MA 10: Spin-dependent Transport Phenomena

Time: Monday 15:00–18:00 Location: HSZ 403

MA 10.1 Mon 15:00 HSZ 403

Anomalous Hall effect in Heusler alloys: native disorder and Fermi-sea term — •Josef Kudrnovsky[1], Ilja Turek[2], and Vaclav Drchal[1] — [1]Institute of Physics AS CR, Prague — [2]Institute of Physics of Materials AS CR, Brno

The anomalous Hall effect of selected Heusler alloys is estimated from first principles. An emphasis is put on the effect of the native disorder which is often present in the stoichiometric samples.

We employ a recently developed fully-relativistic Kubo-Streda approach adapted to disordered multisublattice systems in which the chemical disorder is described in terms of the coherent potential approximation. Both the Fermi-surface [1] and Fermi-sea [2] terms are included.

As case studies we choose half-metallic Heusler alloys Co2CrAl, Co2MnAl, and the spin gapless semiconductor alloy Mn2CoAl.

We demonstrate that a proper inclusion of the disorder significantly improves agreement between the experiment and theory. The importance of inclusion of the Fermi-sea term is also discussed.

[1] J. Kudrnovsky et al., Phys. Rev. B 88 (2013) 014422
[2] I. Turek et al., talk at this conference

MA 10.2 Mon 15:15 HSZ 403

ballistic emission electron microscopy investigation of the spin filtering effect in epitaxial Fe/Au/Fe/GaAs(001) spin valve — •marie hervé[1,2], sylvain tricot[1], yann claveau[1], sophie guézo[1], sergio di matteo[1], gabriel delhaye[1], bruno lépine[1], philippe schieffer[1], and pascal turban[1] — [1]Département Matériaux-Nanosciences - Institut de Physique de Rennes, Rennes, France — [2]Physikalisches Institut, Karlsruhe Institute of Technology (KIT),Karlsruhe, Germany

Ballistic Electron Magnetic Microscopy (BEMM) is a unique experimental tool allowing characterization of electronic properties of buried interfaces with nanometric lateral resolution. In BEMM experiments, hot electrons are injected from an STM tip into a spin-valve/semiconductor heterostructure. The measurement of the hot electron magnetocurrent collected at the back of the substrate gives access to the local magnetoconductance properties of the spin valve. In this communication, we will discuss experimental BEMM investigations on the epitaxial spin-valves Fe/Au/Fe/GaAs(001). In this structure, BEMM measurement show hot electron magnetocurrents as high as 500% at room temperature. This magnetocurrent is observed to be independant on the Fe layers thickness, and is thus dominated by interfacial effects [1]. We demonstrate that these strong magnetoconductance effects are related to the spin filtering effect at the gamma point that was predicted by Autès et al. [2]

[1] M. Hervé et al., Appl. Phy. Lett. 103 (2013) 202408 [2] G. Autès et al., Phys. Rev. B 83 (2011) 052403.

MA 10.3 Mon 15:30 HSZ 403

Generalized Wannier functions for an ab initio description of the electronic structure of chiral magnets — •Jan-Philipp Hanke, Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Complementary to delocalized Bloch functions, Wannier functions provide insight into the nature of crystal bonding and allow for simplified and accurate calculations of the electronic structure due to their spatial localization [1]. Here, we present the formalism of higher dimensional generalized Wannier functions (GWFs) which are obtained by Fourier transformations of Bloch functions that depend on reciprocal **k**-vector and additionally carry a dependence on the spin-spiral vector **q**. We implement the machinery for constructing such GWFs from ab initio within the full-potential linearized augmented-plane-wave code `FLEUR` [2]. Using this formalism, we acquire a minimal and very accurate description of the first-principles Hamiltonian in **k** and **q** space. Additionally, GWFs provide access to efficient calculation of exchange Heisenberg constants and transport properties of chiral magnets.

Financial support by the HGF-YIG Programme VH-NG-513 is gratefully acknowledged.

