Abstracts

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New Generation of strongly correlated electron systems

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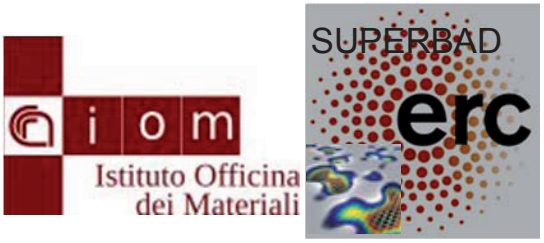

TIME	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
8.45 - 9.00	OPENING				
9.00 - 9.30	Toschi - Lecture	Lake - Lecture	van Heumen - Lecture	Zorko - Lecture	de Medici
9.30 - 10.00	Minola	Perkins	Sordi	Custers	Novelli
10.00 - 10.30	Toschi	Lake	van Heumen	Zorko	Lazarevic
10.30 - 11.00	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK
11.00 - 11.30	Baldasarre - Lecture	Kollar - Lecture	Schiro	Cepas - Lecture	Levallois
11.30 - 12.00	Aichhorn	van Bay	Fausti	Kamiya	Chudzinski
12.00 - 12.30	Baldasarre	Kollar	Avella	Cepas	CLOSING
12.30 - 14.00	LUNCH	LUNCH	LUNCH	LUNCH	LUNCH
14.00 - 14.30	Bascones - Lecture	Giannetti - Lecture	Excursion	Cappelluti	
14.30 - 15.00	Inosov	Bauer	Excursion	Texier	
15.00 - 15.30	Bascones	Giannetti	Excursion	Luders	
15.30 - 16.00	POSTER-flash presentations I	POSTER-flash presentations II	Excursion	COFFEE BREAK	
16.00 - 16.30	POSTER Session	POSTER Session	Excursion	Pfau	
16.30 - 17.00	and COFFEE	and COFFEE	Excursion	Tanaskovic	
17.00 - 17.30	Part I	Part II	Excursion	Prokleska	
17.30 - ...		CONFERENCE DINNER			

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I. Oral Presentations

Why is Sr_2IrO_4 insulating and Sr_2RhO_4 is not? Effects of spin-orbit coupling and structural distortions

Markus Aichhorn[1]

[1] TU Graz

We discuss the notions of spin-orbital polarization and ordering in paramagnetic materials, and address their consequences in transition metal oxides. Extending the combined density functional and dynamical mean field theory (DMFT) scheme to the case of materials with large spin-orbit interactions, we investigate the electronic excitations of the paramagnetic phases of Sr_2IrO_4 and Sr_2RhO_4. We show that the interplay of spin-orbit interactions, structural distortions and Coulomb interactions suppresses spin-orbital fluctuations. As a result, the room temperature phase of Sr_2IrO_4 is a paramagnetic spin-orbitally ordered Mott insulator. In Sr_2RhO_4, the effective orbital degeneracy is reduced, but the material remains metallic, due to both, smaller spin-orbit and smaller Coulomb interactions. We find excellent agreement of our ab-initio calculations for Sr_2RhO_4 with angle-resolved photoemission.

Defect states and electron correlations in multi-orbital Mott insulators

Adolfo Avella[1]

[1] Dip. di Fisica - Univ. di Salerno, Italy

We address the role played by defects in doped Mott insulators with active orbital degrees of freedom. We observe that defects are characterized by rather complex and rich physics which is well captured by a degenerate Hubbard model extended by several terms that describe crystal-field splittings, the orbital-lattice coupling, as well as local terms generated by defects such as the Coulomb potential terms that act both on a doped hole and orbitals of undoped sites (orbital polarization). We show that the multiplet structure of excited states generated in such systems by strong electron interactions is well described in an optimized unrestricted Hartree-Fock approximation, taking into account the usual symmetry breaking by the onset of magnetic and orbital order. More importantly, we show that defect states are responsible for new features that arise within the Mott-Hubbard gap and in the multiplet spectrum at high energy. These states involve active orbital flavors at atoms being nearest neighbors of the defect state, which are modified by the local defect-orbital Coulomb interactions. The present study suggests a new mechanism for the Coulomb gap realized in the presence of defect states and investigates the dependence of the (filled and empty) orbitals on the orbital polarization. As an illustrative example of our general approach, we perform explicit calculations for a model describing three t_{2g} orbital flavors in the perovskite vanadates doped by divalent Ca ions, such as $Y_{1-x}Ca_xVO_3$ perovskites.

Towards metallic states: infrared spectroscopy of strongly correlated systems under pressure

Leonetta Baldassarre[1]

[1] Center for Life NanoScience@LaSapienza, Istituto Italiano di Tecnologia, Viale Regina Elena 295, Roma, Italy

Strongly correlated systems are characterized by rich and often complex phase diagrams that depend on temperature, pressure and doping [1]. By changing lightly one of the aforementioned parameters the properties of these systems change significantly. Chemical substitution, for instance, is a convenient method for changing the properties of a compound. However, it inevitably introduces impurities affecting many of the physical parameters in an uncontrollable way. There is therefore a growing need to find a way of tuning these systems in a more systematic fashion by using high pressure. Indeed, the application of very high pressure typically increases the orbital overlap usually decoupling the effects of different interactions, and, in some cases, to enhance hidden interactions which are too weak at ambient conditions. In recent years high pressure demonstrated to be a useful technique for investigating the physics of strongly correlated electron systems, where the ratio between the electronic Coulomb repulsion and the hopping integral drives the system toward the metal to insulator transition [2,3]. In this talk I will present infrared measurements on strongly correlated systems under pressure, mainly performed at the SISSI beamline @ELETTRA, discussing either the emergence of metallic states from Mott insulators or the evolution of the metallic properties in systems with a moderate degree of correlations (as for example pnictides). At last, I will discuss the pressure-dependence of Cs3C60, following its insulator to metal transition.

[1] M. Imada et al, Rev, Mod. Phys. 70, 1039 (1998).

[2] E. Arcangeletti et al., Phys. Rev. Lett. 98, 196406 (2007).

[3] S. Lupi et al., Nature Communications 1:105 (2010).

Magnetic interactions in iron superconductors - Lecture

Leni Bascones[1]

[1] Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Cantoblanco, E-28049 Madrid, Spain

A major breakthrough happened in 2008 as high temperature superconductivity was discovered in iron compounds. While the phase diagram of these materials resembles that of cuprates, with superconductivity emerging upon suppression of antiferromagnetism, it was soon clear that the starting point for a theoretical description should be different in both systems. Iron superconductors are multiorbital systems and the antiferromagnetic state is metallic, as opposed to the Mott insulating character of cuprates.The antiferromagnetic state shows columnar ordering, i.e. antiferromagnetic along one direction and ferromagnetic along the other one. Based on the metallic character and an approximate nesting of the Fermi surface some theories propose an itinerant origin of magnetism, while others describe the magnetic state in terms of localized spins. Interactions are believed to be intermediate between these two limits. The role of Hund's coupling to

promote bad metallic behavior and to stabilize the antiferromagnetic state is also discussed. The magnetic transition is closely followed by an structural transition, which has led to theoretical proposals based on orbital ordering or magnetic nematicity. The structural transition and a strong dependence of the electronic properties on structural details evidences a strong coupling between lattice and magnetism or superconductivity. While the most accepted model explains superconductivity in terms of magnetic fluctuations, models based on an unconventional electron-phonon coupling have been also proposed. In this talk I will discuss the basic phenomenology of iron superconductors and the present status of theories to explain it.

Magnetic interactions in iron superconductors

Leni Bascones[1]

The antiferromagnetic state of iron pnictides is metallic and shows columnar ordering, i.e. antiferromagnetic (AF) in one direction and ferromagnetic (FM) in the other one. The itinerant or strong coupling origin of magnetism and the role of Hund's coupling are still unsettled. The itinerant picture relies on the nesting of the Fermi surface. The localized description generally assumes AF exchange constants satisfying $2J_2 > J_1$, with J_1 and J_2 referring to first and second nearest neighbors respectively. This condition is necessary to stabilize columnar ordering.

To make connection between the itinerant and localized picture we have analyzed the magnetic interactions of iron superconductors on the basis of a five orbital model treated both within Hartree-Fock and Heisenberg approximations. We have found that the exchange constants strongly depend on the charge and orbital filling and can become FM at large Hund's coupling. Columnar ordering is found for intermediate Hund's coupling. At smaller Hund's coupling an unusual orbital reorganization can stabilize checkerboard ordering, AF along both directions. Ferromagnetism appears at large Hund's coupling. As in experiments ferromagnetic correlations are enhanced with electron doping while large hole doping stabilizes checkerboard antiferromagnetism. Comparing these results with those of the Hartree-Fock approach, which also show a double stripe phase, we are able to differentiate those regions in the phase diagram in which the ground state is determined by nesting from those where strong coupling physics is relevant.

The emergence of superconductivity for systems with competing electron-phonon and electron-electron interactions

Johannes Bauer[1]

[1] Max-Planck Institute for Solid State Research, Stuttgart

We analyze the emergence of superconductivity for systems with an effective short range Coulomb repulsion U and a retarded electron-electron attraction induced by an electron-phonon coupling as described by the Hubbard-Holstein model. We first discuss the case without Coulomb interactions, where Migdal-Eliashberg (ME) theory can be applied. In recent years, the validity of the ME theory for values of the electron-phonon coupling strength $\lambda > 1$ has been questioned by model studies. By distinguishing bare and effective parameters, and by comparing the ME theory with the dynamical mean field theory (DMFT), we clarify the range of applicability of the ME theory. Specifically,

we show that ME theory is very accurate as long as the product of effective parameters, $\lambda\omega_{\rm ph}/D$, where $\omega_{\rm ph}$ is an appropriate phonon scale and D an electronic scale, is small enough [1]. The effectiveness of retardation effects for the competing Coulomb interaction is usually considered based on the lowest order diagram in the perturbation theory. We analyze these effects to higher order and find modifications to the usual result for the Coulomb pseudo-potential μ^*. Retardation effects are weakened due to a reduced effective bandwidth. Comparison with the non-perturbative DMFT corroborates our findings [2]. Our results can help to understand better a number of materials, for which the conventional theory fails. We also extend these calculations to larger coupling strengths and different filling factors to establish a more complete picture.

[1] J Bauer, J Han, and O Gunnarsson, Phys. Rev. B. 84, 184531 (2011).

[2] J Bauer, J Han, and O Gunnarsson, cond-mat/1202.5051 (2012).

Superconductivity in the doped topological insulator $Cu_xBi_2Se_3$

Tran van Bay[1]

[1] Van der Waals-Zeeman Institute, University of Amsterdam

Recently, topological insulators have sparked a wide research interest because they offer a new playground for the realization of novel states of quantum matter. The concept of topological insulators can also be applied to superconductors due to the direct analogy between topological band theory and superconductivity. Here we report a high-pressure study [1] on the superconducting properties of one of the first test-case systems $Cu_xBi_2Se_3$ which is a prime candidate for topological superconductivity. Transport measurements show that superconductivity is depressed smoothly and the metallic characteristic is gradually lost under pressure. More importantly, the upper critical field $B_c2(T)$ collapses onto a universal curve that is at odds with the standard behavior for a weak-coupling, orbital-limited, spin-singlet superconductor, and rather points to spin-triplet superconductivity. We discuss our results in view of the prediction that all topological superconductors are unconventional odd parity superconductors.

[1] T.V. Bay, T. Naka, Y.K. Huang, H. Luigjes, M.S. Golden and A. de Visser, Phys. Rev. Lett. 108, 057001 (2012).

