0.0.1 Psi-k Workshop on KKR and Related Greens Function Methods

Halle, Germany

July 8-10, 2011

Psi-k Network,
Max Planck Institute of Microstructure Physics and
Martin Luther University Halle-Wittenberg

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http://slab.physik.uni-halle.de/kkr_workshop

Scientific Report

The importance of ab initio electronic structure simulations based on Density Functional Theory is well-established in materials science, new approaches and theories are being continuously implemented to study novel problems and materials. The Korringa-Kohn-Rostoker (KKR) method is known to be a highly versatile tool to investigate, e.g., relativistic effects and electron correlations, magnetic and chemical interactions, spectroscopic properties, as well as electric transport in solids ranging from bulk to nanoparticles. This versatility of the KKR method mainly stems from the Greens function formalism it employs.

Back to several decades, leading groups of the KKR method have organized annual or biannual meetings with the aim to exchange experiences in developing computer codes and to discuss scientific achievements and further progress that can be accessed in terms of this methodology. As those groups are mostly located in Europe, Psi-k naturally provided a background to host and support these meetings during the past decade. It was the very purpose of this workshop to continue this tradition and, thus, to keep the KKR method in the forefront of ab initio based computational materials science.

The workshop was intended to continue a regular series of meetings of the KKR research community organized under support of Psi-k (Munich 2004, Bristol 2006, Canterbury 2008, Budapest 2009). A particular feature of the current workshop was that not only the KKR community was presented but as well groups working with other Green function related methods. 73 participant from seven European countries joined the workshop.

Related to recent advances achieved and novel challenges met by the KKR method, the workshop was focused to developments and applications of relativistic electron theory and phenomena driven by spin-orbit interaction:

- The calculation of magnetic anisotropies and magnetic interactions of relativistic origin such as the Dzyaloshinskii-Moriya interaction.
- Advances in understanding the spin and the anomalous Hall effect in terms of Boltzmann's transport equation or of the Kubo formalism.
- Developments with respect to topological phases to consider phenomena like the intrinsic spin and the intrinsic anomalous Hall effect as well as orbital polarization.
- Ab initio vs. multiscale approaches to spin-dynamics to study finite temperature metallic magnetism from simple metals to heterogeneous systems of technological interest.
- Magnetism on the atomic scale: clusters and nanoparticles of different shape deposited on surfaces, beating the superparamagnetic limit for high density magnetic recording.
- Functional materials for spintronics: oxides, half-metals, multi- and nanoferroics.
- Excitations (magnons and phonons) based on the dynamic linear response theory. The latter formalism is particularly well implementable with the KKR method. (viii) Ab initio description of magnon and phonon assisted inelastic transport phenomena.
- First principles description of strongly correlated materials within the multiple-scattering theory.

Beyond the above topics, other research fields commonly accessed by Green function methods (e.g., to alloy theory) were presented during the workshop. In addition, a session was devoted to discuss computational methods and problems with emphasis to recent developments of full-potential KKR method and related Green function methods. Each presentation of the workshop was followed by intensive discussions among the participants of the workshop. The general scientific atmosphere of the discussions and the workshop in general was open and creative.

Programme

Friday, 8th of July			
Time		**Speaker**	**Title**
12:30-13:25			*Coming together, Refreshments*
13:25-13:30			*Opening remarks*
			Magnetism
13:30-14:00	I1	J. Staunton	Competing magnetic interactions in transition metal and rare earth materials from ab-initio electronic structure electronic structure theory
14:00-14:30	I2	L. Udvardi	Finding a non-collinear magnetic groundstate
14:30-15:00	I3	B. Ujfalussy	Exchange interactions on alloy surfaces
15:00-15:30	I4	V. Drchal	Effective magnetic Hamiltonians
15:30-15:50			*Coffee break*
			Superconductivity, Magnons
15:50-16:20	I5	H. Gross	Ab-initio approach to superconductivity
16:20-16:50	I6	P. Buczek	Magnon-elecron scattering in nanoscale transport
16:50-17:20	I7	L. Sandratskii	Interface electronic complexes and Landau damping of magnons in ultrathin magnets
17:20-17:30			*Coffee Break*
			Nanostructures, Surfaces
17:30-18:00	I8	P. Zahn	Transport properties of nanostructured thermoelectric materials
18:00-18:30	I9	V. Stepanyuk	Quantum confinement of electrons in atomic-scale nanostructures
18:30-18:45	C1	O. Brovko	Confined bulk-states as a long-range sensor for impurities and a transfer channel for quantum information
18:45-19:00			*Break*
19:00-21:00			Postersession / *Refreshments*