[1] N. Marzari and D. Vanderbilt, Phys. Rev. B **65**, 12847 (1997)
[2] See http://www.flapw.de

MA 10.4 Mon 15:45 HSZ 403

Transverse charge and spin transport within the Kubo-Bastin formalism — •Kristina Chadova, Diemo Ködderitzsch, and Hubert Ebert — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München

In recent years several first-principles approaches have been established to treat transverse electron transport phenonmena as e.g. the anomalous Hall effect and spin Hall effect. Most of them treat particular contributions to the full conductivity tensor. We present a first-principle approach based on the Kubo-Bastin equation implemented withtin the fully relativistic KKR (Korringa-Kohn-Rostoker) formalism that is able to treat intrinsic and extrinsic contributions on equal footing. Both contributions from states below ("Fermi sea") and at the Fermi level ("Fermi surface") are treated and can be analysed with respect to constituting the full transverse conductivities. The approach is applicable to pure systems as well as metallic and semiconductor alloy systems. Several applications are presented that demonstrate the reliability and the power of the proposed scheme.

MA 10.5 Mon 16:00 HSZ 403

Perpendicular magnetic tunnel junctions with $Mn_{3-x}Ga$ bottom electrode — •Manuel Glas[1], Daniel Ebke[2], Eugen Schellenberg[1], Karsten Rott[1], Jan Schmalhorst[1], and Günter Reiss[1] — [1]Thin Films and Physics of Nanostructures, Bielefeld University, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The integration of $Mn_{3-x}Ga$ thin films with perpendicular magnetic anisotropy into magnetic tunnel junctions was investigated. MgO (001) and $SrTiO_3$ (001) substrates were used to achieve epitaxial (001)-oriented thin films. Crystallographic and magnetic measurements were performed to characterise the $Mn_{3-x}Ga$ electrodes. To overcome the lattice mismatch between the bottom electrode and the MgO barrier, a thin CoFeB interlayer was deposited. A magnetically perpendicular counter electrode was formed by Co/Pt multilayers. To improve the applicability, we replaced the Co/Pt multilayer by a perpendicularly magnetised CoFeB thin film. Additionally, CoFeB based perpendicular magnetic tunnel junction were investigated for comparison. Samples with Co/Pt counter electrode exhibited a TMR effect of only 3 % and samples with CoFeB top electrode showed an effect of 5 %. However, CoFeB based tunnel junctions revealed the highest MR effect with 72 %. The temperature dependent transport measurements of Mn-Ga based tunnel junctions with CoFeB counter electrode exhibited an initial increase of the TMR effect and a maximum effect between 80 and 100 K. For lower temperatures the TMR effect decreases, due to a reversal of the coercivity of both CoFeB electrodes.

15 min. break

MA 10.6 Mon 16:30 HSZ 403

First principles calculation of spin chirality contribution to thermoelectric transport effects — •Jürgen Weischenberg, Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In magnetic systems with a non-collinear configuration of spins, the conduction electrons may acquire a geometrical phase, the so-called Berry phase, which gives rise to a topological contribution to the transverse current in response to an external field. In contrast to the anomalous Hall effect, which originates from the spin-orbit interaction (SOI), the topological contribution also exists in systems without SOI and in which the scalar spin chirality symmetry is non-zero. In this work, we take nano-skyrmionic lattices as such an example and study the influence of SOI on the topological contribution in the presence of an electric field or a temperature gradient. For this purpose, we compute the electronic properties of the spin texture in real space using density functional theory. We then employ the Wannier interpolation technique in order to examine the various thermoelectric transport coefficients within linear response.

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MA 10.7 Mon 16:45 HSZ 403

Emerging Magnetic Order in Pt atomic contacts and chains — •Florian Strigl, Christopher Espy, Maximilian Bückle, Torsten Pietsch, and Elke Scheer — Department of Physics, University of Konstanz, 78475 Konstanz, Germany

Platinum, as bulk metal, is not magnetically ordered, but it is a strong paramagnet close to the Stoner criterion of ferromagnetism. Several theoretical predictions exist about the formation of a magnetically ordered state in reduced dimensions and in particular in atomic chains [Smogunov, Thiess]. This makes it possible to study the influence of magnetic order on conductance properties of atomic contacts without influencing the contact geometry due to magnetostriction [Egle]. In this talk we will show results of a detailed experimental study in which we follow the evolution of magnetoconductance (MC) in atomic platinum contacts. The size, sign, and signature of single MC traces can vary largely even for slight changes on the contact and also show an anisotropic behavior. These features are similar to those found for atomic-size contacts of the 3d band magnets. We discuss how these findings may be put into context with a locally constricted magnetic order in the contact.

