Book of Abstracts

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First order character and observable signatures of topological quantum phase transitions

Topological quantum phase transitions are characterized by changes in global topological invariants beyond the paradigm of spontaneous symmetry breaking. For non-interacting electrons, such transitions are continuous and always accompanied by a gap-closing in the energy spectrum. Here, we demonstrate that sufficiently strong electron-electron interaction can fundamentally change the situation: we discover a topological quantum phase transition of first order character in the genuine thermodynamic sense, which occurs without gap closing. Our theoretical study reveals the existence of a quantum critical endpoint associated with an orbital instability on the transition line between a 2D topological insulator and a trivial band insulator. Remarkably, this phenomenon entails unambiguous signatures associated to the orbital occupations that can be detected experimentally.

Edoardo Baldini

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Evidence for Pre-Formed Cooper Pairs in the Pseudogap Phase of Slightly Underdoped NdBa2Cu3O6+x

In the last years, ultrafast experiments have contributed to shed new light on high-temperature superconductivity. In particular, tailored excitation in the mid-infrared spectral range was demonstrated to suppress competing structural and electronic orders and to promote a highly coherent state in several underdoped cuprates [1 - 4]. In YBa2Cu3O6+x this transient state was found to persist up to room temperature, evidenced by the enhancement of the superfluid strength in the THz response. The question whether the high coherence is the signature of a perfect conducting or of an exotic superconducting state at nonequilibrium still remains open. Here, we address this problem from a spectroscopic point of view, by investigating a slightly underdoped sample of NdBa2Cu3O6+x through ultrafast spectroscopy in the optical regime. The use of a broadband detection scheme enables us to reveal evidence for quasiparticle (QP) excitation in a wide range of temperatures up to the pseudogap temperature scale T*. The existence of a QP spectral signature in the pseudogap phase, together with its peculiar temporal evolution and temperature dependence, can be directly related to the presence of a pairing gap for QP excitation. This observation leads to the hypothesis that the selective melting of a competing order using intense resonant mid-infrared pulses can establish coherence in pre-formed Cooper pairs underlying the pseudogap phase [5].

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Neven Barišić

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Evidence for good metal behavior in normal state of the cuprate high-temperature superconductors

The superconducting state of the cuprates evolves upon cooling from an enigmatic metallic phase that is characterized near optimal hole doping by a planar resistivity with large magnitude and extended linear temperature dependence. Below optimal doping, at temperatures below T^*, there exists an intermediate pseudogap phase with a partially gapped Fermi surface. These unusual properties have motivated proposals to consider unconventional electronic scattering mechanisms and even to abandon the Landau quasiparticle paradigm entirely.

$HgBa_2CuO_{4+\delta}$(Hg1201) may be viewed a model cuprate system due to its relative structural simplicity, minimal disorder effects, and large optimal T_c of nearly 100 K (1). We have found that the planar resistivity of Hg1201 exhibits quadratic temperature dependence, the behavior characteristic of a Fermi liquid, at temperatures below T^{**} ($T^{**} < T^*$) (2). This result motivated optical conductivity measurements that yielded the quadratic frequency dependence and the temperature-frequency scaling of the optical scattering rate expected for a Fermi liquid (3). Furthermore, we demonstrated for Hg1201 (and for $YBa_2Cu_3O_{6+\delta}$) that the magnetoresistance obeys Kohler's rule at temperatures below T^{**} (4). By combining our dc resistivity results for Hg1201 with published data for three structurally more complex cuprates, we obtained the universal sheet resistance throughout most of the temperature-doping phase diagram and arrived at the unexpected conclusion that Fermi-liquid behavior extends to very low doping, close to the Mott-insulating state (2). In contrast to previous approaches that extended ideas developed for the strange metal phase ($T > T^*$) to the pseudogap phase ($T < T^*$), we will discuss the former in the context of the now well-documented pseudogap Fermi-liquid state. A combined analysis of the planar dc-resistivity and Hall-effect measurements demonstrate that the transport scattering rate remains quadratic in temperature across T^{**} and T^*, and moreover doping and compound independent. This universal behavior implies an underlying conventional scattering mechanism throughout the entire phase diagram [5].

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Alice Cantaluppi

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Stimulated superconducting-like properties in K3C60 far above the equilibrium critical temperature

In conventional BCS superconductors, the electron pairing is mediated by the exchange of lattice phonons. Molecular superconductors are peculiar because the coupling of electrons is mediated by intramolecular vibrations with characteristic energies of of tens to hundreds meV. [1] The present experiment is strongly suggestive of a new type of superconductivity that is directly stimulated [3] by the laser field and indicates highly novel emergent physics away from equilibrium.

Alberto Crepaldi

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Optical control of the electronic properties of $ZrTe_5$

Transition metal pentatelluride, $ZrTe_5$, displays a rich set of unique and exotic transport properties. An anomalous peak in resistivity at T^* 160 K [1] is accompanied by the charge carrier switch from holes ($T > T^*$) to electrons ($T < T^*$) [2]. Moreover ZrTe5 exhibits a superconducting state under pressure [3], spin helical surface states have been predicted [4] and magneto-resistance has been reported with both positive [5] and negative sign, thus suggesting the presence of chiral magnetic effect, possible in the case of 3D Dirac semimetal [6]. In this light, we have performed a comprehensive investigation of both the occupied and unoccupied electronic states of $ZrTe_5$ by combining Angle Resolved Photoemission Spectroscopy (ARPES) and time resolved ARPES (tr-ARPES). The dependence of the electronic band structure with temperature has been studied, in order to understand the mechanism at the base of the anomalous resistivity peak. Having clarified the origin of the unique transport properties of $ZrTe_5$, we have experimentally proven the possibility to optically control, at the ultrashort time scale, both the energy position and the electron scattering rate of the bands.

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Eduardo da Silva Neto

University of British Columbia

Charge ordering in hole and electron-doped cuprates

In cuprate high-temperature superconductors, an antiferromagnetic Mott insulating state can be destabilized toward unconventional superconductivity by either hole or electron doping. Besides these two phases, a charge ordering (CO) instability was recently detected in the Y-cuprates [1,2], which echoed the long-known presence of stripe order in the La-based cuprates [3,4]. However, at that point, the universality of the CO to the cuprates and its connection to other phenomena in the cuprate phase diagram (e.g. pseudogap and antiferromagnetism) remained to be determined.

