MA 38: Theory of strongly correlated systems

Time: Thursday 9:30–13:15 Location: H 0110

Topical Talk MA 38.1 Thu 9:30 H 0110

RKKY-induced Kondo breakdown near a magnetic quantum phase transiton — •Johann Kroha — Universität Bonn, Germany — CCM, Zhejiang University, Hangzhou, China

The fate of the fermionic quasiparticles near a magnetic quantum phase transition (QPT) in heavy-fermion (HF) compounds has been controversial for many years. It is generally believed that this Kondo destruction is driven by the critical fluctuations near the QPT. A novel renormalization group treatment of the quantum interference of Kondo and RKKY couplings shows, however, that the HF quasiparticles can be destroyed by the RKKY interaction even without critical fluctuations [1], with far reaching consequences for the QPT scenario: The lattice Kondo temperature, $T_K^*(y)$, is suppressed in a universal way by the dimensionless RKKY coupling y, with a discontinuous breakdown at a critical value $y = y_c$. This agrees quantitatively with STM spectroscopy on continuously tunable two-impurity Kondo systems [2]. We analyze in detail most recent time-resolved THz reflectometry experiments on the HF compound $CeCu_{6-x}Au_x$ across the QPT at x=0.1 [3]. The theoretical as well as the experimental findings point to a new quantum critical scenario, realized in $CeCu_{6-x}Au_x$, where the HF quasiparticles disintegrate in that their spectral weight vanishes continuously, but $T_K^*(y)$ remains finite. This is consistent with ω/T scaling as an indicator for critical Kondo destruction.

[1] A. Nejati, K. Ballmann, J. Kroha, PRL **118**, 117204 (2017)
[2] J. Bork, Y.-H. Zhang, L. Diekhöhner *et al.*, Nature Phys. **7**, 901 (2011)
[3] Ch. Wetli, J. Kroha, K. Kliemt *et al.*, arXiv:1703.04443

MA 38.2 Thu 10:00 H 0110

Dynamics of the magnetic moments in correlated metals: The case of Fe and Ni from ambient to Earth's core conditions — Andreas Hausoel[1], Micheal Karolak[1], Giorgio Sangiovanni[1], Ersoy Sasioglu[2], Alexander Lichtenstein[3], Andrey Katanin[4], Kasten Held[5], and •Alessandro Toschi[5] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425, Germany — [3]Institut für Theoretische Physik, Universität Hamburg, 20355, Germany — [4]Institute of Metal Physics, 620990 Ekaterinburg, Russia — [5]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

The formation of localized magnetic moments and their dynamical screening represents one of the crucial ingredients for the physics of correlated metals. Their fingerprints appear, sometimes in different ways, in transport and spectroscopic experiments. As a relevant example, we present here our most recent ab-initio (DFT) + DMFT calculations [1] for two of the most common ferromagnetic elements: Fe and Ni, both at ambient and Earth's core conditions. The comparison of the results inspires the interesting hypothesis of a more important role played by Ni for the generation of the Earth's magnetic field, than hitherto postulated.

[1] A. Hausoel, M. Karolak, E. Sasioglu, A. Lichtenstein, K. Held, A.A. Katanin, A. Toschi, and G. Sangiovanni, Nature Communications **8**, 16062 (2017).

MA 38.3 Thu 10:15 H 0110

Time-reversal origin of anisotropies for non-Kramers magnetic states — •Bruno Tomasello and Tim Ziman — Institut Laue-Langevin, CS 20156, Cedex 9, 38042 Grenoble, France

Magnetic anisotropies of rare-earth ions characterise unconventional phases in many condensed matter systems. The theoretical effort for describing such phases typically begins by "adjusting" suitable *pseudo-spin* Hamiltonians which can account for complex exotic behaviours and yet involve simple enough mathematics. A case per se are *non-Kramers* bound-ions whose spectra features a *neat* separation of the lowest energy states from the higher ones. In this talk, focusing on non-Kramers magnetic ions, I will discuss the relationship between *time-reversal* properties and the origin of axial anisotropies. Emphasis will be given to identifying the *microscopic* mechanisms of interest from established theoretical frameworks. The analysis will be contextualised in the perspectives of recent dispersive signatures in the low-temperature neutron-scattering experiments on powders of the *garnet* $Tb_3Ga_5O_{12}$, which is well known for detection of *phonon Hall* physics.