Infrared phonon activity and Fano interference in multilayer graphenes

Emmanuele Cappelluti[1]

[1] ICMM, CSIC, Madrid, Spain

The detection and analysis of the spectral properties of optical phonon in single-layer and multilayer graphene provides a powerful tool not only for a careful characterization of the systems but also for investigating the role of the underlying electron-phonon interaction. Recent experiments in gated bilayer graphene revealed a clear phonon resonance at 1590 cm-1 with several interesting features, as for instance a giant enhancement of

the phonon intensity as a function of teh gate voltage as well as a pronounced Fano lineshape asymmetry. In this contribution we will discuss how these features can be analyzed and predicted on a microscopic quantitative level using a charge-phonon theory applied to the specific case of graphene systems. We show in particular how the phonon intensity and the Fano asymmetry are strictly related, stemming out from the quantum interference between the electronic and phononic degrees of freedom. Within this context we are also able to elucidate the relative role of the Eu and Eg phonon modes in regards to the infrared activity and the Fano asymmetry of the observed phonon peaks. We present thus a complete phase diagram for the strength of the phonon modes and their Fano properties as functions of the chemical potential and of the gated-induced electronic gap, showing that a switching mechanism between the dominance of the Eu or Eg mode can be controlled by the external gate voltage. We discuss how the present analysis can be generalized as well to multilayer systems with different stacking order.

Theory of the electron spin resonance in correlated spin systems - Lecture

Olivier Cepas[1]

[1] Institut N´eel, CNRS et Universit´e Joseph Fourier, BP 166, F-38042 Grenoble 9, France

What is the characteristic time scale for the magnetization of a many-body system to relax? Experimentally, it is obtained by measuring the linewidth of the electron spin resonance (ESR) induced by an external ac-field, assuming a relaxation governed by a phenomenological "friction" in the Bloch equations.

However, the friction originates in microscopic processes. The theory that relates the friction (linewidth) to the couplings in the Hamiltonian is difficult because of the strong correlations. Experimentalists often rely on the theory of Kubo and Tomita [1]. We have tested this theory by exact diagonalization of low-dimensional systems at high temperatures [2]. We predict non Lorentzian resonance lineshapes and deviations from the Kubo-Tomita theory, which result from long-memory processes (either "recurrences" in nanomagnets or spin diffusion). The predictions can then be compared with experiments, in particular in $ZnCu_3(OH)_6Cl_2$.

At very low temperatures, on the other hand, the ESR response is dominated by sharp transitions between single quantum levels. Some of them are *forbidden* by selection rules. They are nonetheless observed in a variety of compounds, *e.g.* $CuGeO_3$, NaV_2O_5, $SrCu_2(BO_3)_2$, $Ba_3/Sr_3Cr_2O_8$. I will discuss the issue of the mechanism of the transitions and argue that the ac electric-field may actually play an important role in allowing transitions between magnetic states, thanks to the presence of magneto-elastic couplings similar to those invoked to explain multiferroics [3].

[1] R. Kubo and K. Tomita, J. Phys. Soc. Jpn. 9 (1954).

[2] S. El Shawish, O. Cepas and S. Miyashita, Phys. Rev. B 81, 224421 (2010).

[3] O. Cepas and T. Ziman, Phys. Rev. B 70, 024404 (2004).

Heterogeneous dynamical freezing in geometrically frustrated magnets without disorder

Olivier Cepas[1]

Geometrically frustrated magnets have an interesting variety of phases, such as broken-symmetry phases, spin-liquid phases (which do not break any symmetry), or "frozen" phases.

"Frozen" phases have static order below a temperature T_g with locally frozen spins but no magnetic long-range order. Such transitions were observed experimentally in frustrated compounds, although the chemical disorder is apparently weak. In general, theories of freezing invoke quenched disorder, as in spin glasses, or a slowing-down of the dynamics.

I will present a simple model of constrained classical spin dynamics where the strong correlations of the degrees of freedom slow down the relaxation to equilibrium. I will compare with experimental results in kagome compounds and give some predictions, in particular regarding the heterogeneous nature of the dynamics.

The Luttinger liquid theory of molybdenum purple bronze $Li_{0.9}Mo_6O_{19}$

Piotr Chudzinski[1]

[1] DPMC-MaNEP, Universite de Geneve

We study a quasi-1D material, the purple bronze $Li_{0.9}Mo_6O_{19}$ which becomes superconductor at 1.9K. Firstly, the band structure is calculated by use of ab-initio DFT-LMTO method. The unusual, very 1-dimensional band dispersion obtained in previous band calculations is confirmed and the overall band structure agrees reasonably with existing photoemission data. Dispersion perpendicular to the main dispersive direction is obtained and investigated in detail. Temperature and disorder effects are evaluated, in particular we check their influence on the band broadening. Based on this, in the second part of our work we derive an effective low energy theory within the Luttinger liquid framework. We estimate the strength of possible instabilities and values of charge modes compressibilities. Our aim is to understand experimental findings, in particular the ones which are certainly lying within 1D regime. We discuss the validity of our approach and further perspectives for the lower energy phases.

Exploring the Physics of Quantum Phase Transitions

Jeroen Custers[1]

[1] Dept. Condensed Matter Physics, Charles Univ., Prague, CZ

Matter at absolute zero temperature might undergo a second order phase transition for example from a magnetic to a non-magnetic state. In the vicinity of such a transition point, called quantum critical point (QCP), strong quantum fluctuations exist, that lead to bizarre observations in the physical properties like deviations from expected Fermi liquid behavior or the occurrence of an unconventional superconducting state.

In this presentation focus will be on Yb-based heavy fermion (HF) materials which are close to a QCP. Recent experiments on several of these compounds revealed non-Fermi liquid behavior in a finite zero-temperature region in the magnetic field- or pressure-tuned phase diagram [Ref. 1]. While the canonical view of HF quantum criticality assumes that the transition from magnetically ordered to heavy Fermi liquid takes place via a single QCP, these observations raise the possibility that our underlying scenario for HF quantum criticality may need to be changed. For the case of Ge-doped $YbRh_2Si_2$ we advance arguments that the zero temperature non-Fermi liquid region is a new metallic Quantum Critical ground state and is not due to disorder effects. We discuss the physical properties of this new metallic state and propose a two-dimensional generalization of the Doniach phase diagram for interpreting this, and other recently observed cases of "strange metal phase" of similar character.
Finally it will be shown that similar is observed for Cerium-based HF compounds [Ref. 2].

[1] J. Custers *et al.*, Phys. Rev. Lett., **104,** 186402 (2010).

[2] J. Custers *et al.*, Nature Mat., doi://10.1038/nmat3214 (2012).

Hubbard's exciton revealed by time-domain optical spectroscopy

Daniele Fausti[1]

[1] Università degli Studi di Trieste and Sincrotone S.C.P.A.

By means of ultra-fast time-resolved pump&probe optical spectroscopy, we demonstrate that the twofold feature in the visible optical properties of YVO3, heavily debated as a case-study for insulating transition metal oxides, originates from the same d-d transition. Separating thermal and non-thermal contribution to the optical transients, we show that the total spectral weight of the two bands is conserved at any time giving strong evidence of the excitonic nature of the low energy branch. In this framework, we identify the low energy peak as a bound state between a doublon and a holon, named Hubbard exciton (HE). Finally, we speculate that the pump-driven disorder can be used to quantify the kinetic energy gain of the excitons with respect to the single particles.

Recent advances in ultrafast spectroscopies - Lecture

Claudio Giannetti[1]

[1] Mathematics and Physics Department of the Catholic University in Brescia

In strongly-correlated systems the electronic properties at the Fermi energy are intertwined with those at high energy scales and are strongly affected by different degrees of freedom, such as lattice vibration, bosonic excitations of electronic origin, quasi-particle excitations. Broadband ultrafast spectroscopy is emerging as the premier technique to disentangle the subtle interplay of the different degrees of freedom by their different characteristic timescales and spectral responses. In this talk we will review the latest advances in time-resolved techniques and the basics of broadband ultrafast spectroscopy

[1], as a tool to unravel the elusive physics of strongly-correlated materials and manipulate their physical properties on the femtosecond timescale.

[1] F. Cilento et al., Appl. Phys. Lett. 96, 021102 (2010).

Understanding the complex dynamics of superconducting cuprates by broadband ultrafast spectroscopy

Claudio Giannetti[1]

[1] Mathematics and Physics Department of the Catholic University in Brescia

In this talk we will tackle some of the most important open questions in the physics of superconducting cuprates from the perspective of the ultrafast dynamics triggered by an ultrashort light pulse. By performing optical spectroscopy on Bi2Sr2Ca0.92Y0.08Cu2O8+? crystals, with simultaneous time- and frequency-resolution, we disentangle the electronic and phononic contributions to the total electron-boson coupling function [1] and we demonstrate the interplay between the many-body high-energy CuO2 excitations at 1.5 and 2 eV and the onset of high-temperature superconductivity [2]. These results strongly point to an unconventional mechanism of electronic origin both below and above the optimal hole concentration required to attain the maximum critical temperature (Tc). The microscopic modelling of the non-equilibrium dynamics of correlated superconductors, unveiled by the time-resolved spectroscopy, will be one of the key challenges of the next-years materials science.

[1] S. Dal Conte et al., Science 335, 1600 (2012).

k-space microscopy of quantum electron matter

Erik van Heumen[1]

[1] van der Waals - Zeeman Institute, University of Amsterdam

Angle resolved photoemission spectroscopy (ARPES) offers a direct method for the investigation of the electronic band structure of quantum matter. In the last two decades the technique has seen a tremendous improvement in resolving power driven by its capability to give a unique k-space view on interactions and correlation effects. I will give an overview of the type of questions that can be answered with traditional photoemission spectroscopy and its angle resolved counterpart. In this first part basic notions about the technique will be explained:

- From photoelectric effect to photoemission processes.
- Many-body effects: probing the single particle spectral function.

In the second part I will show how ARPES can be used to elucidate the electronic structure of materials ranging from weak to strongly interacting systems. Topological insulators are bulk insulators with robust, topologically protected surface states. The topological nature of these materials is best seen from k-space, making ARPES the ideal technique for their study. The iron-pnictide superconductors will be used as an example of systems where moderate correlation effects introduce deviations from the

non-interacting particle picture. Finally I will discuss colossal magneto resistance materials as an example of a system where strong electron-phonon interactions can destroy the ubiquitous Fermi liquid ground state in condensed matter physics.

Magnetic Resonant Mode in the Superconducting Phase of $A_xFe_{2-y}Se_2$ (A = K, Rb) Single Crystals

Dmytro Inosov[1]

[1] Max-Planck-Institute for Solid State Research

We employ inelastic neutron scattering to study the reciprocal-space structure and dispersion of magnetic excitations in the normal and superconducting states of single-crystalline $Rb_{0.8}Fe_{1.6}Se_2$ and $K_{0.8}Fe_{1.8}Se_2$. In the superconducting state of both samples, we observe a magnetic resonant mode centered at an energy of $\hbar\omega_{\rm res} = 14$ meV near the commensurate wave vector (1/2 1/4 1/2), which differs from the ones characterizing magnetic resonant modes in other iron-based superconductors. Our finding suggests that the 245-iron-selenides are unconventional superconductors with a sign-changing order parameter, in which bulk superconductivity coexists with the $\sqrt{5} \times \sqrt{5}$ magnetic superstructure. The estimated ratios of $\hbar\omega_{\rm res}$ / $k_{\rm B}T_{\rm c} = 5.1 \pm 0.4$ and $\hbar\omega_{\rm res}/2\Delta = 0.7 \pm 0.1$, where Δ is the superconducting gap, indicate moderate pairing strength in this compound, similar to that in optimally doped 1111- and 122-pnictides. We also found that the magnetic resonant mode has a quasi-two-dimensional character, similar to overdoped iron-pnictide superconductors. Moreover, it exhibits a rich in-plane structure that is dominated by four elliptical peaks, symmetrically surrounding the Brillouin zone corner, without the $\sqrt{5} \times \sqrt{5}$ reconstruction. We also present evidence for the dispersion of the resonance peak, as its position in momentum space depends on energy. Comparison of our findings with the results of band structure calculations provides strong support for the itinerant origin of the observed signal. It can be traced back to the nesting of electronlike Fermi pockets in the doped metallic phase of the sample in the absence of iron-vacancy ordering.