In this talk I will discuss a combined scanning tunneling microscopy (STM) and resonant x-ray scattering (RXS) experimental approach that established the formation of CO in the high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212) [5]. The CO in this system occurs with the same period as those found in Y-based or La-based cuprates and displays the analogous competition with superconductivity – therefore showing its universality to hole-doped cuprates [5-7]. Doping- and temperature-dependent measurements of the CO fingerprints in RXS and in spectroscopic imaging STM in will be used to discuss its phenomenological relationship to pseudogap and Mott physics. Still, if this unusual CO is truly a phenomenon stemming from the doping of a Mott insulator, the lack of evidence for CO in the electron-doped materials remained a puzzle. Here I will also discuss recent RXS measurements that demonstrate the presence of a similar CO in the electron-doped (n-type) cuprate $Nd_{2-x}Ce_xCuO_4$ (NCCO) [8]. In contrast to the hole-doped materials, the CO onset in NCCO is higher than the pseudogap temperature, and is actually in the same temperature range where antiferromagnetic fluctuations are first detected – thereby showing that CO and antiferromagnetic fluctuations are likely coupled in electron-doped cuprates. Beyond the already published results, a comprehensive RXS doping-dependent study of NCCO allows us to further probe the relationship between CO and the ARPES measured Fermi surface [9].

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Alberto de la Torre

University of Geneva

Emergence of a nodal liquid in the pseudospin-1/2 antiferromagnet Sr2IrO4 from ARPES

The insulating ground state of the layered perovskite iridates is often described in a single band Jeff=1/2 Hubbard model [1,2]. Iridates were thus proposed as analogues to the cuprates and as such, a potential platform for engineering high-temperature superconductivity under electron doping [2]. However, it proved difficult to dope iridates in the bulk and to date little is known about the evolution of their electronic structure with increasing carrier concentration. Here we report the successful growth of La doped single crystals of Sr2IrO4. Angle resolved photoemission measurements on single layer (Sr(1-x)Lax)2IrO4 show a collapse of the Mott gap for x > 0.06. At the highest doping level of x=0.1, quasiparticle like excitations forming a large circular Fermi surface centered at Gamma emerge. As in cuprates, we find a strongly anisotropic quasiparticle residue and a momentum dependent pseudogap that increases in magnitude towards the antinode resulting in a Fermi arc-like contour. However, our data show significant weight on the backside of the arcs, which we attribute to backfolding due to the structural distortion of the IrO2 plane. We conclude that lightly doped Sr2IrO4 does indeed share much of the electronic structure phenomenology with cuprates and that anisotropic pseudogaps are a generic property of two-dimensional doped Mott insulators rather than a unique hallmark of cuprate high temperature superconductivity.

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Tadeusz Domanski

Marie Curie Sklodowska University, Poland

Superconductivity in nanoscopic systems

Superconducting state (manifested by dissipationless charge transport and ideal diamagnetism) has been so far observed in various bulk materials driven by the pairing mechanisms related to phonons, magnons or other 'gluing' particles. Recently there have been intensive attempts to obtain similar superconducting state in the ultra-small (nanoscopic) objects such as molecules, nanowires or other kinds of the 'quantum dots' via the proximity effect. Thus induced electron pairing can lead to a number of very spectacular effects. For instance it can: 1) invert direction of the Josephson current (0-π transition), 2) produce the spatially entangled charge carries (using the Cooper pair splitters), 3) generate the exotic Majorana or Weyl-type quasiparticles, 4) enable a changeover from the positive to negative resistance/conductance (in multitermina junctions) and

plethora of other fantastic phenomena. I shall give a brief overlook of these phenomena, with an emhasis on their potential future applications.

Claudia Giuseppina Fatuzzo
EPFL

Spin-orbit-induced orbital excitations in Sr2RuO4 and Ca2RuO4: a resonant inelastic X-ray scattering study

Ruthenate-oxide materials attract much attention due to the interesting ground states they exhibit, such as unconventional superconductivity in Sr2RuO4 or Mott physics in Ca2RuO4. The role of electron correlations, Hund's coupling and spin-orbit interactions is still being debated and explored [1,2]. In this talk [3] we present a study on the Ru 4d-orbital occupation and excitations in (Ca/Sr)2RuO4, performed through a combination of X-ray Absorption Spectroscopy (XAS) and high resolution oxygen K-edge Resonant Inelastic X-ray Spectroscopy (RIXS). The ruthenium 4d orbital occupation and excitations were probed through their hybridization with the oxygen p-orbitals. A minimal model, taking into account crystal field splitting and spin-orbit coupling, is presented to account for the observations. Implications on electronic structure, Mott physics and superconductivity are discussed.

Katharina J. Franke
Freie Universität Berlin

Electron transport through Shiba states induced by magnetic adsorbates on a superconductor

Magnetic adsorbates on a superconductor create a magnetic scattering potential for the quasiparticles of the superconductor. A single spin gives rise to so-called Shiba states. These can be observed in scanning tunneling spectroscopy (STS) as a pair of resonances at positive and negative bias voltages in the superconducting gap. The energetic position inside the gap reflects the magnetic coupling strength, whereas the intensity has been interpreted in terms of a density of states. Here, we investigate Manganese (Mn) atoms and Mn-phthalocyanine (MnPc) molecules deposited on a Pb(111) surface. In both cases, we resolve multiple Shiba states inside the gap. The Mn atoms present a stable tunneling junction over several orders of magnitude in conductance [1]. We observe two different transport regimes: at large tip-sample distance, the tunneling current is dominated by single-electron processes. However, these require the relaxation of electrons/holes from the Shiba states into the superconductor. At small tip- sample distance, the relaxation processes are not fast enough for an efficient depopulation of the states, and thus Andreev processes become important, which resonantly transfer a Cooper pair into the superconductor. MnPc molecules adsorb in a variety of different adsorption sites with different

magnetic coupling strengths on a Pb(111) surface. This is reflected by the energetic position of the Shiba states inside the gap [2]. At 1.2 K, we resolve a characteristic splitting of the Shiba states, which is present throughout a wide range of coupling strengths. We explain this splitting as a result of magnetic anisotropy, which has been theoretically predicted [3].

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Philipp Hansmann

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Electronic interactions in effective cuprate models beyond a Cu Hubbard U

Current theoretical studies of electronic correlations in transition metal oxides typically only account for the local repulsion (Hubbard U) between d-electrons even if oxygen ligand p-states are an explicit part of the effective Hamiltonian. Interatomic interactions such as Upd between d- and (ligand) p-electrons, as well as the local interaction between p-electrons, are neglected. Often, the relative experimentally obtained information. By applying the merger of local density approximation and dynamical mean field theory to the prototypical case of the three-band Emery dp model for the cuprates, we demonstrate that, without any 'ad hoc' adjustment of the orbital splitting, the charge transfer insulating state is stabilized by the interatomic interaction Upd. Our study hence shows how to improve realistic material calculations that explicitly include the p-orbitals.

