describes the magnetooptic response of a material. We performed ab-initio calculations of the permittivity tensor in bcc Fe by the WIEN2k code [1]. We also model the intraband contributions via the Drude term [2]. The results are then compared to experiment. This work further includes detailed investigation of key bands contributing to the MOKE signal and their visualisation in Brillouin zone.

[1] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, WIEN2k

[2] Š. Višňovský, Optics in Magnetic Multilayers and Nanostructures, Taylor and Francis Group, Boca Raton, Florida 2006

**15 min. break.**

MA 38.6 Wed 11:00 HSZ 403

**Coherence and stiffness of spin waves in diluted ferromagnets** — •Ilja Turek[1], Josef Kudrnovsky[2], and Vaclav Drchal[2] — [1]Institute of Physics of Materials, Acad. Sci. Czech Rep., Brno, Czech Republic — [2]Institute of Physics, Acad. Sci. Czech Rep., Prague, Czech Republic

We present results of a numerical analysis of magnon spectra in supercells simulating low-dimensional and bulk random diluted ferromagnets with long-ranged pair exchange interactions [1]. We show that low-energy spectral regions for these strongly disordered systems contain a coherent component leading to interference phenomena manifested by a pronounced sensitivity of the lowest excitation energies to the adopted boundary conditions. The dependence of configuration averages of these excitation energies on the supercell size can be used for an efficient determination of the spin-wave stiffness $D$. The developed formalism is applied to the ferromagnetic Mn-doped GaAs semiconductor with optional incorporation of phosphorus; the obtained

concentration trends of $D$ are found in reasonable agreement with recent experiments. Moreover, a relation of $D$ to the Curie temperature has been studied for Mn-doped GaAs and GaN semiconductors.
[1] I. Turek et al., arXiv: 1611.06691 (2016).

MA 38.7 Wed 11:15 HSZ 403

**Electron dynamics of correlated materials** — •Viktor Valmispild[1,2], Vladimir Antropov[3], Evgeny Gorelov[4], Alexander Joura[1], Martin Eckstein[5], and Alexander Lichtenstein[1,2] — [1]Institute of Theoretical Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [2]The Hamburg centre for ultrafast imaging, 22761 Hamburg, Germany — [3]Ames Laboratory, Ames, IA 50011, USA — [4]European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany — [5]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

The work is focused on theoretical description of electron dynamics in correlated materials. The report consists of two sections:

In the first part we study the single-band Hubbard model on a infnite-dimensional lattice in the presence of a large spatially uniform electric field out of equilibrium. We study the model out of equilibrium using the Keldysh formalism and perturbation theory in the Coulomb interaction U. This work present numerical results for the total energy of the system on an infinite-dimensional hypercubic lattice with nearest-neighbor hopping.

The second part of investigations conducted dynamic magnetic susceptibility simple transition metals Iron, Cobalt and Nickel.

MA 38.8 Wed 11:30 HSZ 403

**Ab-initio modelling of spin-fluctuations in classical regime for itinerant ferro- and antiferromagnetics.** — •Sergii Khmelevskyi — CMS, IAP, Vienna University of Technology, Vienna, Austria

We present an ab-initio scheme of calculating high-temperature magnetic properties of the itinerant electron systems with strong thermally induced longitudinal fluctuations of the magnetic moments. The scheme is based on the disordered local moment formalism and magnetic force theorem for the calculation of the inter-atomic magnetic exchange interactions. The single-site theory and constrained first-principle calculations has been used for setting the parameters of the mean-field like Heisenberg Hamiltonian with varying amplitude of the spin moment. The transverse (spin-rotation) degrees of freedom, however, have been treated beyond mean-field (Monte-Carlo simulations). We discuss a problem of choosing of a proper statistical measure for the integration over the spin degrees of freedom in classical configurational space. We compare different approaches to the problem for various systems: bcc Fe, fcc Ni, fcc Co, novel itinerant high temperature antiferromagnetic V3Al [1] and "nearly ferromagnetic" FeSi semiconductor. The comparison is done by calculating the magnetic ordering temperatures and high temperature behavior of the susceptibility entirely from first principles. [1] S. Khmelevskyi, Phys. Rev. B 94, 024420 (2016).

MA 38.9 Wed 11:45 HSZ 403

**Dzyaloshinskii-Moriya interaction parameters calculated by means of the relativistic KKR Green function method** — •Sergiy Mankovsky and Hubert Ebert — Dept. Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany

A new scheme to calculate the inter-atomic Dzyaloshinskii-Moriya (DM) interaction parameters by means of the relativistic KKR (Korringa-Kohn-Rostoker) Green function method is presented. For this purpose, perturbation theory is used to express the change in energy $\Delta E$ caused by a helimagnetic modulation – characterized by a small wave vector $\vec{q}$ – of a magnetically ordered system. The corresponding derivative $\frac{\partial E}{\partial q_\alpha}$ in the limit $q \to 0$ gives access to the various components of the DM vector [1]. Making use of the real space representation of the electronic Green functions as supplied by the KKR formalism an expression for the inter-atomic DM interaction parameters is obtained. The present approach avoids the calculation of the full exchange coupling tensor [2,3] and allows to calculate the components of the DM vector using just one magnetic configuration. Test calculations have been performed for various 3D and 2D systems. The corresponding results are compared with results obtained previously using other schemes suggested in the literature [1,2,3].

[1] F. Freimuth, S. Blügel and Y. Mokrousov, J. Phys.: Condens. Matter **26**, 104202 (2014)

[2] L. Udvardi, L. Szunyogh, K. Palotas, and P. Weinberger, Phys. Rev. B **68**, 104436 (2003)

[3] H. Ebert and S. Mankovsky, Phys. Rev. B **79**, 045209 (2009)

MA 38.10 Wed 12:00 HSZ 403

**Bosonic excitations observed at the transition to helical magnetic phases in PrPtAl** — •Jean-Philippe Reid[1], D Sokolov[2], C Oneill[3], C Lithgow[3], A Walker[1], M Lizaire[1], S Codsi[1], E Yelland[3], P Wahl[1], and Andrew Huxley[3] — [1]School of Physics and Astronomy, University of St. Andrews, St. Andrews, UK — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]School of Physics and CSEC, University of Edinburgh, Edinburgh, UK

Transport and thermodynamic measurements were performed on the rare earth platinum aluminide PrPtAl through the helical magnetic phases, located in a narrowed temperature range between the ferromagnetic and paramagnetic phases. We detected an additional bosonic contribution to the thermal conductivity which can only be related to the helical magnetic phase. This additional bosonic contribution accounts for most of the increase of the density of states observed in the specific heat. It suggests that the emergence of the helical magnetic phases is accompanied by strong bosonic fluctuations which not only induce scattering, but also contribute to the thermal conductivity. Quantum order-by-disorder theory effectively integrates over boson modes and considers fermionic quantum fluctuations. Our findings suggests direct consideration of the boson modes may provide greater insight.