Soliton Crystallization in $Ca_3Co_2O_6$

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We study a frustrated quantum Ising model relevant for $Ca_3Co_2O_6$ that comprises a triangular lattice of weakly-coupled ferromagnetic chains. According to our quantum Monte Carlo simulations, the chains become ferromagnetic and form a three-sublattice "up-up-down" structure below a temperature $T = T_{\rm CI}$. In contrast, long-period spin-density-wave (SDW) modulations along the chains are stabilized for $T_{\rm CI} < T < T_c$ in agreement with recent experiments by Agrestini et al [1]. Our mean field solutions reveal quasi-continuous change of the periodicity as a function of T, implying the existence of metastable states in the SDW phase that may explain the very slow low-temperature dynamics that has been observed in $Ca_3Co_2O_6$ [2]. Closely related multiferroic material Ca_3MnCoO_6 [3] will also be discussed briefly.

[1] S. Agrestini et al., Phys. Rev. Lett., 101, 097207 (2008).

[2] T. Moyoshi and K. Motoya, J. Phys. Soc. Jpn., 80, 034701 (2011).

[3] Y. J. Jo et al., Phys. Rev. B. 79, 012407 (2009).

Correlated electrons in nonequilibrium - Lecture

Marcus Kollar[1]

[1] University of Augsburg

How is a new stationary state reached in an isolated quantum-mechanical many-body system after it has been forced out of equilibrium? What are the properties of this new state, in particular, is it the thermal state expected from statistical mechanics? For correlated electrons in condensed matter, which are not independent of each other because of the Coulomb interaction, such questions can be investigated with time-resolved femtosecond spectroscopy, where shortly after a first laser pulse the response to a second pulse is measured. Theoretical approaches that describe the real-time dynamics of correlated systems are discussed, in particular nonequilibrium dynamical mean-field theory for Hubbard-type models. We discuss the formation of stationary states and the relaxation towards thermal states, which is also of interest in view of experiments with cold atomic gases in optical traps.

Relaxation dynamics of weakly interacting quantum systems

Marcus Kollar[1]

[1] University of Augsburg

An isolated quantum many-body system that is suddenly forced out of equilibrium is said to thermalize if it relaxes to a new equilibrium state, and if this is the thermal state predicted by statistical mechanics. Weakly interacting systems are usually first trapped in a prethermalized state and can thermalize only at a later stage [1]. We discuss several examples for which this prethermalized state shares some properties with the nonthermal steady state that emerges in the corresponding free system. These examples support the notion that nonthermal steady states in integrable systems may be viewed as prethermalized states that never decay further. Furthermore we show that prethermalization plateaus can be correctly predicted by generalized Gibbs ensembles built from approximate constants of motion in the vicinity of the noninteracting point [2].

[1] M. Moeckel and S. Kehrein, Phys. Rev. Lett. 100, 175702 (2008).

[2] M. Kollar, F. A. Wolf, and M. Eckstein, Phys. Rev. B 84, 054304 (2011).

Neutron Scattering in Quantum and Frustrated Magnets

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In quantum and frustrated magnets quantum fluctuations are strong and suppress long-range magnetic order, giving rise to exotic behaviours not found in conventional magnets. It is possible to make model materials engineered to exhibit specific quantum features which can then be measured using the technique of neutron scattering. This presentation will discuss a number of different quantum and frustrated magnets. Neutron scattering investigation of several of one-dimensional antiferromagnets will be presented including the spin-1/2 Heisenberg chains which has fractional spinon excitations and spin-1/2 spin-ladders which have gapped magnon states and bound modes. Frustrated magnets will also be discussed including triangular and kagome systems. Neutron scattering can be used to accurately test theoretical models and several examples will be given.

Raman scattering study of $K_xFe_{2-y}Se_2$ single crystals

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Coexistence of antiferromagnetism and superconductivity in newly discovered family of iron based superconductive materials ($A_xFe_{2-y}Se_2$, A = K, Rb, Cs and Tl) invoke a lot of debate in scientific community. It is shown that antiferromagnetism in this class of materials is a consequence of the Fe vacancy ordering. We present temperature dependent polarized Raman scattering spectra of $K_xFe_{2-y}Se_2$ single crystals. The spectra were analyzed in terms of peculiarities of both I4/m and I4/mmm space group symmetries. We found 16 Raman-active modes corresponding to the vibrations of the atoms of the I4/m symmetry structure. Two additional modes, for which we believe that originates from the vibrations within the FeSe layer of the I4/mmm symmetry, have also been observed. Some of the phonon modes of the both structures showed energy and broadening change anomalies at semiconductor to metal crossover temperature.

Hybridization gap and anisotropic far-infrared optical conductivity of URu2Si2

Julien Levallois[1]

[1] Université de Genève

A long standing mystery encountered in the cuprate high-Tc superconductors is formed by the pseudogap: Well above the critical temperature, where the Cooper-pairs form, a partial gap in the density of states is observed by low energy spectroscopic probes including tunneling, ARPES and optical spectroscopy. This partial suppression of density of states is commonly referred to as the pseudogap. No change of specific heat has been observed at the temperature where the pseudogap forms. While various different models have been proposed for the exact nature of the pseudogap, it is universally regarded as a key dowel to the puzzle of high Tc superconducting materials.

Our recent studies of the heavy fermion compound URu2Si2 have revealed a similar pseudogap in the optical conductivity. This compound is fascinating because it presents (at least) two phase transitions: one occurs at 1.5 K and is associated to a superconducting transition, the other takes place at THO=17.5 K and is attributed to a hidden

order transition whose order parameter, despite numerous theoretical and experimental efforts, is still unidentified.

We measured the optical conductivity for both axis of the tetragonal structure. It appears that the conductivity exhibits a partial suppression of spectral weight around 12 meV and below 30 K, that is to say well above the transition at 17.5 K. This suppression is very clear in the temperature dependence of the reflectivity in the energy range 20-30 meV, which presents an abrupt suppression when the temperature is lowered below 30 K. After the first diffusion of our work, the presence of a pseudogap in URu2Si2 has been confirmed by a number of other experimental groups. Understanding the pseudogap in URu2Si2 may help us to identify the nature of similar phenomenon in other materials including high-Tc superconductors.

Interplay between structural and electronic properties in $LaVO_3/SrVO_3$ superlattices

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Superlattices of $LaVO_3/SrVO_3$, where one monolayer of $SrVO_3$ is inserted between thicker layers of $LaVO_3$, have shown some interesting properties, as room temperature magnetism, an oscillating magnetization with the $LaVO_3$ layer thickness, and a combined structural and electronic transition. The origin of these original properties, which are not observed in the bulk systems, is probably the strong electronic correlations combined with a deformation of the unit cell due to the strained growth of the superlattices and the finite thickness of the involved layers. In order to understand the observed properties, we have studied in depth the structural deformations and the octahedral rotations of $LaVO_3$ thin films and the superlattices, providing information on the V-O-V bond angles and length. On this basis, we have calculated the band structure of different superlattice geometries. The calculations show a marked anisotropy between superlattices with an even or odd number of $LaVO_3$ layers, where a confinement of the charges is possible only in the even case, and a magnetic phase can emerge only in the odd case. We can explain this anisotropy by considering the octahedral rotations of the $LaVO_3$ layers, which cannot build up in a film of an odd number of monolayers, leading to a buckling of the VO_2 sublayers and therefore different physics for both geometries.

Hund's coupling effects in correlated materials

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Hund's rule coupling plays a surprisingly crucial influence on the metallicity properties of correlated materials. Three main effects of this coupling are isolated in the multi-orbital Hubbard model: it tunes the proximity to the Mott metal-insulator transition, it renormalizes the Fermi-liquid coherence temperature and it acts as a "band-decoupler". These effects can cooperate or compete to enhance or suppress the metallicity properties of materials for which this model captures the low-energy physics. A simple rule of thumb to know if metallic, bad-metallic or Mott insulating behaviours are promoted is found, depending on the filling of the system. Ab-initio LDA+DMFT calculations allow to compare these predictions with actual materials (mainly 3d and 4d transition

metal oxides) and check that this concise classification allows to capture some important material trends, and explains why very similar materials (such as $SrVO_3$, $SrCrO_3$ and $SrMnO_3$) can display very different behaviors. It also explains the occurrence of bad-metallicity in Sr- and Cr- oxides, and the recently reported record T_{Neel} of $SrTcO_3$. Last but not least these three aspects give a simple rationale behind the bad metallic properties of the normal state of Fe-based superconductors.

[1] L. de' Medici, PRB 83, 205112 (2011).

[2] L. de' Medici, J. Mravlje and A. Georges, arXiv: 1106.0815.

Period 3 charge modulation in $R Ba_2Cu_3O_{6+x}$ superconductors observed with energy resolved resonant soft x-ray scattering

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In high-T_c cuprate superconductors a gap opens below $T^* > T_c$ in the underdoped part of the phase diagram. The origin of this pseudogap is still highly debated and electronic instabilities are serious candidates. A particular case is the one of stripes: for doping levels close to 1/8, static antiferromagnetic stripes separated by ribbons of holes with a period of 4 lattice units have been predicted theoretically and observed with neutron and x-ray scattering experiments in the $(La, X)_2CuO_4$ family (X=Ba, Sr). However it is still not clear if this microscopic phase separation helps superconductivity or is in competition with it. Here we report the experimental evidence of charge ordering in $RBa_2Cu_3O_{6+x}$ (R=Nd, Y) over a wide doping range (x=6.5 to 6.9), obtained by soft x-ray scattering at the Cu L_3 resonance. This is the first proof of the coexistence of charge-density wave in CuO2 planes with superconductivity in the RBCO family. The modulation has a periodicity close to 3 lattice units for all doping levels. The elusive nature of the associated incommensurate peak is probably due to the non-static nature of stripes, impossible to seize by techniques slower than x-ray scattering. The peak intensity is maximum at T_c and its width diverges at high temperature, suggesting a competition with superconductivity. These results for the RBCO family eventually confirm longstanding theoretical predictions, but the new periodicity challenges the universality of period-4 stripes seen in the LXCO family, hopefully giving new insights to understand the origin of the pseudogap state.

THz pump white light probe time domain spectroscopy

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We report on a novel time domain pump-probe experiment based on pump pulses in the THz regime and white light supercontinuum probes. Ultrashort THz pulses with energy exceeding 100 nJ/pulse, corresponding to fluence of about 10 ?J/cm2 and peak electric field larger than 100 KV/cm, are generated by means of high-efficiency tilted wave-front optical rectification in $LiNbO_3$ crystals (starting from 1mJ, 800 nm, t=100fs

light pulses) and combined in a pump-probe experiment with white light supercontinuum probes. This novel spectroscopic tools allow for the measurements of the evolution of the high energy optical constants (1<E<3.5 eV) following excitation with ultrashort THz pulses (t<1 ps) and is used here to investigate the transition between quasi-static and dynamical regime in the Franz-Keldysh Effect, which is revealed by the measured collapse of the semiconducting gap, in slightly doped GaAs.