F. Hardy

Karlsruhe Institute of Technology

Strong correlations and new magnetic phases in $Ba_{1-x}K_xFe_2As_2$ and $Ba_{1-x}Na_xFe_2As_2$ iron pnictides

High-Tc superconductivity in the cuprates occurs at the crossover from a correlated Mott insulating state to a weaker correlated Fermi liquid as a function of doping. The Fe-pnictides were initially thought to be weakly correlated. However, we have recently shown that KFe_2As_2 is in fact a highly correlated metal and that these correlations are even further enhanced in Rb- and $CsFe_2As_2$. Whereas the correlations in the cuprates result from a large value of the Hubbard U, recent works have stressed the particular relevance of Hund's coupling J in the pnictides.

Our data may be interpreted in terms of a close proximity to an orbital-selective Mott transition. We now have good thermodynamic data covering

both the hole and electron doping sides of the $BaFe_2As_2$ system and we will discuss how these correlations are modified by doping. We have also re-examined in greater detail the underdoped region of $Ba_{1-x}K_xFe_2As_2$ and $Ba_{1-x}Na_xFe_2As_2$. We find a small region of C4 symmetry inside the SDW state of $Ba_{1-x}K_xFe_2As_2$, similar to that of $Ba_{1-x}Na_xFe_2As_2$, followed by a reentrance to the C2 phase. In $Ba_{1-x}Na_xFe_2As_2$, this rentrance is absent and the phase diagram is shown to be considerably more complex than previously reported. Differences and similarities between the $Ba_{1-x}Na_xFe_2As_2$ and $Ba_{1-x}K_xFe_2As_2$- systems will be discussed and we will show how these new phases interact with superconductivity.

Rainer Härtle

Institut für theoretische Physik, Georg-August-Universität Göttingen, Germany

Hierarchical quantum master equations and driven long-term impurity dynamics

The hierarchical quantum master equation technique is a promising method to describe nonequilibrium impurity problems. It employs a hybridization expansion of the time evolution of the impurities density matrix from a product initial state. Using an advanced and systematic truncation scheme, convergence can be achieved if the temperature of the environment is not too low. Thus, numerically exact results can be obtained. This is corroborated by a direct comparison with the continuous-time quantum Monte Carlo approach. In particular, the nonequilibrium dynamics of interacting quantum dot systems is studied that can be described by Anderson impurity models. The focus is on effects and phenomena that emerge on long time scales such as, for example, the steady-state magnetization or the complex build-up of coherences.

Andreas Hausoel

University of Wuerzburg

Ab-initio study of the finite temperature magnetism in iron and nickel

The calculation of the ferromagnetic transition temperature of itinerant ferromagnets like iron and nickel has been a very hard problem for theory ever since. This is due to the interplay between strong local interactions and the itinerant character of the electrons. Here we show fully ab-initio DFT+DMFT calculations for bcc-iron and fcc-nickel, using the numerically exact Continuous Time Quantum Monte Carlo method in hybridization expansion. We consider the full cubic Coulomb interaction from cRPA and discuss the effects of different commonly used approximations, i.e. density-density and Slater-Kanamori. Besides interaction-dependent ab-initio estimates of the transition temperatures of iron and nickel we also discuss their magnetism at the 2-particle level.

Aldo Isidori

Royal Holloway University of London

Coexisting electronic orders in the ultra-quantum limit of graphite

Semimetals like graphite have recently received compelling interest as they not only are able to host topologically non-trivial phases but also can be driven into the ultra-quantum limit by magnetic fields now achievable in modern-day laboratories. Thus, they provide insight into quantum-Hall physics and the physics of massless Dirac fermions in three dimensions. They also represent ideal model systems for studying magnetic-field driven density wave instabilities, as the onset field for such collective excitations is suppressed in semimetals. Using pulsed high-magnetic fields up to 60 T applied to a single crystal of natural Tanzanian graphite, we find a series of field-induced phase transitions into collinear charge-density wave states resulting from enhanced interactions between the lowest four Landau levels. By analysing magneto-transport data and calculating the renormalized Landau level structure at high fields, we establish the phase diagram of graphite in its ultra-quantum limit. Our results imply the existence of a topologically-protected chiral edge state at high fields supporting both charge and spin currents.

Michael Karolak

University of Wuerzburg

Tunable Kondo effect of Pc Molecules on noble metal surfaces

We present a detailed investigation of spectroscopic features located at the central metal ion of a Pc molecule on a noble metal surface (Ag(001)). STS data taken close to the Fermi level reveal an asymmetric feature that cannot be fit with a single Fano function representing a one-channel Kondo effect. Instead, our data indicate the existence of a second superimposed feature. Two potential physical origins, a second Kondo channel related to the dxz/yz -orbitals, and a spectral feature of the dz2 -orbital itself, are discussed. A systematic experimental and theoretical comparison of MnPc with CoPc and FePc indicates that the second feature observed on MnPc is caused by the dz2-orbital. This conclusion is corroborated by STM- induced dehydrogenation experiments on FePc and MnPc which in both cases result in a gradual shift towards more positive binding energies and a narrowing of the Kondo resonance. Theoretical analysis, using a combination of DFT with an Anderson Impurity Model, reveals that the latter is caused by the reduced hybridization between the d-orbital and the substrate. Thus, Pc-Molecules on noble metal surfaces are a perfect playground for the study and manipulation of parameters governing the physics of the Kondo effect in both theory and experiment.

Dante Kennes

RWTH Aachen

Dynamics in dissipative quantum systems

Coherence is an integral part of quantum mechanics giving rise to many fascinating effects in mesoscopic systems. Perfect coherence however is usually not encountered in any realistic setup as coupling to the environment introduces decoherence effects, or dissipation. How coherence and decoherence do interplay thus poses an particularly interesting question. One of the most prominent prototype models for quantum dissipative dynamics is the so called spin-boson model, which has been studied intensively throughout the last decades. It features quite rich physics depending on the parameter regime under consideration. In this talk we will (a) report on some recent progress in understanding the transition from coherent (damped oscillatory) to decoherent (monotonic) transient dynamics in the spin-boson model by usage of two complimentary renormalization group schemes and (b) present results on quantum quenches and the influence of (markovian) memory, onto the dynamics found in this model.

Jelena Klinovaja

University of Basel

Engineering Topological Quantum States: From 1D to 2D

I will present results on exotic bound states in one-dimensional (Majorana fermions and parafermions) and two-dimensional (edge states in topological insulators) condensed matter systems that have attracted wide attention due to their promise of non-Abelian statistics believed to be useful for topological quantum computing. I discuss systems in which topological properties could be engineered per demand. For example, Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. Here, I will discuss candidate materials such as semiconducting nanowires [1-2], graphene nanoribbons [3], atomic magnetic chains or magnetic semiconductors [4]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [5,6]. In the second part of my talk, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [6-8], where interaction effects in the wires can be treated non-perturbatively via bosonization. I will demonstrate that such systems can exhibit the integer or fractional quantum Hall effect [6], spin Hall effect [7], and anomalous Hall effect [8]. In the fractional regimes, the quasiparticles have fractional charges and non-trivial Abelian braid statistics.