MA 38.4 Thu 10:30 H 0110

Electronic entropy in finite-temperature Green's-function calculations — •Ilja Turek[1,2], Josef Kudrnovsky[3], and Vaclav Drchal[3] — [1]Institute of Physics of Materials, Czech Acad. Sci., Brno, Czech Rep. — [2]Charles University, Faculty of Mathematics and Physics, Prague, Czech Rep. — [3]Institute of Physics, Czech Acad. Sci., Prague, Czech Rep.

Reliable evaluation of thermodynamic potentials of metallic materials and itinerant magnets at finite temperatures (free energy, grand-canonical potential) requires investigation of systems with perturbed translation invariance. For this purpose, Green's-function techniques are often applied, which use a complex energy variable and integrations over contours in the complex plane. However, for quantities related to the electronic entropy, the branch cut of the complex logarithmic function prevents standard deformations of the integration paths. We have derived and numerically implemented an alternative expression for the electronic entropy, which is not affected by the multi-valued nature of the complex logarithm. In this contribution, the developed theoretical formalism will be presented and its efficiency and accuracy in selected cases (on model and *ab initio* levels) will be discussed.

MA 38.5 Thu 10:45 H 0110

Asymmetry of the density of states and magnetic exchange interactions in Hund's metals — •Andrey Katanin[1,2], Alexander Belozerov[1,2], and Vladimir Anisimov[1,2] — [1]Institute of Metal Physics, Ekaterinburg, Russia — [2]Ural Federal University, Ekaterinburg, Russia

We discuss the effect of the asymmetry of the density of states on a possibility of Hund's metal behaviour and the way of calculation of the respective exchange interactions between frozen-spin states, corresponding to local moments. We find that quasiparticle damping and the formation of local magnetic moments due to Hund's exchange interaction are enhanced by asymmetry of the density of states; the properties of Hund's metal are mainly observed close to half filling, on the same side of half filling as the maximum of the density of states, and become stronger with increasing asymmetry. We also suggest the way to calculate the magnetic exchange interaction of Hund's metals within the supercell DMFT approach. We discuss implication of the obtained results to alpha-iron, for which ab initio calculations show a possibility of realization of Hund's metal behavior, and obtain the respective momentum- and temperature dependences of the magnetic susceptibilities and magnetic exchange interaction in this substance.

15 minutes break

MA 38.6 Thu 11:15 H 0110

Source-free exchange-correlation magnetic fields in density functional theory — •John Kay Dewhurst, E. K. U. Gross, Antonio Sanna, and Sangeeta Sharma — Max Planck Inst. of micro structure physics, Halle, Germany

Spin-dependent exchange-correlation energy functionals in use today depend on the charge density and the magnetization density: $E_{\rm xc}[\rho, \mathbf{m}]$. However, it is also correct to define the functional in terms of the curl of $\mathbf{m}$ for physical external fields: $E_{\rm xc}[\rho, \nabla \times \mathbf{m}]$. The exchange-correlation magnetic field, $\mathbf{B}_{\rm xc}$, then becomes source-free. We study this variation of the theory by uniquely removing the source term from local and generalized gradient approximations to the functional. By doing so, the total Kohn-Sham moments are improved for a wide range of materials for both functionals. Significantly, the moments for the pnictides are now in good agreement with experiment. This source-free method is simple to implement in all existing density functional theory codes.