Finite temperature phase diagram of the classical Heisenberg-Kitaev model

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We study finite-temperature properties of classical version of the Heisenberg-Kitaev model on the honeycomb lattice. This model is a prominent example of anisotropic spin-orbital models, which can possibly describe the low-energy physics of Na2IrO3 and Li2IrO3. In these systems, the spin-orbit coupling is a dominant interaction leading to a strong entangling of spin and orbital degrees of freedom into localized states which interact quite anisotropically. Our main result is a finite-temperature phase diagram obtained by classical Monte-Carlo simulations. Because of highly anisotropic Kitaev interaction, the spin symmetry of the model is reduced to the discrete Z6 symmetry. As the discrete symmetry can be broken at finite temperature even at 2D, the model undergoes phase transitions as a function of temperature. At low temperature phase, thermal fluctuations induce order-by-disorder, just as the quantum fluctuations do at zero temperature. Magnetically ordered states persist up to a certain critical temperature. We find out that there is an intermediate phase between the low-temperature ordered phase with the spontaneously broken Z6 symmetry and the high-temperature disordered phase. The final size scaling analysis suggests that the intermediate phase is a critical Kosterlitz-Thouless-like phase characterized by the continuously variable exponents. Finally, we discuss the relevance of obtained results for experimental findings in Na2IrO3 and Li2IrO3.

High-field thermoelectric transport in $YbRh_2Si_2$

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The heavy fermion compound $YbRh_2Si_2$ has attracted much interest as an example of an unconventional quantum critical point that can be approached using very small magnetic fields. However, there are also anomalous features at higher fields that have not been well explored, and these may give us further insights into the electronic state of this unusual material. We report thermopower measurements on the best available single crystals of $YbRh_2Si_2$ at temperatures down to 0.1K and magnetic fields up to 12T oriented in the ab-plane. We found two step-like features in the field dependence at 9T and 11T, the region where a suppression of the heavy fermion state was reported [1]. Additionally, another step appears at 3.5T. These steps in thermopower correspond to features found in electrical transport. The experimental results are supported by recently published renormalized bandstructure calculations [2] which show two features in the field dependent quasiparticle density of states at around 4T and at 10T. According

to that, the anomalies at 10T in various quantities are caused by a van-Hove-type singularity below the Fermi energy. However, the separation into two features in thermopower and in resistivity remains unexplained as well as the origin of the clear 3.5T-signature.

[1] P. Gegenwart et al, New. J. Phys. 8, 171 (2006).

[2] G. Zwicknagl, J. Phys.: Condens. Matter 23, 094215 (2011).

Physics of CeRuSn studied on a single crystal

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[1] DCMP, Charles University in Prague, Ke Karlovu 5, CZE

The recently reported hysteretic anomalies of electrical resistivity and magnetic susceptibility of CeRuSn between 160 K and 290 K are most likely associated with crystal structure transitions caused by charge ordering at one Ce ion of unstable valence [1,2]. We have grown a single-crystal and measured single crystal X-ray diffraction (SXRD), thermal expansion, susceptibility, resistivity, Hall effect, thermal conductivity and specific heat in the temperature range of interest. The temperature dependence of resistivity was also measured at various hydrostatic pressures. Two step-like anomalies have been observed in all bulk properties at 290 and 220 K, respectively, when cooling and at about 15-20 K higher temperatures, respectively, when heating. The size of corresponding anomalies is identical for cooling and heating but strongly anisotropic with respect to the direction of electrical current, applied magnetic field and direction of measured thermal expansion, respectively. The crystal shrinks by 0.7 % along the c-axis between 300 and 200 K but changes slightly along a- and b-. The hydrostatic pressure shifts the both resistivity anomalies to higher temperatures by more than 11 K/kbar. This would corroborate the scenario considering Ce ion valence changes. SXRD data collected below 160 K can be best conceived in terms of a superstructure formed by a tripled room-temperature CeCoAl-type unit cell along c. The real structure, however, may be more complex [2].

[1] J. A. Mydosh, et al., Phys. Rev. B 83, 054411 (2011).

[2] R. Feyerherm, et al., Phys. Rev. B 85, 085120 (2012).

Out of Equilibrium Dynamics of the Hubbard Model

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Transient time dependent phenomena in correlated electron systems are attracting a great deal of interest in a number of different physical contexts, ranging from ultracold atomic gases to pump probe experiments on correlated materials. Indeed when brought far from equilibrium by extensive energy perturbations strongly correlated electron systems can display non trivial dynamical behaviours or even be trapped into long lived metastable states that differ substantially from their low-energy counterparts. In this

talk I will focus on the single band Hubbard Model and show that physical properties of these metastable states, including possible short-time crossovers or dynamical transitions, can be captured by a Gutzwiller time dependent variational approach. As opposite, the long time dynamics where relaxation and thermalization will eventually arise crucially requires coupling to quantum fluctuations. I will discuss how these can be included using different theoretical approaches. Finally, I will comment on the role of lattice degrees of freedom and surface effects on the non equilibrium dynamics of the Hubbard Model induced by sudden excitations such as those realized in modern pump-probe experiments.

Strong coupling superconductivity, pseudogap and Mott transition

Giovanni Sordi[1]

[1] Institut Laue-Langevin

An intricate interplay between superconductivity, pseudogap and Mott transition, either bandwidth-driven or doping-driven, occurs in materials. Layered organic conductors and cuprates offer two prime examples. We provide a unified perspective of this interplay in the two dimensional Hubbard model within cellular dynamical mean-field theory on a 2×2 plaquette. Both at half-filling and at finite doping, the metallic normal state close to the Mott insulator is unstable to d-wave superconductivity. Superconductivity can destroy the first-order transition that separates the pseudogap phase from the overdoped metal. Yet that normal state transition leaves its marks on the dynamic properties of the superconducting phase. For example, as a function of doping one finds a rapid change in the particle-hole asymmetry of the superconducting density of states. In the doped Mott insulator, the dynamical mean-field superconducting transition temperature T_c^d does not scale with the order parameter when there is a normal-state pseudogap. T_c^d corresponds to the local pair formation temperature observed in tunneling experiments and is distinct from the pseudogap temperature.

[1] G. Sordi et al., PRL 104, 226402 (2010).

[2] G. Sordi et al., PRB 84, 075161 (2011).

[3] G. Sordi et al., arXiv:1110.1392 (2011); G. Sordi et al., arXiv:1201.1283 (2012).

Phase diagram, energy scales and nonlocal correlations in the Anderson lattice model

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[1] Institute of Physics Belgrade, Serbia

We study the Anderson lattice model with one f-orbital per lattice site as the simplest model which describes generic features of heavy fermion materials. The resistivity and magnetic susceptibility results obtained within dynamical mean field theory (DMFT) for nearly half-filled conduction band show the existence of a single energy scale T^* which is similar to the single ion Kondo temperature T_K^o. To determine the importance

of inter-site correlations, we have also solved the model within cellular DMFT (CDMFT) with two sites in a unit cell. The antiferromagnetic region on the phase diagram is much narrower than in the single-site solution, having smaller critical hybridization V_c and Néel temperature T_N. At temperatures above T_N the nonlocal correlations are small, and the DMFT paramagnetic solution is in this case practically exact, which justifies the ab initio LDA+DMFT approach in theoretical studies of heavy fermions. Strong inter-site correlations in the CDMFT solution for $T < T_N$, however, indicate that they have to be properly treated in order to unravel the physical properties near the quantum critical point.

NMR in the iron-selenides : Phase separation between a Mott-antiferromagnet and a homogeneous superconductor in the 245 family

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Iron-based superconductors are often described in the limit of moderate to weak electronic correlations: the parent antiferromagnetic state is a spin-density wave due to nesting of the Fermi Surface, and superconductivity develops under carrier doping of applied pressure. But the recent discovery of superconductivity in the 245 iron-selenide family has put this scenario into question. Indeed, this family of compounds with nominal composition $A_xFe_{2-y}Se_2$ (with A = K, Rb, Cs) shows insulating antiferromagnetism with large moments and no nesting, better described in a Mott picture. Unexpectedly, this AF order seems to coexist with superconductivity with T_c of about 30 K. These findings would favor a strong coupling scenario instead, where the physics could be captured by the carrier-doping of a Mott insulator as in high T_c cuprates. We studied this phase using ^{87}Rb and ^{77}Se NMR in $Rb_{0.74}Fe_{1.6}Se_2$. Our experiment provides clear evidence for a phase separation between antiferromagnetism and superconductivity. We further demonstrate that the superconducting phase is surprisingly homogeneous and does not contain any Fe-vacancies nor magnetic moments. These results bring a new light on the origin of superconductivity in the Fe-based superconductors, suggesting that they cannot be described as carrier-doped Mott insulators.

[1] arXiv:1203.1834

Towards a theoretical spectroscopy": Dynamical mean field theory and beyond - Lecture

Alessandro Toschi[1]

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While the exact calculation of systems of correlated electrons still represents a formidable task, a great step forward in mastering their many-body physics have been achieved since the early Nineties by means of the dynamical mean field theory (DMFT)[1]. In fact, DMFT captures a very important part of electronic correlations, namely the local ones, which play a pivotal role, e.g., in the physics of the Mott-Hubbard

metal-insulator transition. Moreover, merging DMFT with ab-initio density-functional-based approaches has turned out to be a very successful scheme (LDA+DMFT) for explaining - and even for predicting- the results of several spectroscopic experiments performed on correlated electron systems (as in the prototypical cases of SrVO3 or V2O3). Eventually, I will also discuss the most recent perspectives of the methods based on extensions of DMFT, aimed at the inclusion of non-local spatial correlations beyond the mean field level.

[1] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989); A. Georges and G. Kotliar, Phys. Rev. B 45 6479 (1992); A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).

Selected Applications of DMFT: magnetism and superconductivity from weak- to strong-coupling

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In this talk, I will present some selected applications of DMFT, beyond the mere calculation of photoemission or ARPES spectral functions, to study the evolution of magnetic[1] and superconducting[2] phases as a function of the strenght of electronic correlation. Finally, if time is enough, I will also discuss the corrections to the DMFT description of second-order magnetic phase-transitions due to long-range spatial correlations, which have been recently computed[3] by means of the Dynamical Vertex Approximation[4].

[1] C. Taranto, G. Sangiovanni, K. Held, M. Capone, A. Georges, and A. Toschi, Phys. Rev. B 85, 085124 (2012).

[2] A. Toschi, M. Capone, C. Castellani, Phys. Rev. B 72, 235118 (2005).

[3] G. Rohringer, A.Toschi, A.A. Katanin, and K. Held, Phys. Rev. Lett. 107 256402 (2011).

[4] A. Toschi, A.A. Katanin, and K. Held, Phys. Rev. B 75, 045118 (2007).

Electron Magnetic Resonance in Strongly Correlated Electronic Systems – Experimental Aspects - Lecture

Andrej Zorko[1]

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Electron magnetic resonance (EMR) is a highly powerful technique that facilitates direct detection of electronic correlations on a local scale [1]. The first detection of the EMP signal was performed by Zavoisky already in 1944 and predates the nowadays more commonly used nuclear magnetic resonance (NMR). ESR is often superior to other spectroscopic techniques that can detect electronic correlations only indirectly (e.g., NMR) and bulk techniques that do not provide local insight. In principle, resonant

absorption of electromagnetic waves is possible in insulators containing paramagnetic species or imperfections which may trap electrons or holes, in ordinary metals, as well as in magnetically ordered states. Experiments can be performed with either continuous-wave (CW) or pulsed irradiation, however, extremely short spin relaxation times render the latter inoperative in the case of strongly correlated electronic systems.

In this lecture, we will focus on the CW EMR method applied to strongly correlated systems. Basic principles on the magnetic resonance absorption will be presented, introducing the concepts of a spin Hamiltonian, exchange narrowing, critical slowing down of spin correlations and detection of collective excitations in magnetically ordered states. We will demonstrate that accurate information on essential interaction terms and temperature evolution of spin correlations can be extracted from EMR spectra; i.e., from EMR line widths and line shifts.