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Igor Kuzmenko

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Carbon Nanotube Quantum Dot: Realization of Two-Channel Kondo Effect

We consider Kondo tunneling through a junction composed of two semi-infinite carbon nanotubes (CNT) that serve as left and right leads (CNTL and CNTR, respectively) attached on both sides of a short CNT quantum dot with an atom A having an s-wave valence electron of spin 1/2 implanted on its axis (CNTQDA). The two wave numbers (valleys) K and K′ (located on the two corners of the hexagonal Brillouin zone of the CNT) serve as two symmetry protected flavor quantum numbers. The CNTQDA is gated such that its (neutral) ground state consists of the caged atom with spin up or down while its lowest excited (charged) states are singlet and triplet states. The energy of the singlet state is above the energy of the triplet state. The Anderson model hybridizes lead and dot electrons with the same flavor and spin projection, and the Schrieffer-Wolf transformation, while mixing spin projections does not mix flavors, thereby realizing a two-channel Kondo physics. Perturbative renormalization group analysis exposes a finite weak-coupling two-channel fixed point, where the Kondo temperature is estimated as 0.5 - 5 K.

Nenad Lazarevic

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Vacancies and phase separation in pure and transitional metal doped $K_xFe_{2-y}Se_2$: The Raman scattering study

Understanding the origin and mechanism of superconductivity in iron-based materials pose one of the main challenges in the condensed matter physics today. The presence of vacancies and intrinsic phase separation in alkali-doped iron-selenides make these questions even more challenging. We present the results of a comprehensive polarization and temperature dependent Raman scat-

tering study of pure and transitional metals (Co and Ni) doped $K_xFe_{2-y}Se_2$. The Raman modes, originating from both the high symmetry (superconducting) and low symmetry (antiferromagnetic) domains, have been identified. By analysing these modes we were able to follow the phase separation evolution throughout the series in the full doping range. Rather low intrinsic linewidth for the high symmetry Raman modes in $K_xFe_{2-y}Se_2$ indicates the absence of vacancies in these domains. On the other hand, in both $K_xCo_{2-y}Se_2$ and $K_xNi_{2-y}Se_2$ analysis of Raman modes intrinsic linewidth and the lineshape revealed the presence of disordered vacancies in the high symmetry phase. The $K_xFe_{2-y}Se_2$ temperature dependent Raman scattering study revealed the sudden change of the A_{1g} mode energy near superconducting transition temperature due to the rearrangement of the electronic states. The phonon modes renormalization due to the electron-phonon and spin-phonon interactions at Curie temperature in $K_xCo_{2-y}Se_2$ have also been discussed.

Natalia Lera

CIC nanoGUNE, 20018 Donostia-San Sebastian, Spain and Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Madrid 28049, Spain

Superconductivity from the unconventional metallic state of $Li_{0.9}Mo_6O_{17}$

Superconductivity in the quasi-one-dimensional material $Li_{0.9}Mo_6O_{17}$ is analyzed based on a multiorbital extended Hubbard model. Superconductivity is found near charge order transitions for different couplings. The order parameter is a p-wave with nodes in the Fermi surface. The metallic state displays a characteristic charge collective mode with spectral weight in two different momentum $\mathbf{Q_1}$ and $\mathbf{Q_2}$. Within this model, strong charge fluctuations at $\mathbf{Q_1}$ drives the system into the superconducting phase in the triplet channel in $Li_{0.9}Mo_6O_{17}$. We found a region of coexistence between charge order at $\mathbf{Q_2}$ and superconductivity in $p-$wave channel.

Tobias Meng

TU Dresden

Quantum LEGO: from quantum wires to three-dimensional topological phases

While the understanding of fractionalized topological phases has impressively developed in two dimensions (2D), much less is known in three dimensions (3D). In this talk, I present a 3D system of coupled quantum wires that exhibits fractional topological phases composed of closed loops and open planes of two-dimensional fractional quantum Hall subsystems, and discuss that the coupled-wire approach provides a new, and powerful tool for the analysis of interacting topological physics in 3D.

In the array of wires considered in this talk, the coupled wire approach

allows to identify the protected edge states associated with the topologically non-trivial bulk gapped phases. It also shows that these phases are separated by exotic quantum phase transitions corresponding to a rearrangement of fractional quantum Hall edge modes. Also an extended exotic critical phase may exist. Without electron-electron interactions, similar but unfractionalized bulk gapped phases based on coupled integer quantum Hall states exist. They are separated by an extended critical Weyl semimetal phase.

Michael Mulligan

Stanford University

A 2D Metallic Phase at Half-Filling

Composite fermions provide a fruitful intuitive picture for much of the physics that occurs in the 2D electron gas. Gapped fractional quantum Hall states are viewed as instabilities of a gapless non-Fermi liquid parent state in which an electron is replaced by a composite fermion that strongly interacts with an emergent Chern-Simons gauge field. In other words, exotic electronic states are traded for "conventional" orderings of the composite fermion. This behavior is analogous to other strongly correlated materials in which unconventional order emerges from a novel parent state. Remarkably, while the gapless composite (non-)Fermi liquid state has only short-ranged single-electron correlations, it exhibits Friedel-like oscillations and a logarithmic violation of the entanglement entropy area law indicative of a Fermi surface of neutral composite fermions.

Much remains to be understood about this composite (non-)Fermi liquid parent state, despite a great deal of both experimental and theoretical work. For instance: what is the character of the composite fermion effective mass; what is the correct charge assignment of the composite fermion quasiparticle excitations; what is the nature and explanation of the crossover from weak anti-localization observed in some materials to linear in temperature resistivity behavior; does the composite (non-)Fermi liquid provide an example a state that is gapless, but continues to exhibit a type of topological order? In this talk, I will describe a new theoretical approach to the characterization of this state in which we approach the isotropic 2D limit via a collection of interacting 1D quantum wires arranged on the plane. This provides a controlled, albeit anisotropic, starting point to describe the 2D non-Fermi liquid physics. I will provide numerical evidence of the formation of the composite (non-)Fermi liquid state within the wire construction through density matrix renormalization group studies and variational Monte Carlo, along with an analytical understanding of these results.