[Smogunov] Phys. Rev. B 78, 014423 (2008) [Thiess] Phys. Rev. B 81, 054433 (2010) [Egle] Phys. Rev. B 81, 134402 (2010)

MA 10.8 Mon 17:00 HSZ 403

Symmetry of spin transport coefficients — •Marten Seemann, Diemo Ködderitzsch, and Hubert Ebert — Universität München, Dept. Chemie, Butenandtstraße 5-13, D-81377 München, Germany

The symmetry of the coefficients appearing in the description of charge, spin and thermo transport is important when discussing experimental setups and theoretical calculations for ordered two- or three dimensional systems. Starting from Kubo's linear response theory, Kleiner [1] devised a scheme that provides the symmetry of transport coefficients for pairs of operators in perturbation/response providing generalized Onsager relations. We extended this scheme to describe the symmetry of conductivity tensors appearing in spin- and thermo-magneto-galvanic transport. Implications for the appearance of interesting effects described by non-zero elements of the respective conductivity tensors are outlined. Several examples (anomalous Hall and Nernst as well as spin Hall and Nernst conductivities) are given to illustrate this analysis in combination with numerical results obtained using the spin-polarized KKR electronic structure method.

[1] W. H. Kleiner, Phys. Rev. **142**, 318 (1966), *ibid.* **153**, 726 (1967)

MA 10.9 Mon 17:15 HSZ 403

Spin transport and magnetoresitance in metal | phthalocyanine | metal vertical heterostructures investigated by first principle methods — •Hahn Torsten — Institute for Theoretical Physics, TU Freiberg, D-09596 Freiberg

Based on density functional theory electronic structure calculations we used the nonequilibrium Green's function formalism (NEGF) to study finite bias quantum transport in metal | metal-phthalocyanine | metal heterostructures. The investigated structures model phthalocyanine layers sandwiched between two semi-infinite metal electrodes. We study the quantum transport and thus the magnetoresitance of such devices as a function of the applied bias voltage. By varying the type of the Phthalocyanine in the junction we show that one can tune the magnitude of the magnetoresistance. Furthermore we can show that even with the strong coupling between Phthalocyanine and metal electrodes it is possible to reach reasonable magnetoresistance values which could make those molecules suitable for prototypical spin-transport based devices.

MA 10.10 Mon 17:30 HSZ 403

Magnon-phonon dynamics in the heat transport in low dimensional quantum antiferromagnetic cuprates. — •Matteo Montagnese[1], Ekaterina Khadikova[2], Xenophon Zotos[3], Oleg Mityashkin[4], Christian Hess[4], Alexandre Revcolevschi[5], Romuald Saint-Martin[5], and Paul H M van Loosdrecht[1] — [1]II. Physikalisches Institut der Universität zu Köln, D-50937 Köln, Germany — [2]Zernike Institute for Advanced Materials, Rjiksuniversiteit Groningen, Groningen, Tmohe Netherlands — [3]Department of Physics, University of Crete and Foundation for Research and Technology-Hellas, 71003 Heraklion, Greece — [4]IFW-Dresden, Institute for Solid State Research, D-01171 Dresden, Germany — [5]Laboratoire de Physico-Chimie de L'Etat Solide, ICMMO, UMR8182, Université Paris-Sud, 91405 Orsay CEDEX, France

Low dimensional cuprate antiferromagnets such as the spin chain SrCuO2 and the spin ladder Ca9La5Cu24O41 are notable for their quantum disordered ground state and their intriguing magnetic excitation spectrum . Moreover, they show an unusual magnon-dominated thermal conduction over a wide temperature range, partly due to extremely long magnetic mean free paths, eventually in the micron range. At the same time, space and time-resolved optics is emerging as an optimal tool to probe thermal transport at the microscale. We have applied different space- and time-resolved optical methods to study the magnetic thermal transport dynamic, aiming at detecting its ballistic component and clarifying the kinetics and interaction of AFM excitations in low dimensions.

MA 10.11 Mon 17:45 HSZ 403

Superconducting proximity effect and zero-bias anomaly in quantum dots weakly attached to ferromagnetic leads — •Piotr Trocha and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland

The Andreev transport through a quantum dot coupled to two external ferromagnetic leads and one superconducting lead is studied theoretically by means of the real-time diagrammatic technique in the sequential and cotunneling regimes. We show that the tunnel magnetoresistance (TMR) of the Andreev current displays a nontrivial dependence on the bias voltage and the level detuning, and can be described by analytical formulas in the zero temperature limit. The cotunneling processes lead to a strong modification of the TMR, which is most visible in the Coulomb blockade regime. We find a zero-bias anomaly of the Andreev differential conductance in the parallel configuration, which is associated with a nonequilibrium spin accumulation in the dot triggered by Andreev processes.