[1] A. Abragam and B. Bleaney, Electron Paramagnetic Resonance of Transition Ions (Clarendon, Oxford, 1970).

Electron Magnetic Resonance in Strongly Correlated Electronic Systems – Experimental Aspects

Andrej Zorko[1]

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Electron magnetic resonance (EMR) can be effectively employed to yield quantitative information on dominant exchange interactions in exchange coupled systems as well as on major magnetic anisotropy terms, which are usually crucial in determination of a particular ground state of a strongly correlated electronic system. Such information can either be extracted from the EMR spectra in the paramagnetic phase or in a magnetically ordered state, where collective magnon excitations are detected.

First, we will focus on recent examples of low-dimensional quantum spin systems [1,2], where EMR in the paramagnetic phase has yielded essential information for understanding their ground-state properties. This includes the spin-liquid states of the frustrated Shastry-Sutherland lattice SrCu2(BO3)2 [1] and the first “geometrically perfect” kagomé lattice ZnCu3(OH)6Cl2 [2]. In the second part, we’ll show examples of EMR detection of collective magnon modes of geometrically frustrated Ba3NbFe3Si2O14 [4] and FeTe2O5Br. Here EMR has been used for extracting their spin Hamiltonians, as a highly sensitive alternative to the more conventional inelastic neutron scattering.

[1] A. Zorko et al., Phys. Rev. B 69, 174420 (2004).

[2] A. Zorko et al., Phys. Rev. Lett. 101, 026405 (2008).

[3] A. Zorko et al., Phys. Rev. Lett. 107, 257203 (2011).

[4] M. Pregelj et al., submitted for publication.

II. Poster Presentations - Part A - Monday

Poster A1

Lattice vs continuum in the BCS-BEC crossover: The Legacy of broken Galilean invariance

Antonio Privitera[1]

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Lattice approaches to systems in continuum space are ubiquitous in modern science, ranging from lattice QCD to QMC simulations of strongly-interacting Fermi gases. A common issue shared by all these approaches is how to perform a controlled extrapolation to the continuum limit. In this talk we focus on a specific application, namely how the properties of fermionic lattice models with short-range attractive interactions converge,in the dilute limit, to those of a dilute Fermi gas in continuum space through the whole BCS-BEC crossover. This is directly relevant for the physics of ultracold Fermi gases and of the BCS-BEC crossover in these systems.We investigate this connection using both static and dynamical mean-field theory to address the low-density properties of the attractive Hubbard model on different lattices. We show that the existence of a finite lattice spacing has consequences down to very small densities. Our results place strong constraints on current lattice QMC extrapolations of dilute Fermi gas properties.

Poster A2

Signature of antiferromagnetic long-range order in the optical spectrum of strongly correlated electron systems

Ciro Taranto[1]

[1] Vienna University of Technology

We show how the onset of a non-Slater antiferromagnetic ordering in a correlated material can be detected by optical spectroscopy. Using dynamical mean-field theory we identify two distinctive features: The antiferromagnetic ordering is associated with an enhanced spectral weight above the optical gap, and well-separated spin-polaron peaks emerge in the optical spectrum. Both features are indeed observed in LaSrMnO4 [A. Gössling et al. Phys. Rev. B 77 035109 (2008)]. Published in Phys. Rev. B 85, 085124

(2012)

Poster A3

Reduced Density Matrix Functional Theory- A suitable vehicle to import explicit correlations.

Ebad Kamil[1]

[1] Institute for Theoretical Physics, University of Goettingen

A variational formulation for the calculation of interacting fermions system based on density matrix functional theory is presented. This formulation allows importing explicit many particle effects into standard density functional theory based calculations and also avoids ambiguities of double counting terms inherent to other approaches. Local approximation for explicit correlations is introduced and the resulting quantum impurity problem is solved using self consistent Liouvillian perturbation theory within the resolvent formalism.

Poster A4

Organic molecular crystals: materials with competing orders

Gianluca Giovannetti[1]

[1] Sissa (Trieste)

In recent years, organic molecular crystals have emerged as a fascinating class of materials with immense potential for applications. Structures in these materials are held together by van der Waals and hydrogen bonding as opposed to much stronger covalent and ionic bonding in conventional crystals. As a consequence, these systems present complex phases and phenomena which still require a microscopic understanding, ranging from anomalous positive and negative thermal expansion [1] to high-temperature ferroelectricity with large polarization [2] and even superconductivity [3,4]. Moreover, their light, flexible and nontoxic character makes them ideal candidates for future applications. By means of ab-initio and model calculations, we show instabilities towards magnetism in different families of organic molecular crystals driven by electronic correlations. In the tendency to magnetic ordering they share a common feature which is however only a side in their rich and different phase diagrams.

[1] D. Das et al. , Nature Mater. 9, 36 (2010).
[2] S. Horiuchi et al. , Nature 463, 789 (2010).
[3] R. Mitsuhashi et al. , Nature 464, 76 (2010).
[4] A.Y. Ganin et al. , Nature Mater. 7, 367 (2008).

Poster A5

Quantum Critical Transport Near the Mott Transition

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We perform a systematic study of incoherent transport in the high temperature crossover region of the half-filled one-band Hubbard model. We demonstrate that the family of resistivity curves displays characteristic quantum critical scaling of the form $\rho(T,\delta U)=\rho_c(T)f(T/T_o(\delta U))$, with $T_o(\delta U)\sim|\delta U|^{z\nu}$, and $\rho_c(T)\sim T$. The corresponding β-function displays a "strong coupling" form $\beta\sim\ln(\rho_c/\rho)$, reflecting the peculiar mirror symmetry of the scaling curves. This behavior, which is surprisingly similar to some experimental findings, indicates that Mott quantum criticality may be acting as the fundamental mechanism behind the unusual transport phenomena in many systems near the metal-insulator transition.

Poster A6

Universal exchange-driven phonon splitting in antiferromagnets

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We report a linear dependence of the phonon splitting $\Delta\omega$ on the non-dominant exchange coupling constant J_{nd} in the antiferromagnetic transition-metal monoxides MnO, FeO, CoO, NiO, and in the frustrated antiferromagnetic oxide spinels $CdCr_2O_4$, $MgCr_2O_4$, and $ZnCr_2O_4$. It directly confirms the theoretical prediction of an exchange induced splitting of the zone-centre optical phonon for the monoxides and explains the magnitude and the change of sign of the phonon splitting on changing the sign of the non-dominant exchange also in the frustrated oxide spinels. The experimentally found linear relation $\hbar\Delta\omega=\beta J_{nd}S^2$ with slope $\beta=3.7$ describes the splitting for both systems and agrees with the observations in the antiferromagnets $KCoF_3$ and $KNiF_3$ with perovskite structure and negligible next-nearest neighbour coupling. The common behavior found for very different classes of cubic antiferromagnets suggests a universal dependence of the exchange-induced phonon splitting at the antiferromagnetic transition on the non-dominant exchange coupling.

Poster A7

Phase separation and charge orderings in the extended Hubbard models

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Electron charge orderings phenomena in strongly correlated electron systems are currently under intense investigations. Charge orderings (COs) are relevant to a broad range of important materials, including manganites, cuprates, magnetite, several nickel, vanadium and cobalt oxides, heavy fermion systems (e.g. Yb_4As_3) and numerous organic compounds. We present studies of the extended Hubbard model with both (i) the effective on-site interaction U and (ii) the intersite density-density interactions W. In the analysis of the phase diagrams and thermodynamic properties of this model in the atomic limit we have adopted the variational approach, which treats the on-site interaction term exactly and the intersite interactions within the mean-field approximation. We also studied the finite bandwidth limit of the model using diagonalization method

by Lanczos algorithm within the dynamical mean field theory. Our investigation of the general case depending on the values of the interaction parameters and the electron concentration, the system can exhibit not only several homogeneous charge ordered (CO) phases, but also various phase separated states (CO-CO and CO-nonordered). One finds that the model considered exhibits very interesting multicritical behaviours and features, including among others bicritical, tricritical, critical-end and isolated critical points.

Poster A8

Superconducitivity and Charge Density Wave: Comparative Raman Spectroscopy Study of the Dichalcogenides2H-NbS2 and 2H-NbSe2

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Whereas the dichalcogenide 2H-NbSe2 exhibits coexisting superconducting (7K) and charge density wave (33K) orders, its isostructural brother 2H-NbS2 presents only the superconducting state (6K). Comparative studies of both compounds provide a playground to explore the longstanding question of the origin of the CDW instability as well as the question of the interplay between superconductivity and CDW order. We have performed Raman spectroscopy on 2H-NbSe2 and 2H-NbS2 versus temperature down to 1.7K and versus magnetic field up to 8T. A superconducting peak is observed in NbS2, consistent with STM measurements [Guillamon]. The intensity of the peak associated with the superconductivity is much larger in NbSe2 [Sooryakumar]. A precise study of the superconducting and the CDW peaks in 2H-NbSe2 versus temperature and magnetic field will be presented. The behavior of the phonons is investigated. The energy scale of the double phonon process in both compounds is consistent with the soft mode observed by inelastic X-ray scattering [Weber, Leroux]. However, in 2HNbSe2, the phonon peak freezes below Tcdw.

[Sooryakumar] R. Sooryakumar et al, PRL 45, (1980) 660.
[Guillamon] I. Guillamon et al., PRL 101, (2008) 166407.
[Weber] F. Weber et al., PRL 107, (2011) 107403.
[Leroux] M. Leroux et al., to be published

Poster A9

Pressure tuning of the incoherent holon-doublon decay in a 1D Mott-insulator

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We report a near-infrared pump-probe experiment at high static pressures aimed to the measurement of the pressure scaling of the incoherent many-body relaxation in a Mott insulator. The organic compound ET-F2TCNQ, is a room-temperature 1D Mott insulator characterized by a weak electron-lattice interaction and a high correlation energy (1 eV). This features makes it an ideal material for the investigation of purely

electronic excitations in presence of strong active correlations. The optical spectrum displays a narrow CT resonance along the a axis and it has been recently shown that its photoexcitation induces a metallic state modulated on the 10 fs scale by the coherent evolution of double occupancies (doublons) and empty sites (holons). Our goal is to describe how these many-body excitations' lifetimes are related to the microscopic parameters of this compound, namely the onsite correlation energy U, the intersite correlation V, and the hopping t. Experiments in fermionic optical lattices suggest that in 3D the relaxation time depends exponentially from the ratio U/t, and in our case high pressures represent an ideal tuning parameter. We observe that the relaxation process becomes faster when pressure is applied and simultaneously the CT band shifts towards low frequencies because of the increased overlap in the system. By relating the holon-doublon relaxation to the microscopic parameters of the system our work establishes a neat connection between a solid state problem and its quantum simulation via fermionic optical lattices.

Poster A10

Pressure dependence of optical exitations in tetragonal Sr2VO4

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The Mott-Hubbard insulator Sr_2VO_4 shares the crystal structure of the archetypal cuprate high Tc superconductor La_2CuO_4, with a $3d^1$ configuration of the V^{4+} ions. The near degeneracy of the three t_{2g} orbitals is responsible for a rich magnetic phase diagram with a high temperature non-ordered state and a low temperature spin-orbital ordered phase, subject of recent theoretical efforts. Our optical data reveal the presence of two excitations at 36 meV and 104 meV, associated to spin-orbit and crystal-field splitting. Applying hydrostatic pressure modifies the inter-atomic distances and thus allows tuning of the interactions. With our newly developed diamond-anvil pressure cell for infrared spectroscopy from 20-300 K and pressure up to 20 GPa, we have measured the optical transmission spectrum in the frequency windows from 12 to 40 meV and 62 to 140 meV. The data show a strong sensitivity of these optical absorption band energies to the pressure (i.e. to crystal field).