Yusuke Nomura

Centre de Physique Théorique (CPHT) École Polytechnique

Fully ab-initio calculation of transition temperature for alkali-doped fullerene superconductors

The alkali-doped fullerides (A3C60, A = K, Rb, Cs) show the highest superconducting transition temperature (Tc) among the molecular solids. The existence of a Mott-insulating phase next to an s-wave superconducting phase is surprising since the s-wave superconductivity is believed to be severely suppressed by the strong correlations. The Mott phase is a low-spin state characterized by dynamical Jahn-Teller effect, indicating a nontrivial interplay between strong correlations and phonons [1].

In the present study, we perform fully ab initio studies for fullerides [2,3]. We apply a recently-formulated downfolding scheme [4] to fcc A3C60 systems and construct realistic low-energy models including phonon degrees of freedom. We find that the alkali-doped fullerides are unique strongly-correlated systems with effectively negative exchange interactions: The usual Hund's rule is inverted because of the Jahn-Teller phonons.

This work is done in collaboration with S. Sakai, M. Capone, and R. Arita.

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Petra Pudleiner

Johannes Gutenberg-University, Mainz

Momentum-space structure of the self-energy in the two-dimensional Hubbard model

Strongly correlated systems exhibit a wide range of interesting properties (such as Mott metal-insulator transition or superconductivity). As the self-energy maps noninteracting onto interacting Green functions, it necessarily encodes all such phenomena. We compute the self-energy in the half-filled Hubbard model on a square lattice using quantum Monte Carlo and analytic continuation techniques. We find (i) a quite strong momentum dependence and (ii) a very peculiar structure, not previously seen in literature: Except for pseudogap features right at the Fermi edge, the self-energy can be parametrized via the noninteracting dispersion $\epsilon_{\mathbf{k}}$, i.e., it can be written as $\Sigma(\epsilon, \omega)$, with two energy-like parameters. In my talk, I will also link our work to a recent study of the structure of the self-energy in three dimensions [Schäfer et al., Phys. Rev. B 91, 121107 (2015)] and discuss the impact of anisotropy and doping.

Jonathan Rameau

Brookhaven National Lab

Ultrafast Self Energy Dynamics via Time Resolved Photoemission in the Cuprates

One of the more notable contributions of angle resolved photoemission spectroscopy (ARPES) to the study of correlated electron materials has been the identification of electron mass enhancements, or dispersion particle self energy. The identification of several such features in the electronic spectra of cuprate high T_c superconductors and their likely reflection of the pairing mechanism responsible for the high T_c phenomenon has led to intense debate about their origin. The recent introduction of non-equilibrium degrees of freedom to the problem in the form of time resolved ARPES (trARPES) has added renewed vigor, and qualitatively new information, to efforts aimed at resolving this long-standing problem. In my talk I will discuss the results of a series of trARPES experiments examining the physics of the famous 70 meV nodal kink in the normal state of optimally doped and underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$. In particular part of the photoelectron spectrum. I will also discuss more recent developments in examining the imprint of kink physics on the unoccupied part of the photoexcited spectrum and how, in conjunction with cutting edge theoretical modeling, these effects can be related to the equilibrium self energy. Finally, I will show how, by summarizing our understanding of both sets of experimental results within a single theoretical framework, we are able to arrive at a below T_c and make some statements about how this impacts our understanding of high T_c superconductivity in these materials.

Tobias Ritschel

Leibniz Institute for Solid State and Materials Research IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

Electronic self-organization in layered transition metal dichalcogenides

We present a study of the charge density wave order in the prototypical material 1T-TaS2 which combines density-functional theory, x-ray diffraction and angle-resolved photoemission spectroscopy. Most importantly, this study reveals a remarkable and surprising feature of charge density waves, namely their intimate relation to orbital order. We not only show that the charge density wave within the 2D TaS2-layers involves previously unidentified orbital textures of great complexity. We also demonstrate, by considering the 3D character of the charge density wave, that two metastable stackings of the orbitally ordered layers allow to manipulate salient features of the electronic structure. Indeed, these orbital effects provide a route to switch the properties on 1T-TaS2 nanostructures from metallic to semiconducting with technologically pertinent gaps of the order of 200 meV. Furthermore, our results indicate that the previous paradigm of a Mott-gap in this system needs to be reconsidered. Instead we find firm evidence that the corresponding gap is predominantly due to the

hybridization between the orbitally ordered TaS2-layers. We discuss our results in relation to recent time-resolved experiments.

Thomas Schaefer

Institute of Solid State Physics, TU Wien

Fluctuation diagnostics of the electron self-energy: Origin of the pseudogap physics

We demonstrate how to identify which physical processes dominate the low-energy spectral functions of correlated electron systems. We obtain an unambiguous classification through an analysis of the equation of motion for the electron self-energy in its charge, spin and particle-particle representations. Our procedure is then employed to clarify the controversial physics responsible for the appearance of the pseudogap in correlated systems. We illustrate our method by examining the attractive and repulsive Hubbard model in two dimensions. In the latter, spin fluctuations are identified as the origin of the pseudogap, and we also explain why d-wave pairing fluctuations play a marginal role in suppressing the low-energy spectral weight, independent of their actual strength.

Phys. Rev. Lett. 2015 (in press)

Michael Sentef

Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

Theory of laser-driven nonequilibrium superconductivity

The study of the real-time dynamics dynamics of solids perturbed by short laser pulses is an intriguing opportunity of ultrafast materials science. Previous theoretical work on pump-probe photoemission spectroscopy revealed spectroscopic signatures of electron-boson coupling [1, 2], which are reminiscent of features observed in recent pump-probe photoemission experiments on cuprate superconductors [3, 4]. Here we investigate the ordered state of electron-boson mediated superconductors subject to laser driving [5, 6] using Migdal-Eliashberg theory on the Kadanoff-Baym-Keldysh contour. We extract the characteristic time scales on which the non-equilibrium superconductor reacts to the perturbation, and their relation to the coupling boson and the underlying order.

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Priyanka Seth

Ecole Polytechnique, France

Advances in ab-initio DFT+DMFT treatment of strongly-correlated systems

The application of DFT+DMFT to strongly-correlated systems has given us much insight into the physics of such materials. However, there remain materials for which a fully ab-initio treatment continues to be a challenge. I will describe advances on this front in two separate issues. First, I will present a new scheme to compute interaction parameters for low-energy models that take into account inter-shell interactions. Secondly, I discuss algorithmic advances in continuous-time hybridization expansion impurity solvers that make hitherto impossible calculations now tractable. Finally, I will present results showcasing the improvements for both d- and f- electron systems.