MA 38.7 Thu 11:30 H 0110

Electronic structure and antiferromagnetism in a three-orbital model for iron pnictides. — •Sayandip Ghosh — Institute for Theoretical Physics, TU Dresden

The iron pnictides are the new class of high T_c superconductors after cuprates. They exhibit a rich temperature-doping phase diagram in which the parent compounds go through a structural transition and a magnetic phase transition to stripe antiferromagnetic (AFM) state. The electronic structure from first-principle techniques and ARPES

experiments reveal two nearly circular hole pockets and two elliptical electron pockets. The magnetic excitations in the magnetic state examined by inelastic neutron scattering measurements yield well defined spin wave excitations with a maximum at the ferromagnetic zone boundary. Towards understanding the electronic and magnetic properties, we propose and investigate a three-orbital itinerant-electron model and show that essential features of electronic structure and magnetism can be understood in this model. We also demonstrate how the effective spin couplings are generated from particle-hole propagator explaining microscopic origin of ferromagnetic spin coupling along b direction required to understand spin wave dispersion.

MA 38.8 Thu 11:45 H 0110

Theory of noncollinear interactions beyond Heisenberg exchange: Applications to bcc Fe — •Attila Szilva[1], Danny Thonig[1], Pavel Bessarab[2], Yaroslav Kvashnin[1], Debora Rodrigues[3], Ramon Cardias[1], Manuel Pereiro[1], Lars Nordström[1], Anders Bergman[1], Angela Klautau[3], and Olle Eriksson[1] — [1]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [2]Science Institute of the University of Iceland, 107 Reykjavik, Iceland and Department of Nanophotonics and Metamaterials, ITMO University, 197101 St. Petersburg, Russia — [3]Faculdade de Física, Universidade Federal do Pará, Belém, 66075-110, Brazil

We show for a simple noncollinear configuration of the atomistic spins (in particular, where one spin is rotated by a finite angle in a ferromagnetic background) that the pairwise energy variation computed in terms of multiple-scattering formalism cannot be fully mapped onto a bilinear Heisenberg spin model even in the absence of spin-orbit coupling. The non-Heisenberg terms induced by the spin-polarized host appear in leading orders in the expansion of the infinitesimal angle variations. However, an Eg-T2g symmetry analysis based on the orbital decomposition of the exchange parameters in bcc Fe leads to the conclusion that the nearest-neighbor exchange parameters related to the T2g orbitals are essentially Heisenberg-like: they do not depend on the spin configuration, and can, in this case, be mapped onto a Heisenberg spin model even in extreme noncollinear cases.

DOI: 10.1103/PhysRevB.96.144413

MA 38.9 Thu 12:00 H 0110

Calculation of micromagnetic parameters and spin-wave stiffness using the SPR-KKR method — •Sergiy Mankovsky[1], Ondrej Šipr[2], Sebastian Wimmer[1], Svitlana Polesya[1], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, D-81377 Munich, Germany — [2]Institute of Physics ASCR v. v. i., CZ-162 53 Prague, Czech Republic

We present an approach for the calculation of the micromagnetic exchange stiffness ($A_{\alpha\beta}$) as well as the closely related spin-wave stiffness, and Dzyaloshinskii-Moriya ($D_{\alpha\beta}$) tensors, based on the fully relativistic multiple scattering Korringa-Kohn-Rostoker (KKR) formalism. Results for ordered systems and for disordered alloys are compared with experimental results as well as with results based on the parameters of the relativistically extended Heisenberg model, that were calculated within the same ab-initio framework. In general a good agreement between the micromagnetic parameters calculated directly and those derived from other parameters, as well as from experiment, is found.

MA 38.10 Thu 12:15 H 0110

Comparison of different approaches to ab-initio calculations of the spin wave stiffness — •Ondřej Šipr[1], Sergey Mankovsky[2], and Hubert Ebert[2] — [1]Institute of Physics, Czech Acadademy of Sciences, Praha, Czech Republic — [2]Ludwig-Maximilians-Universität München, Germany

The spin waves stiffness constant D is one of the basic quantities characterizing magnetism in solids. Ab-initio calculations of spin wave stiffness reported in the literature have been performed within the scalar relativistic approximation. Usually D is evaluated either (i) in real space as a weighted sum of exchange coupling constants or (ii) in reciprocal space by fitting the spin-wave dispersion in the long-wave limit to a parabola. Even though both approaches look conceptually simple, theoretical values of D obtained for Fe and Ni by different groups show considerable spread of 50–100 %. We present results for the spin waves stiffness constant D of Fe, Ni, and permalloy $Fe_{0.2}Ni_{0.8}$ obtained by explicit summation of weighted exchange coupling constants as well as by fitting the spin-wave dispersion. We demonstrate that both procedures yield similar values when properly converged and we discuss which issues are crucial in this respect (especially concerning the summation of weighted exchange coupling constants and its extrapolation to the limit of zero damping). We inspect to what extent the energies of spin spirals can be described within the magnetic force theorem. In addition, we show how the spin waves stiffness changes if spin-orbit coupling is taken into account.