Poster A11

Wigner-Mott scaling of transport near the two-dimensional metal-insulator transition

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Electron-electron scattering usually dominates the transport in strongly correlated materials. It typically leads to pronounced resistivity maxima in the incoherent regime around the coherence temperature T^*, reflecting the tendency of carriers to undergo Mott localization following the demise of the Fermi liquid. This behavior is best pronounced in the vicinity of interaction-driven (Mott-like) metal-insulator transitions, where the T^* decreases, while the resistivity maximum ρ_{max} increases. Here we show

that, in this regime, the entire family of resistivity curves displays a characteristic scaling behavior $\rho(T)/\rho_{max} \approx F(T/T_{max})$, while the ρ_{max} and $T_{max} \sim T^*$ assume a powerlaw dependence on the quasi-particle effective mass m^*. Remarkably, precisely such trends are found from an appropriate scaling analysis of experimental data obtained from diluted two-dimensional electron gases in zero magnetic fields. Our analysis provides strong evidence that inelastic electron-electron scattering – and not disorder effects – dominates finite temperature transport in these systems, validating the Wigner-Mott picture of the two-dimensional metal-insulator transition.

Poster A12

Lanczos algorithm with Matrix Product States for dynamical correlation functions

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We reconsider the oldest approach within the Density Matrix Renormalization Group (DMRG) to calculate dynamical correlation functions: the Lanczos algorithm. We use an formulation of the DMRG in matrix product states (MPS). The direct use of matrix product states combined with an ex-post reorthogonalization method allows to avoid several shortcomings of the original approach, namely the multi-targeting and the approximate representation of the Hamiltonian inherent in earlier Lanczos-method implementations in the DMRG framework, and to deal with the ghost problem of Lanczos methods, leading to a much better convergence of the spectral weights and poles. We present results for the dynamic spin structure factor of the spin-1/2 antiferromagnetic Heisenberg chain. A comparison to Bethe ansatz results in the thermodynamic limit reveals that the MPS-based Lanczos approach is much more accurate than earlier approaches at minor additional numerical cost.

Poster A13

Ultrafast Spectroscopy of charge/orbital ordering in La0.5Sr1.5MnO4

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Nearly single-cycle, 4 femtosecond near-infrared laser pulses are used to photo-excite the charge transfer in single-layer half-doped manganite, probing the dynamics of orbital ordering within time resolution shorter than the lattice response time.

La0.5Sr1.5MnO4 compound shows orbital (OO), charge (CO) and magnetic ordering at low temperatures (T CO/OO = 220K, TN = 110K). Orbitals align themselves along ferromagnetic zig-zag chains, coupled antiferromagnetically to the other chain. This ordering is stabilized by cooperative Jahn-Teller distortions and electronic exchange interactions, tied strongly to each other. Furthermore, it is associated with optical anisotropy in the ab-plane, allowing for sensitive optical probing.

We aim to know which of the two mechanisms stabilizes the orbitally and magnetically ordered states. As there is an intrinsic bottleneck in the response time of the

crystal lattice, only the ultrashort photo-excitation can disentangle the dynamics of these two different phenomena. In our experiments, 4fs near-infrared pump pulses, resonant with the charge transfer band, delocalize electrons from one of the Mn3+ sites to nearby Mn4+ sites along the ferromagnetic chains. Degenerate probe pulses measure the induced change in the OO associated optical birefringence.

We find that the ultra-fast reduction of birefringence is limited only by the cross-correlation between the pump and probe pulse. It strongly suggests that OO is dominantly stabilized by fast exchange interactions, while lattice effects like Jahn-Teller phonon seems to be of minor importance in OO state. Our work shows a promising way to investigate individual dynamics of otherwise treated coupled parameter.

Poster A14

Electronic Correlation at the Two-Particle Level

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Electronic correlated systems often can be successfully described by dynamical mean field theory (DMFT). If DMFT is applied to finite-dimensional systems it is self-consistent at the one-particle level. Extensions of DMFT based upon the systems' two-particle properties have been developed such as the dynamical vertex approximation (DΓA) [1] or the dual fermion approach [2]. In addition, the understanding and the calculation of two-particle quantities are crucial within DMFT to compute momentum-dependent response functions that can be compared directly with experiments. As hitherto the investigation of local and non-local two-particle properties has been merely sporadic, we provide a systematic analysis [3,4] of the reducible and irreducible two-particle vertex functions by applying DMFT and the dynamical cluster approximation (DCA) to the two-dimensional Hubbard model.

[1] A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. B 75, 045118 (2007)

[2] A. N. Rubtsov, M. I. Katsnelson, and A.I. Lichtenstein, Phys. Rev. B 77, 033101 (2008)

[3] G. Rohringer, A. Valli, A. Toschi, arXiv:1202.2796.

[4] T. Schaefer, G. Sangiovanni, G. Rohringer, O. Gunnarsson, K. Held, A. Toschi - in preparation

Poster A15

Unusual properties of the insulator [Mn(Imz6)2+(NO3-) where, Imz = imidazole: A polarised and non-polarised neutron diffraction, EPR study

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For the free ion Mn(II), represented by the 6A1g ground state, the spin density distribution of the five unpaired electrons is expected to be spherical within [Mn(Imz)6]2+(NO3-)2 on the basis of the ionic model for metal-ligand interaction. In this respect the spin density for Mn(II) may be modelled by a superposition of expanding one-centered spherical orbital functions centered on manganese. Through polarised neutron diffraction on a 2*2.5*5 mm^3 (40 mg) crystal of the deuterated complex on the D3 instrument at the ILL, we have found however that the Fourier reconstructed spin density distribution for the complex is unpexpectedly non-spherical but trigonal, which indicates intriguingly that dative pi (and sigma) ligand-to-metal interactions are likely responsible for the non-spherical spin density distribution. The DFT modelling of the system also showed a trigonal distribution of the spin density, and that the complex is an insulator from the density of states analysis. Continuous wave EPR (X-band), High Field Multi-Frequency measurements on both single crystal and powder samples of the complex showed no significant frequency dependency. The PND, DFT, EPR, analyses indicate that the complex is a potential candidate for new generation of strongly correlated electron systems.

1. Garrett et al. Acta Cryst. 1983. C39, 1031-1034

Poster A16

Exotic phase diagrams of d^9 Kugel-Khomskii model in two and three dimensions

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We present the results of cluster mean-field approach to the spin-orbital Kugel-Khomskii model for transition metal compounds: K_2CuF_4 with the two-dimensional (2D), and recently investigated [1] $KCuF_3$ with three dimensional (3D) lattice geometry. The zero-temperature phase diagrams are presented depending on crystal field splitting E_z (playing the role of an uniaxial pressure along the c direction) and Hund's exchange coupling $\eta \equiv J_H/U$. These are compared to: (*i*) single-site mean-field approach, (*ii*) results obtained for the bilayer system [2], and (*iii*) the phase diagram for $KCuF_3$ obtained using spin-wave theory and variational wave functions [3]. Both phase diagrams include phases with spin-orbital entanglement, alternating spin singlets and exotic chiral, helicoidal or striped magnetic order separating standard magnetic phases with ferro-orbital or alternating orbital order. We present effective, perturbative spin-only models explaining such behaviors, characteristic for AF-FM transitions in different lattice directions. We show the order parameters, spin and orbital correlation functions and a measure of spin-orbital entanglement as functions of E_z or η for different cuts of the phase diagrams. Finite-temperature behavior of different phases of 2D and 3D systems is also investigated.

[1] J. Deisenhofer *et al.*, Phys. Rev. Lett. **101**, 147601 (2008).
[2] W. Brzezicki and A.M. Oleś, Phys. Rev. B **83**, 214408 (2011).
[3] L.F. Feiner, A.M. Oleś, and J. Zaanen, Phys. Rev. Lett. **78**, 2799 (1997).

Poster A17

Infrared and THz spectroscopy in multiferroic $Eu_{1-x}Ho_xMnO_3$

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We investigated $Eu_{1-x}Ho_xMnO_3$ with the concentration varying from 0.1 to 0.5. On cooling, $Eu_{0.9}Ho_{0.1}MnO_3$ enters an incommensurate antiferromagnetic phase, which turns into an commensurate antiferromagnetic one at lower temperatures. Doping leads to ferroelectricity with polarization parallel to the a-axis, which flips to P//c by further doping. In order to detect the coupling between low energy phonons and electromagnons [1-4], we performed systematic polarization dependent IR and THz studies. The data will be compared to $TbMnO_3$ and the related system $Eu_{1-x}Y_xMnO_3$.

[1] A.Pimenov et al., Nature Phys.,2, 97(2006)
[2] A.Pimenov et al., Phys. Rev. B, 77, 014438(2008)
[3] N.Kida et al., Phys. Rev. B, 78, 104414(2008)
[4] R.Valdés Aguilar et al., Phys. Rev. Lett., 102, 047203(2009)

Poster A18

Raman Scattering study of the Hidden Order state of URu_2Si_2

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The unconventional superconductivity appears usually inside or nearby a magnetic phase, however more exotic cases exist. The heavy fermion compound URu_2Si_2 exhibits a superconductivity phase (TC=1.5K) inside a so-called Hidden Order phase (T0=17.5K). Despite over 25 years of research, the microscopic origin of the Hidden Order is not yet well known. Neutron scattering experiments reveal small antiferromagnetically ordered moment below T0 about 0.02 ?B. However, this moment is too weak to explain the large anomaly and the loss of entropy visible in specific heat at T0 [Mydosh]. As for optical investigation on URu_2Si_2, mainly far-infrared reflectance experiments exist [Bonn, Levallois]. And only few Raman scattering studies have been performed [Cooper, Lampakis] and only for c axis. We have studied URu_2Si_2 for both a and c axes, down to low temperature (2K). We have probed the phononic and electronic properties and their interaction. Softening of phonon modes together with Fano-shape were observed, implying that a phonon-electron coupling is at play. At low energy, electronic Raman signal shows either fluctuations or more conventional Drude shape for different symmetry. We have studied both signals through the Hidden Order temperature.

J. A. Mydosh et al., Reviews of Modern Physics 83, 1301 (2011)

D.A. Bonn et al., PRL 61, 1305 (1988)

J. Levallois et al., PRB 84, 184420 (2011)

S. Cooper et al., PRB 36, 5743 (1987)

D. Lampakis et al., Physica B 378-380, 578 (2006)

III. Poster Presentations - Part B - Tuesday

Poster B1

Non-equilibrium stationary state formation in driven correlated systems

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We investigate the dynamics of a two-dimensional Hubbard model in a static electric field in order to identify the conditions to reach a non-equilibrium stationary state. For a generic electric field, the convergence to a stationary state requires the coupling to a thermostating bath absorbing the work done by the external force. Following the real-time dynamics of the system, we show that a non-equilibrium stationary state is reached for essentially any value of the coupling to the bath. We map out a phase diagram in terms of dissipation and electric field strengths and identify the dissipation values in which steady current is largest for a given field.

Poster B2

Magnetic soft modes in the distorted triangular antiferromagnet α-$CaCr_2O_4$

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α-$CaCr_2O_4$ is a spin-3/2, distorted triangular lattice antiferromagnet with a simple 120° spin structure that masks the complex pattern of exchange interactions [1]. The magnetic excitation spectrum has been measured using inelastic neutron scattering on powder and single crystal samples. It reveals unusual low energy modes which can be explained by linear spin-wave theory assuming nearest and next-nearest neighbor interactions. The mode softening is due to the next-nearest neighbor interactions and indicates a new magnetic phase nearby as revealed by the phase diagram constructed for this system. The extracted direct exchange interactions correlate well with the Cr3+-Cr3+ distances and are in agreement with other chromium oxide delafossite compounds.