Saturday, 9th of July			
Time		**Speaker**	**Title**
		Rashba effect	
08:30-09:00	I10	L. Szunyogh	Generalized Bychkov-Rashba Hamiltonians
09:00-09:30	I11	J. Braun	Actual trends in ARPES: Correlation, disorder and Rashba physics
09:30-09:45	C2	F. Freimuth	Spin-orbit mediated torque in Rashba systems
09:45-10:00	C3	O. Sipr	Induced magnetic moments make MAE calculation fun or nightmare
10:00-10:30		*Coffee break*	
		Anisotropies, topological insulators	
10:30-11:00	I12	H. Ebert	Fully relativistic calculations of the magnetic shape anisotropy and of the Gilbert damping parameter
11:00-11:30	I13	I. Turek	Tunneling anisotropic magnetoresistance in Fe/GaAs/Ag(001)
11:30-12:00	I14	J. Henk	Properties of the undoped and magnetically doped 3D topological insulator Bi_2Te_3
12:00-12:15	C4	M. Garcia Vergniory	Ab initio study of the surface properties of a new ternary compound topological insulator
12:15-12:30	C5	H. Zhang	Electrically tunable quantum anomalous Hall effect in 5d transition-metal adatoms on graphene
12:30-13:30		*Lunch break*	
		Spin Hall effect, spin relaxation	
13:30-14:00	I15	M. Gradhand	The Berry curvature and the spin Hall effect calculated with the KKR
14:00-14:30	I16	D. Ködderitzsch	Spin and anomalous Hall effect in transition-metal alloys
14:30-15:00	I17	P. Mavropoulos	Spin relaxation due to impurity scattering in non-magnetic metallic systems
15:00-15:30	I18	D. Fedorov	Elliott-Yafet spin relaxation mechanism within the KKR method
15:30-16:00		*Coffee break*	
		Excitations	
16:00-16:30	I19	Y. Mokrousov	Recent advances in ab initio theory of transverse scattering-independent transport
16:30-17:00	I20	B. Gyorffy	The Berry phase of Dirac electrons and spin-orbit coupling
17:00-17:30	I21	S. Lounis	Dynamical magnetic excitations of nanostructures
17:30-18:00	I22	Chr. Heiliger	Spin transfer torques in magnetic tunnel junctions
19:30-23:00		*Conference dinner*	

Sunday, 10th of July			
Time		**Speaker**	**Title**
		Methods	
08:30-09:00	I23	L. Vitos	The EMTO method: Implementation and demonstration
09:00-09:30	I24	R. Zeller	Projection potentials, Loyd's formula and angular momentum convergence of total energies in full-potential KKR
09:30-10:00	I25	H. Akai	Total energy calculation within EXX+RPA
10:00-10:30	I26	R. Hammerling	The non-relativistic full potential single site problem
10:30-10:50		*Coffee break*	
		Order - Disorder - Electronic Structure	
10:50-11:20	I27	M. Ogura	First-principles calculation of structural transformation
11:20-11:50	I28	J. Kudrnovsky	Quaternary Heusler alloys (Ni, Cu)$_2$MnSn: Electronic, magnetic, and transport properties
11:50-12:20	I29	C. Etz	Ab initio study of strongly correlated materials
12:20-12:35	C6	A. Marmodoro	A multi-sublattice extension of the non-local coherent potential approximation
12:35-12:50	C7	S. Mankovsky	Spin spirals in ordered and disordered solids
12:50-13:00			*Closing remarks*
13:00-14:00		*Lunch*	

List of Participants

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