MA 38.11 Thu 12:30 H 0110

First-principles study of the magnetic and electronic properties of cubic GdCu compound — •Vikas Kashid[1], Ersoy Şaşioğlu[2], Gustav Bihlmayer[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum, Jülich and JARA, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We investigate the structural and magnetic properties of bulk GdCu (CsCl type) using spin density functional theory, where highly localized $4f$ orbitals are treated within LDA+U and GGA+U methods. The calculated magnetic ground state of GdCu exhibits a C-type antiferromagnetic configuration representing a propagation vector $\mathbf{Q} = (\pi, \pi, 0)$. The estimated Néel temperature of the cubic GdCu using GGA+U and LDA+U density functionals is 161 and 115 K, respectively within the mean field approximation (MFA). In particular, the theoretical understanding of Gd and Cu core level shift observed in photoemission spectroscopic experiments are investigated in detail. We find that, the shift of Gd-$4f$ states in GdCu with respect to bulk Gd, is due to the extra correlation (Hubbard U) of $4f$ electrons in the GdCu lattice. The core level shift in GdCu is studied using the Random Phase Approximation (RPA) and found sensitive to the choice of lattice parameters and the exchange functional.

MA 38.12 Thu 12:45 H 0110

Anatomy of the magnetic anisotropy energy mediated by tight-binding Rashba electrons — Gaurav Chaudhary[1], •Manuel dos Santos Dias[2], Allan H. MacDonald[1], and Samir Lounis[2] — [1]Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Perpendicular magnetic anisotropy (PMA) is one of many properties that can arise from the interface between a ferromagnetic layer and a heavy-metal one. The free-electron Rashba model, often used to describe the properties of such interfaces, has been shown not to support PMA [1]. We reprise the tight-binding model of Ref. [1], describing spin-orbit-coupled electrons exchange-coupled to a background ferromagnetic order. The band energy differences approach is compared with a new description based on the static uniform spin susceptibility of the electronic system, and with a proposal of Antropov based on the spin-orbit energy [2]. We investigate not only their compatibility but also what physical insights can be gained from each of them.

This work was supported by a DAAD–RISE internship and by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] K.-W. Kim *et al.*, Phys. Rev. B **94**, 184402 (2016)
[2] V. Antropov *et al.*, Solid State Commun. **194**, 35–38 (2014)

MA 38.13 Thu 13:00 H 0110

Calculated Curie temperatures of metallic ferromagnets — •Roman Kováčik, Phivos Mavropoulos, Konstantin Tillmanns, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We analyze the predictive power of the local density approximation, generalized gradient approximation, and disordered local moment method in connection with the classical Heisenberg model to determine the critical temperature of the magnetic phase transition for a large set (about 100) of bulk materials from the Heusler family alloys. To obtain the electronic structure we employ the *ab initio* Korringa-Kohn-Rostoker Green function method [1] where the exchange parameters are calculated by the method of infinitesimal rotations [2]. The magnetization curve as a function of temperature is simulated by the Monte Carlo method. The fourth-order cumulant is used to determine the critical temperature while its convergence is ensured with respect to the exchange parameters cut-off distance and the supercell size of the Monte Carlo simulation. Finally, we evaluate the effective magnetic moment and analyze our results in comparison with the experimental

data. Support from JARA-HPC (jara0051) is gratefully acknowledged.
[1] H. Ebert *et al.*, Rep. Prog. Phys. 74, 096501 (2011), also see: www.kkr-gf.org. [2] A. I. Liechtenstein *et al.*, J. Magn. Magn. Mater. 67, 65 (1987).