[1] S. Toth, B. Lake et. al., Phys. Rev. B, 84, 054452 (2011)

Poster B3

High superconducting critical temperatures depend universally on the electron-phonon interaction strength

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The pairing mechanism at the origin of high-temperature superconductivity is still the subject of passionate debate. Ample experimental evidence suggests that in high-temperature superconductors the electrons interact strongly with two types of collective (bosonic) excitations: lattice vibrations (phonons), and collective electronic excitations, such as spin fluctuations. However, evidence for strong interaction is not sufficient to identify the pairing mechanism. Here we show that the superconducting critical temperature of pnictides, cuprates, and bismuthates depends universally on the strength of the electron-phonon interaction as measured by the electron energy relaxation rate 1/ e-ph, showing a characteristic maximum at 1/ e-ph 15 ps-1, Tc $>$ 130 K. This dependence demonstrates that the electron-phonon interaction is fundamental for the pairing. Among the many scenarios that have been proposed for the high-Tc mechanism, we find that only bipolaronic pairing is consistent with the experimental results.

Poster B4

2DEG-like behavior in $SrTiO_3$ with Oxygen Vacancies

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The $SrTiO_3/LaAlO_3$ (STO/LAO) interface has been the focus of much attention due to metallic conduction reported as due to the formation of a 2D electron gas (2DEG). However, STO itself becomes metallic when annealed in a low oxygen environment. By vacuum annealing bare STO we are able to replicate transport properties, including resistivity, Hall effect, and thermopower, that are frequently ascribed to a 2DEG at the STO/LAO interface. We discuss the implications of this work for STO-based 2DEGs and investigate tuning STO's electronic and thermal transport properties via oxygen doping and electrostatic gating. This work was supported by the Ministerio de Ciencia e Innovación (Spain), grant MAT2010-16157, and the European Research Council, grant ERC-2010-StG 259082 2D THERMS.

Poster B5

Magnetic Properties of the Haldane Spin-Chain Compound $SrNi_2V_2O_8$: Effects of inter-chain couplings and anisotropy

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The spin-1 Heisenberg antiferromagnetic chains - also known as Haldane chains have attracted considerable attentions in recent years due to their novel quantum mechanical

behaviors. For these chains, the ground state is a spin singlet and the excitations are a gapped S = 1 triplet of magnons (where the gap is known as the Haldane gap) which is in contrast to gapless continuum of spinon (S-1/2) excitations for a half-integer spin-chain system. Under an applied magnetic field, Haldane chains undergo a quantum phase transition from the gapped spin-liquid phase to a gapless ordered phase at some critical value Hc. The presence of anisotropy and inter-chain interactions lead to more complex behavior and a richer phase diagram. To understand the effects of anisotropy and the inter-chain interactions, we have carried out magnetization and heat capacity study on the single crystal of new Haldane spin-chain compound $SrNi_2V_2O_8$. We have grown the first single crystals of $SrNi_2V_2O_8$. The compound crystallizes in the tetragonal crystal structure [a = b 12.1660(3) Å and c 8.3286(2) Å; Sp. Gr. I41cd]. It consists of an array of edge-shared NiO6 (Ni2+; 3d8, S=1) octahedra, forming screw chains along the c-axis. The screw chains are separated by nonmagnetic VO4 (V5+; 3d0, S=0) tetrahedra and Sr2+ ions. Magnetization and heat capacity study on the single crystal confirmed a non-magnetic (spin-liquid) ground state down to 2 K. The field-dependent magnetization curves at 4.2 K for both H $\parallel$ c and H $\perp$ c show an abrupt change of slope at critical fields Hc($\perp$) = 11.6 T and Hc($\parallel$) = 16.4 T, suggesting field-induced magnetic ordering. From the critical field values, the gap energies are calculated to be $\Delta_{\parallel}$ = 0.95 meV and $\Delta_{\perp}$ = 1.9 meV, respectively, by considering the perturbation approach [1]. High temperature series expansion analysis of the temperature dependent susceptibility data yields the intra-chain exchange constant (J) 102.19±0.01 K (8.8 meV). For the present system $SrNi_2V_2O_8$, the value of the mean gap energy (1.58 meV) is considerably smaller than the theoretically predicted Haldane gap value of 0.41J (= 3.6 meV), expected for a system having no inter-chain interactions and anisotropy [1, 2]. The observed lower values of gap energies suggest the presence of substantial inter-chain interactions in $SrNi_2V_2O_8$. Based on the present studies we have proposed a phase diagram in the HT-plane. References

[1] O. Golinelli, Th. Jolicoeur, and R. Lacaze, J. Phys. Condens. Matter 5, 7847 (1993).
[2] T. Sakai and M. Takahashi, Phys. Rev. B 42, 4537 (1990).

Poster B6

Designing microwave experiments for milikelvin temperatures

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[1] Vienna University of Technology

Correlation effects of electrons in solids are responsible for many intensively studied phenomena like superconductivity and quantum criticality. These effects involve low energy scales and their experimental investigation therefore requires specialized conditions: on the one hand, the studied materials have to be cooled to low temperatures; on the other hand, any kind of non-thermal excitation to the system also has to be in a low-energy range. One very direct way to study the response of the electronic system to a low-energy excitation is using electromagnetic radiation in the microwave range. Implementing a microwave experiment into a low-temperature environment is challenging from a technical point of view since high sensitivity has to be achieved without heating the sample and the system by the radiation itself or by thermal conduction through the microwave cables. We present different experimental approaches to measure electronic

properties of metallic samples with microwave radiation down to temperatures in the mK range.

We gratefully acknowledge financial support from the European Research Council/ERC Advanced Grant No 227378.

Poster B7

Magnetic properties and structure evolution along R_2RhIn_8 series

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Intermetallic compounds R_2RhIn_8 (R = rare earth) are structurally related to a class of Ce-based heavy-fermion superconductors. Study of their magnetic structure and behavior is important for understanding mechanism of the unconventional heavy-fermion superconductivity. We have successfully grown single crystals of these compounds with R = Nd, Tb, Dy, Ho, Er and Tm from the melt in the In flux. We report the evolution of the magnetic properties of this series. All studied compounds exhibit antiferromagnetic behavior with the Néel temperatures up to 43 K for Tb compound. Magnetization and specific heat measurements have revealed metamagnetic transitions to another antiferromagnetic phase for Tb, Dy and Ho compounds. We show detailed magnetic phase diagrams for all these compounds and compare with results reported for Nd_2RhIn_8 [1]. Low temperature magnetic structures were studied by neutron diffraction at the Institute Laue-Langevin on VIVALDI Laue diffractometer and four-circle D10 diffractometer. From these experiments, propagation vector $k = (1/2, 1/2, 1/2)$ and magnetic structure of studied compounds were determined. We present comparison of our results with the magnetic structure of Ce_2RhIn_8 and other isostructural compounds from RRhIn$_5$ [2] and R_2CoGa_8 [3] series.

[1] J. G. S. Duquea, et al., J. Magn. Magn. Mater. 323 (2011) 954-956
[2] N. V. Hieu, et al., J. Phys. Soc. Japan 75 (2006) 074708
[3] D. A. Joshi Phys. Rev. B 77 (2008) 174420

Poster B8

Disentangling the non-equilibrium dynamics in the pseudogap phase of Y-Bi2212 cuprate superconductors, by the time-resolved optical spectroscopy.

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The pseudogap state is the most exotic and elusive phase of the phase diagram of High Critical Temperature Superconductors (HTSCs), and the comprehension of the microscopic electronic mechanisms behind is of paramount importance to reveal the nature of this intriguing phase. By exploiting a novel, non-equilibrium all-optical experimental technique, the time-resolved spectroscopy, I demonstrate that the non-equilibrium dynamics underlying this phase are more complex than those observed for the normal

state phase, suggesting that the pseudogap in HTSCs is a state of matter where the fermionic quasiparticles and the bosonic excitations are strongly intertwined. Several Y-Bi2212 (Bi2Sr2Y0.08Ca0.92Cu=8+delta) superconducting samples, differing in the doping level, have been probed with the time-resolved optical spectroscopy, to map the evolution of the time-resolved optical signal through the phase diagram of the compound. In particular, for the non-equilibrium dynamics of samples in the pseudogap phase, measurements are performed at T=100 K, the pseudogap extending between T* (140 K for OP samples and 200 K for UD samples) and Tc. In this region of the doping-T phase-diagram, the transient frequency resolved optical response is different from what observed in the normal state and a pure non thermal scenario does not account for the results. Exploiting the time- and frequency-resolution of our technique and the differential analysis based on a differential dielectric function approach, I demonstrate that, on the femtosecond timescale, the transient optical response at T=100 K is dominated by an excitation-dependent bosonic glue and by an impulsive quench of a gap in the density of states.

Poster B9

Electrical resistivity and magnetization measurements of the Kondo insulator $CeRu_4Sn_6$

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Recently, specific heat and magnetization measurements on single crystalline $CeRu_4Sn_6$ have revealed pronounced anisotropies [1], suggesting that this compound may be a nodal Kondo insulator. Anisotropy was not only found along the principal crystal directions (tetragonal a- and c-direction), but also within a quasi-cubic cell arising in this compound because the lattice parameter c in the [001]-direction matches the lattice spacing c' in the [110]-direction by Δ(c-c')/c = 0.2 %.

Here we present results of electrical resistivity and magnetization measurements on single crystalline $CeRu_4Sn_6$ samples between 25 mK and several hundred degree above room temperature along the different crystal directions (a, c, and c'). The anisotropy in the electrical resistivity and magnetization is seen over the whole temperature range: almost isotropic behaviour within the tetragonal a-a plane (including c'), but clearly distinct behaviour for the out-of-plane direction c. These findings are analyzed in terms of a doubly-gapped state and a nodal or directional gap of this compound, and discussed in the context of previous results on polycrystals [2-4].

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[1] S. Paschen et al., J. Phys.: Conf. Ser. 200, 012156 (2010).
[2] A.M. Strydom et al., J. Magn. Magn. Mater. 310, 377 (2007).
[3] E.M. Brüning et al., J. Magn. Magn. Mater. 310, 393 (2007).
[4] E.M. Brüning et al., Phys. Rev. B 82, 125115 (2010).

Poster B10

Thermoelectric properties of the Kondo insulator CeRu4Sn6

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Kondo insulators represent a special class of heavy fermion systems where a half-filled conduction band hybridizes with an almost dispersionless 4f level resulting in a heavy quasiparticle band with a small energy gap of a few meV at the Fermi level [1]. The tetragonal crystal structure [2] of the Kondo insulator $CeRu_4Sn_6$ places it inbetween the archetypal cubic Kondo insulators like YbB_{12} or $Ce_3Bi_4Pt_3$ and the orthorhombic "Kondo semimetals" CeNiSn and CeRhSb. Investigations of possible anisotropies - or even nodes - of the Kondo insulating gap in $CeRu_4Sn_6$ are of central interest.
Previous measurements on single crystalline $CeRu_4Sn_6$ showed a large anisotropy of physical properties, namely of the electrical resistivity, the magnetic suscpetibility and the specific heat [3]. Interestingly this anisotropy is observed not only in the tetragonal, but also in a quasi-cubic unit cell formed by the c-axis and the diagonal of the a-a-plane, c'. In this work we present thermopower and thermal conductivity data of single crystalline $CeRu_4Sn_6$. A large anisotropy between the c-axis and the tetragonal plane is observed. We compare the thermoelectric figure of merit ZT of our single crystals with that of polycrystals. In addition, we present our new setup for measurements of thermal conductivity and thermopower in a dilution refrigerator.

References

[1] G. Aeppli and Z. Fisk, Comments Condens. Matter Phys. **16**, 155 (1992).
[2] I. Das and E. V. Sampathkumaran, Phys. Rev. B **46**, 4250 (1992).
[3] S. Paschen, H. Winkler, T. Nezu, M. Kriegisch, G. Hilscher, J. Custers, and A. Prokofiev, J. Phys.: Conf. Ser. **200**, 012156 (2010).