Giovanni Sordi

Royal Halloway University of London

Remnant of the first-order Mott transition at finite doping as an organizing principle for strongly correlated superconductors

An intricate interplay between superconductivity, pseudogap and Mott transition occurs in cuprates. In this talk, I compare experiment with theoretical results obtained from extensions of dynamical mean-field theory for the two-dimensional Hubbard model. In the normal state, at finite doping, a first-order transition between a metal and a pseudogap phase ends at a critical point. In the supercritical region, a Widom line and its precursor determine the crossovers seen experimentally. We demonstrate that much of the phase diagram, including superconductivity, is controlled by this first-order transition, a finite-doping signature of the Mott transition.

Damien Stricker

University of Geneva

Fermi liquid behaviour in strongly correlated metals

A reference point for research on a wider range of correlated behaviour is provided by the so-called Fermi liquids, characterized by a relaxation rate $(\hbar\omega)^2 + (p\pi k_B T)^2$. The theoretical prediction for the relaxation rate appearing in the optical conductivity is $p = 2$ when considering the experimentally most accessible range $\hbar\omega > k_B T$. A number of recent optical studies have addressed the issue of Fermi-liquid characteristics, reporting indeed ω^2 and T^2 for the optical scattering rate of a number of different materials. However, a perfect match to the prediction $p = 2$ has not been observed. One possible scenario that has been proposed to explain this discrepancy is the presence of magnetic impurities. In a recent study we have investigated Sr2RuO4, a ma-

terial which can be synthesized in very pure form, with well established T^2 resistivity below 25 K. Here we observe a perfect scaling collapse of $1/\tau$ as a function of $(\hbar\omega)^2 + (p\pi k_B T)^2$ for $\hbar\omega < 36meV$, and temperature below 40K, with $p = 2$. We also observe features in the spectrum at higher energy, which are manifestly beyond the Fermi-liquid model. The sign and size of these features agree quantitatively with the notion of resilient quasiparticles predicted by dynamical mean field theoretical calculations for this compound.

Maksym Surmach

Technische Universität Dresden

Superconducting properties and pseudogap from preformed Cooper pairs in the triclinic (CaFe(1-x)Pt(x)As)10Pt3As8

Using μSR, INS and NMR, we investigated the novel Fe-based superconductor with a triclinic crystal structure density from the μSR measurements indicates the presence of two superconducting gaps. Our INS data revealed commensurate spin fluctuations at the (π, 0) wave vector. Their intensity remains unchanged across Tc, indicating the absence of a spin resonance typical for many Fe-pnictides. Instead, we observed a peak around ω_0 = 7 meV at the same wave vector, which persists above Tc and is characterized by the ratio $\omega_0/k_B T_c \approx 6.2$, i.e. significantly higher than typical values for the magnetic resonant modes in iron pnictides (4.3). The T-dependence of magnetic disappearance of this new mode. A suppression of the spin-lattice

Agnese Tagliavini

Institut für Festkörperphysik, Technische Unviversität Wien

Critical analysis of the preformed pair physics: the attractive Hubbard model under a paring forcing field

The preformed pair physics often originates controversial interpretations, especially about its relation with pseudogap features in the spectral properties of correlated systems. In this work we aim at a fundamental understanding of the hallmarks, which can prove the presence or the absence of preformed pairs. To this aim, we have performed a dynamical mean field theory study of the attractive Hubbard model which allows for one of the cleanest, and not controversial, realization of a preformed pair phase, associated with a spectral pseudogap. From this perspective, the most interesting information is extracted by studying how the system reacts upon the application of an external pairing field. By comparing our dynamical mean field theory results to the ones obtained in opposite situation of the repulsive Hubbard model, and to corresponding analytical calculations for the non-interacting case, the atomic limits and the two sites model, we identify some characteristic features of the reaction of a preformed pair phase to the external field, appearing beyond the

linear response regime. Our findings provide a solid testbed for the interpretation of similar analyses performed for studying the d-wave preformed pairs of the doped Hubbard model in the framework of the (underdoped) cuprates, as well as of future experiments performed far away from the thermodynamic equilibrium.

Irakli Titvinidze

TU Graz

Non-equilibrium inhomogeneous DMFT for correlated Heterostructures

Due to the experimental progress made in different microscopically controlling quantum mechanical systems quantum many body systems out of equilibrium have recently attracted increasing interest.

In this talk we present new developments of a recently introduced [1] theoretical scheme to deal with correlated system out of equilibrium. This approach allows to efficiently investigate steady-state behavior of the system based upon dynamical-mean-field theory (DMFT) within the nonequilibrium (Keldysh) Green's functions formalism [2].

The main novelty of the method is in the solution of the impurity problem. Here the idea is that the baths coupled to the interacting impurity are replaced by a finite number of bath sites coupled to Markovian reservoirs [1, 3]. Up to now the method has been applied to a single correlated layer sandwiched between two metallic leads at different chemical potentials. Here we show how to extend it to more complex geometries to treat more physically relevant heterostructures. In articular we present results for the steady-state current, spectral function and self-energy. First, we will review the case of a single correlated layer and show the effect of the local Hubbard interaction and bias voltage for weak and the intermediate hybridization strength to the leads. Afterwards we present results for systems of particular interest, such as charge modulated super-lattices, modulated doping close to the Mott insulator, and resonance effects.

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Jan Tomczak

TU Wien

Separability of dynamical and non-local correlations in three dimensions

Several iconic phenomena in many-body physics –e.g., the Kondo effect & the Mott metal-insulator transition– can be described by local correlations. Yet, effects of non-local self-energies are ubiquitous in both, real materials and many-body models, and sometimes they can modify the physics even on the qualitative level. Going beyond dynamical mean-field theory in order to include a description of non-local correlations is however a generally formidable task. It is therefore paramount to gather as much as possible a priori knowledge of the analytical structure of the self-energy –such as limiting cases, asymptotics or sum-rules–to constrain a theoretical approach or reduce its complexity.

While second-order phase transitions always cause strong non-local fluctuations (evident in two-particle quantities), their effect on spectral (one-particle) properties crucially depends on the dimensionality. For the important case of three dimensions, we show that the electron self-energy is well separable into a local dynamical part and static non-local contributions. In particular, our non-perturbative many-body calculations for the three-dimensional Hubbard model at different fillings demonstrate that the quasi-particle weight remains essentially momentum independent, also in the presence of overall large non-local corrections to the self-energy. Relying on this insight into the structure of the self-energy, we propose a space-time-separated scheme for many-body perturbation theory that is up to ten times more efficient than current implementations. Besides these implications for state-of-the-art electronic structure schemes, our analysis might also provide guidance to the quest of going beyond them.

Krzysztof Wohlfeld

University of Warsaw

Is charge and spin degree of freedom effectively decoupled in the 2D Hubbard model?