Poster B11

Antiferromagnetism, structural instability, frustration and quantum critical point in intermetallic $A\mathrm{Fe}_4X_2$ systems

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Magnetic systems with reduced dimensionality or frustration are attracting strong interest because these features lead to an increase of quantum fluctuations which often results in unusual properties. While such effects have been widely investigated in insulating systems, much less work has been done on frustrated and/or low dimensional metallic systems, mainly because of very limited number of appropriate compounds. Here we present a detailed study of the intermetallic $A\mathrm{Fe}_4X_2$ compounds (A = Sc, Y, Lu, Zr; X = Si, Ge) crystallizing in the $ZrFe_4Si_2$ structure type. In this tetragonal structure Fe atoms form chains of edge-linked tetrahedra along the c direction, a configuration which is prone for frustration and low dimensional fluctuations. Our results indeed evidence this family of compounds to cover the whole regime from frustrated

antiferromagnetic (AFM) order up to the quantum critical point (QCP) separating the magnetic ordered ground state from the paramagnetic ground state. We synthesized polycrystalline samples of all these compounds and investigated their magnetic, thermodynamic, structural, and transport properties. In addition we performed preliminary μSR and NMR measurements. In all compounds we observed a Curie-Weiss behavior in $\chi(T)$ at high temperatures indicating a paramagnetic Fe-moment $\mu_{eff} \cong 3\mu_B$/Fe. All compounds with trivalent A elements presents a magnetic transition coupled to a large structural transition. Low T_N´s and large Θ_{CW}/T_N ratios confirm the relevance of frustration. Replacement of trivalent A by tetravalent Zr results in a strong suppression of the AFM order, putting $ZrFe_4Si_2$ close to a QCP.

Poster B12

Electronic structure of the heavy-fermion superconductor $Ce_2Ni_3Ge_5$ and its reference compound $Ce_2Ni_3Si_5$ by ab initio calculations

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Band structures of pressure-induced, heavy-fermion superconductor $Ce_2Ni_3Ge_5$ [1] and its non-superconducting, mixed-valence counterpart $Ce_2Ni_3Si_5$ [2] have been calculated employing the full-potential local-orbital (FPLO) code [3] in the local density approximation (LDA). Both compounds crystallize in the orthorhombic (Ibam) symmetry. These investigations were focused particularly on the Fermi surfaces (FSs) topology. Our LDA results show that the FSs are quite similar in both compounds and exist in four bands, containing three-dimensional holelike and electronlike sheets. Interestingly, the specific FS nesting properties has been revealed only in $Ce_2Ni_3Ge_5$. They support a previously postulated presence of antiferromagnetic (AFM) spin fluctuations in the heavy-fermion superconducting state ($T_{SC} = 0.26K$) of this germanide, particularly in the region above the critical pressure of 3.9 GPa where the long range AFM ordering disappears, as observed experimentally [1]. However, probably still existing magnetic fluctuations can be responsible for the pressure-induced unconventional superconductivity in this system. We present also a comparison between the electronic structures of $Ce_2Ni_3Ge_5$ and rather BCS-like $Lu_2Ni_3Si_5$ [4].

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[1] M. Nakashima et al., J. Phys. CM **17**, 4539 (2005); Physica B **378-380**, 402 (2006).

[2] Ch. Mazumdar et al., Phys Rev. B **46**, 9009 (1992).

[3] FPLO9.00-34, K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999); www.FPLO.de.

[4] M. Samsel-Czekala and M.J. Winiarski, Intermetallics **20**, 63 (2012).

Poster B13

Investigation of the new heavy fermion compound Ce_2PtIn_8

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$Ce_nT_mIn_{3n+2m}$ ($n = 1, 2$; $m = 1$; T = transition metal) type compounds are subject of intense interest in the condensed-matter community. By adding an additional $CeIn_3$-stacking layer the dimensionality changes from 3D to more 2D. While selecting the proper transition metal, the compound might either order antiferromagnetically or becomes superconducting. It has been shown, that the superconducting state is closely linked to the presence of a quantum critical point. The group of $Ce_nT_mIn_{3n+2m}$ compounds is predestinated to investigate the interplay between magnetism and superconductivity. Recently, two new compounds from the $Ce_nT_mIn_{3n+2m}$ heavy fermion family have been found. Ce_2PdIn_8 is an ambient pressure superconductor while $CePt_2In_7$ orders antiferromagnetically. Here, we report on the existence of a new heavy fermion ($\gamma \approx 370 mJ/mol Ce \cdot K^2$) compound Ce_2PtIn_8. Similar to Ce_2PdIn_8, the synthesis of Ce_2PtIn_8 is rather complicated. However, from our recent studies of solution growth of Ce_2PdIn_8 supported by differential thermal analysis optimal conditions for growing Ce_2PtIn_8, single crystals could be deduced. Single crystal X-ray diffraction confirmed that Ce_2PtIn_8 crystallizes in Ho_2CoGa_8–type structure with lattice parameters $a = 4.699$ Å and $c = 12.185$ Å. We will present specific heat, resistivity (ambient and under hydrostatic pressure) and magnetization measurements. Ce_2PtIn_8 orders magnetically below 2.1 K. A second, magnetic order-to-order transition is observed just below at 2 K. Contrary to Ce_2RhIn_8, both transitions merge at magnetic field around 4 T and split again in higher magnetic fields showing on different character of magnetic ordering. The magnetic field-temperature phase diagram will be discussed in the context of superconductivity and magnetism evolution in related compounds.

Poster B14

Strongly correlated quantum systems out of equilibrium: A variational cluster approach

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The theoretical understanding of the non-equilibrium behavior of strongly correlated quantum many body systems is a long standing challenge, which has become increasingly relevant with the progress made in the fields of molecular- and nano- electronics, spintronics or quantum optics and simulation. Besides seeding the fundamental concepts for promising future applications, developing a sound understanding of the plethora of previously unrecognized effects, arising in a non-equilibrium situation, is currently at the forefront of theoretical research. We report on the development of non-equilibrium cluster perturbation theory [1], and its variational improvement, the non-equilibrium variational cluster approach [2]. The non-equilibrium extensions of the well-established cluster perturbation theory and the variational cluster approach are based on the Keldysh Green's function method which allows, in this case, accessing single particle dynamic quantities on the whole complex plane. These flexible and versatile techniques can in principle be applied to any lattice Hamiltonian with local interactions, including multi-band and multi-impurity systems. Within this framework it is possible to work in the thermodynamic limit and therefore exchange particles with a bath and/or dissipate energy. We will highlight the importance of the self-consistently determined variational parameters, introduced in the non-equilibrium variational cluster approach. We will discuss the performance, open issues and limitations as well as the advantages of the non-equilibrium variational cluster approach on the basis of a single impurity system. Based on the good performance of the variational cluster approach for the single Impurity Anderson model

in the equilibrium situation [3], results obtained for the steady state current density as well as the non-equilibrium density of states of a strongly correlated single quantum dot will be presented [4]. These will be benchmarked against data for the quasi stationary state from a real time evolution using matrix product states.

[1] M. Knap, W. von der Linden and E. Arrigoni, Phys. Rev. B 84, 115145 (2011)
[2] M. Balzer and M. Potthoff, Phys. Rev. B 83, 195132 (2011)
[3] M. Nuss, E. Arrigoni, M. Aichhorn and W. von der Linden, arXiv:1110.4533 (2011)
[4] M. Nuss, E. Arrigoni and W. von der Linden, to appear in: AIP Conf. Proc. XVI TCPSCS (2012)

Poster B15

Electronic structures of iron $(Lu;Y;Sc)_2Fe_3Si_5$ and relative nickel 235 superconductors from first principles

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Band structures of several superconductors (SCs), such as the unconventional $R_2Fe_3Si_5$ (R = Lu;Y;Sc), BCS-like $Lu_2Ni_3Si_5$ [1] and heavy-fermion $Ce_2Ni_3Ge_5$, have been computed by the FPLO method [2]. Analogous calculations were performed also for their non-superconducting counterparts. The investigated SCs exhibit relatively low transition temperatures $T_{SC} < 7$ K and only $Ce_2Ni_3Ge_5$ is magnetically ordered [3,4]. In the studied iron-based SCs, the DOSs at the Fermi level are both diminished and dominated by the Fe 3d electrons, similarly to those in other iron-based high-TSC SCs. The Fermi surfaces (FSs) of three studied $R_2Fe_3Si_5$ sillicidies are almost identical, existing in four bands and containing both electronlike and holelike sheets. This fact supports their multi-band superconductivity as concluded earlier from various kinds of measurements [3]. Contrary to quasi-2D cylindrical FS sheets, occurring in high-T_{SC} iron- or nickel-based 1111 and 122 families, the FS sheets of the considered here 235 systems have rather a 3D character. In $Ce_2Ni_3Ge_5$ the revealed FS nesting features can be responsible for a presence of antiferromagnetic spin fluctuations which may act as a pairing mechanism in this pressure-induced superconductor [4].

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[1] M. Samsel-Czeka?a, M.J. Winiarski, Intermetallics **20**, 63 (2012); PRB, submitted.
[2] FPLO9.00-34; www.FPLO.de.
[3] Y. Nakajima et al., PRL **100**, 157001 (2008); R.T. Gordon et al., PRB **78**, 024514 (2008); A.E. Karkin et al., PRB **84**, 054541 (2011).
[4] M. Nakashima et al., J. Phys. CM **17**, 4539 (2005).

Poster B16

Surface-sensitive time-resolved optical spectroscopy

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Pump-probe technique is relevant for the investigation of many ultrafast processes on the time scale of ps and fs, e.g., the ultrafast charge- and energy-transfer in single nanoparticles, the complex electron dynamics in strongly-correlated materials and the dynamics of molecules and more complex biological systems during chemical reactions (femtochemistry). However, the investigation of most of the chemical reactions and biological or physical processes, that are confined to the vicinity of surfaces, is prevented by the lack of suitable time-resolved techniques with surface sensitivity. In this work we realized a surface-sensitive time-resolveld optical setup with the aim of measuring the molecular ps relaxation dynamics during the kinetics of the formation of complex structures. The high surface-sensitivity is achieved by exploiting the evanescent wave generated on the surface of a fused silica prism in the total internal reflection configuration. To perform measurements with a very short acquisition time we used an asincronous optical sampling (ASOPS) technique. We validated our setup on a gold film of 4 nm obtaining a surface-sensitivity 1 order of magnitude larger than in convention setups. Furthermore, this technique paves the way to the investigation of complex solid-state materials (e.g., 2 dimensional electron gas at oxide interfaces, topological insulators) exhibiting exotic electronic properties at the surface.

Poster B17

The lattice Kondo effect - a fabric for superconducting correlations?

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Although the simple Kondo lattice model constitutes one of the paradigms for understanding the physics of heavy-fermion materials, a reliable theoretical investigation of superconductivity in this model is still lacking. We present results based on the dynamical mean-field approximation in combination with the numerical renormalization group as impurity solver. While superconducting order is commonly not expected for a correlated lattice model without additional bosonic degrees of freedom, we observe strong superconducting order in the plain Kondo lattice model away from half filling. The possible origin of this superconducting order is discussed in view of the frequency dependence of the order parameter. In addition, close to half filling we find this ordered phase to appear most pronounced in the vicinity of the antiferromagnetic quantum critical point. Since a characterization of quantum criticality within dynamical mean-field theory is not possible, we rather discuss questions of principle such as the actual nature of the ordered states, that is, local moment or heavy-fermion physics. The latter issue is of considerable interest addressing the question whether the ordered states stay in direct competition or even cooperate with the coherent Kondo effect in the lattice.