One of the most interesting aspects of the 2D Hubbard model, the 'standard model' of the cuprate oxides' physics, is the strong coupling between electron's charge and spin degrees of freedom. This is perhaps best visible in the so-called spin polaron problem: a single hole doped into the antiferromagnetic ground state of the half-filled Hubbard model moves by coupling to the spin excitations and therefore forms a rather heavy quasiparticle – the spin polaron.

In this contribution I would like to challenge this old paradigm. Firstly, I will discuss the recent experimental results which show that the high energy spin excitations in the cuprates are very weakly affected by doping. While this counterintuitive result stays in contrast with the idea of strong coupling between doped carriers and spin excitations, the apparent paradox is resolved by invoking the frequently forgotten 'three-site terms' which allow for the effec-

tively free motion of holes doped into the antiferromagnet [1]. Secondly, I will argue that these three-site terms are responsible for the onset of the most dispersive and (to a large extent) also most intensive feature of the spectral function of the Hubbard model [2]. Finally, I will discuss the implications of these results on the understanding of the unconventional superconductivity of the cuprates.

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Posters

Mark Barber

University of St. Andrews

Effect of Uniaxial Strain on the Quantum Critical Phase of $Sr_3Ru_2O_7$

$Sr_3Ru_2O_7$ has a metamagnetic quantum critical endpoint, which in highly pure samples is masked by a novel phase. This phase is isotropic in the absence of symmetry-breaking fields, but weak in-plane magnetic fields are well-known to induce strong resistive anisotropy, leading to speculation that the phase intrinsically breaks the tetragonal symmetry of the lattice. Here I will show results from a new uniaxial strain technique, capable of applying both compressive and tensile strain. We find a dramatic response: compression by 0.1%, for example, induces a resistive anisotropy of 2.5. We argue that the overall behaviour can be most easily explained by microscopic coexistence of orthogonal density waves, that are only weakly stabilised and hence highly susceptible to perturbation.

Krzysztof Bieniasz

Jagiellonian University

Green's Functions and Orbital Polarons in $KCuF_3$

Hole doping of a Mott or charge-transfer insulator with ground state magnetic and orbital order [1] poses numerous challenging questions. We present a variational calculation of the spectral properties of a single charge doped at the Cu(3d) sites of the Cu-F plane in $KCuF_3$. A superexchange model, designed to represent the physics behind $KCuF_3$, describing interacting $S = 1/2$ spin and eg orbital degrees of freedom is developed [2]. The problem is treated by generating the equations of motion for the Green's function by means of subsequent Dyson expansions, up to a certain degree of interaction [3]. The resulting set of equations is then solved as a linear system, yielding the desired Green's functions. We then compare this method to the Self Consistent Born Approximation (SCBA), successfully used before to study the problem in question [4], and further corroborate the results by checking the sum rules for the first couple of moments. We find that our method gives a similar result for the ground state, although it could be argued that it is both more dependable as well as more flexible, owing to the fact that it is a systematic expansion allowing one to carefully choose the leading terms and also to take into account the real-space constraints coming from the exclusion of double-occupancy states. This is underlined by its good agreement with the sum rules, in contrast to SCBA. Further, the variational approach offers a detailed microscopic insight into the mechanism of hole propagation and could be easily applied to other models, especially in polaron physics research.

Work supported by the Polish National Science Center (NCN) Project 2012/04/A/ST3/00331.

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Lorenzo Fratino

Royal Holloway University of London

d-wave superconducting phase diagram of the two dimensional Hubbard model

(Lorenzo Fratino, Patrick Sémon, Giovanni Sordi and André-Marie Tremblay)

Superconductivity and Mott insulating phase intertwine in materials such as cuprates and organic conductors. We study the d-wave superconducting phase at finite temperature in the two-dimensional Hubbard model on the square lattice within cellular dynamical mean-field theory and continuous-time quantum Monte Carlo. The whole phase diagram as a function of temperature, doping and interaction strength shows that a transition to the superconducting state from a Mott insulator is obtained at the cellular dynamical mean-field level, whether the transition is bandwidth or doping driven.

Dorota Gotfryd

Institute of Theoretical Physics, Warsaw University

of cluster mean field method. Detailed examination of average spins and ground state energies leads to the said phase diagrams. While the diagram for 6 sites confirms part of recently published results for Gamma=0 [1] (zigzag, stripy, spin liquid, ferromagnetic and antiferromagnetic phases) we argue that minor differences in the boundaries of the phases appear due to the shape of 6-sites cluster and specifics of cluster mean field method. The results of [1] and [2] are compared with a recently developed analysis for N=24 cluster which preserves the lattice symmetry and also find the above phases, with somewhat extended range of Kitaev spin liquid phase. Furthermore the examination of Gamma different from 0 (extended KH model) region [1],[3] in phase space is presented.

Work supported by the Polish National Science Center (NCN) Project No. 2012/04/A/ST3/00331.

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Dmytro Inosov
TU Dresden

Magnetic excitations in heavy-fermion metals with multipolar ordering

Recent years have seen tremendous progress in understanding the spin dynamics of highly correlated f-electron systems known as heavy-fermion compounds. Our neutron scattering measurements focused on two compounds with a cubic crystal structure, CeB_6 and $Ce_3Pd_{20}Si_6$, that are both famous for an enigmatic hidden-order phase stabilized at low temperatures. This phase can be ascribed to antiferroquadrupolar ordering, yet numerous studies also emphasized the importance of itinerant-spin magnetism. In an attempt to unravel this complex problem, we performed neutron-spectroscopy and angle-resolved photoemission measurements on pure and La-doped CeB_6 compound and its structurally more complex sibling material $Ce_3Pd_{20}Si_6$. The results of these experiments revealed a very rich and unexpected structure of field-dependent magnon modes that will be discussed in this presentation.

Jure Kokalj
Jozef Stefan Institute, Ljubljana

Bad-metallic behavior of doped Mott insulators

By using the finite temperature Lanczos method (FTLM) for the Hubbard model near and at half-filling I explore the behavior of the resistivity, charge susceptibility or compressibility and diffusion constant. These are all related via Nernst-Einstein relation. The results show that in the regime of high T and small dopings of Mott insulator, the large and linear-in-T resistivity obtains a natural explanation in terms of charge susceptibility. In the bad-metallic regime charge susceptibility shows strong T and doping dependence and it approaches insulating like values with increasing T, which can in addition result in the resistivity crossing the Mott-Ioffe-Regel limit. On the other hand, diffusion constant, which is related to scattering rate, shows rather weak T and doping dependence. I further discuss the simple model capturing the bad-metallic behavior of resistivity and at length the relation to experiments.

Jernej Mravlje

Jozef Stefan Institute, Ljubljana

Electronic correlations in hcp Fe

Within LDA + DMFT approach we calculated the equilibrium volume, the equation of state and bulk modulus of hcp Fe. Unlike in LDA that fails dramatically in the description of experimentally observed properties within the paramagnetic state and predicts a ferromagnetic state, LDA+DMFT accounts for the experimental data within the paramagnetic state well. Despite the good agreement of the thermodynamic data the calculated jump of resistivity on entering the hcp phase is small, poimting to important role of nonlocal correlations for transport but not the equilibrium properties of Fe.

Jovan Odavic

Aachen University

From Number Theory to Charge Density Waves

Frenkel-Kontorova model with asymmetric deformable substrate potential is a classical model used to describe spin and charge density waves. It exibits a step-like(or staircase) behaviour in the response function which is a key feature of this nonlinear dynamical model. We will focus on these harmonic and subharmonic step features and explore an interesting connection with number theory.

Key reference: J. Odavic, P. Mali, J. Tekic, Farey sequence in the appearance of subharmonic Shapiro steps, Phys. Rev. E 91, 052904

Yevhen Onykiienko

TU-Dresden

Spin-excitation spectrum of the insulating skyrmion compound Cu_2OSeO_3

In the multiferroic Cu_2OSeO_3 system, the interplay of interatomic exchange and the Dzyaloshinskii-Moriya (DM) interactions leads to the twisting and canting of magnetic moments and, consequently, to the formation of a spinspiral ground state. An exotic skyrmion-lattice arrangement can be further stabilized by the application of magnetic field. Here we employed a combination of time-of-flight and triple-axis neutron spectroscopy to investigate the complete spectrum of spin excitations in Cu_2OSeO_3 over energies ranging from sub-meV to 50-60 meV. Several magnon bands are observed, in qualitative agreement with theoretical predictions, although a significant quantitative adjustment of exchange interaction parameters is required to match the neutron-scattering data. The experimentally measured dynamical structure factor of the magnons will be also discussed in relationship to the real-space crystal structure of the material.

Žiga Osolin

Jozef Stefan Institute

Wilson chain construction for a generic lattice problem

The NRG can be used as a single site impurity solver in conjunction with the DMFT. If one wants to use the NRG with the cluster DMFT, new techniques are required to transcribe the lattice problem to a more general Wilson chain that also involves internal site indices and complex coefficients. We present how such a discretization can be achieved with a minimal effect on the NRG systematic errors. The steps involve comparing the action of the lattice to an appropriate continuous Hamiltonian, the logarithmic discretization of the continuous Hamiltonian, extraction of the interval coefficients with the minimization procedure, and finally the transformation from the impurity coupled to all intervals into chain basis, where coefficients fall of approximately exponentially, as required by the NRG to be effective. Special care must be taken with symmetries, complex number, re-orthogonalization and precision of calculations to render the procedure stable. The method gives the same results as currently used discretization techniques but provides a natural, non ad-hoc, extension to the discretization when the Hamiltonian is not real: this happens for cluster impurity problems, superconductivity and magnetic field in y-direction to name a few.

Thomas Pruschke

Theoretical Physics, University of Goettingen, D-37077 Goettingen

Dual-fermion approach to correlated electron systems with disorder

Using a replica expansion, the dual fermion approach introduced recently to access non-local properties of correlated electron systems beyond the dynamical mean-field approximation is extended to add disorder to the system. The disorder generates, on the dual fermion level, additional interaction vertices, which can be calculated from the local two-particle self-energies of DMFT. We present results for the Anderson-Falicov-Kimball and Anderson-Hubbard model regarding metal-insulator transitions, localization and the influence of disorder on magnetic properties.

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Francesco Randi

University of Trieste

Phase separation and fluctuations in equilibrium and photo-induced insulator-to-metal transition in Fe_3O_4

The intrinsic sensitivity of transition metal oxides (TMO) to any small variation of external parameters, which is at the core of the intricate phase diagrams often displayed, makes TMO the ideal playground to achieve light-driven phase transformations. In my contribution I will review the case study of the equilibrium and light-induced insulator-to-metal transition in magnetite. The phase transition mechanism and the role of fluctuations will be studied by equilibrium and transient optical properties and benchmarked with recently reported x-ray characterisation. Finally, a feature that may be generally linked to out-of-equilibrium phase separation provides us with a way to directly address the nucleation processes in non-equilibrium transient states.

Georg Rohringer

Institute for Solid State Physics, Vienna university of Technology

Destruction of the Fermi liquid by nonlocal correlations in three dimensions: A Dynamical Vertex Approximation study

By means of DGA, a diagrammatic extension of the dynamical mean field theory (DMFT), we study how the Fermi-liquid properties are gradually destroyed by approaching the antiferromagnetic instability in the two- and three-dimensional Hubbard model. We observe, that long-range nonlocal correlations reduce the transition temperature of DMFT. The focus of the talk is, however, the analysis of spectral and thermodynamic quantities when reducing T in the paramagnetic phase. Specifically we study the temperature- and interaction-dependence of the spectral functions and the quasiparticle scattering rate. The latter exhibits a non-monotonous behavior as a function of temperature in the vicinity of the antiferromagnetic phase transition in three dimensions. This marks the onset of Fermi liquid breakdown. Secondly we analyze the temperature dependence of the kinetic and potential energies of the system, as well as "interacting density of states" which can be measured in photoemission spectroscopy. While their low-T behavior demonstrate how the fluctuating antiferromagnetic islands above T_N already strongly influence the thermodynamic properties of the system, the effects are less pronounced than in the two-dimensional case, where the fluctuation effects extend to a large region of the phase diagram (see PRB 91, 125109).

Markus Ternes

Max-Planck Institute for Solid State Research

Quantum Engineering of Spin and Anisotropy in Magnetic Molecular Junctions

In recent years inelastic spin-flip spectroscopy using a low-temperature scanning tunneling microscope has been a very successful tool for studying not only individual spins but also complex coupled systems. When these systems interact with the electrons of the supporting substrate correlated many-particle states can emerge, making them ideal prototypical quantum systems. Here we will show that experiments in conjunction with model Hamiltonians which takes the coupling to the environment into account enables to achieve a profound understanding of the underlying mechanism which influences the magnetic anisotropy and leads to the emergence of correlations and entanglement.

Yuliia Tymoshenko

TU Dresden

Spin-spiral structure in $ZnCr_2Se_4$ across the whole field-temperature phase diagram

The spinel compound $ZnCr_2Se_4$ is characterized by an incommensurate spin-spiral ground state. Motivated by the magnetic phase diagram reported from magnetization and ultrasound measurements on $ZnCr_2Se_4$, we investigated this material by small-angle neutron diffraction (SANS). Our goal was to establish the nature of the enigmatic high-field phase persisting for 6 T < B < 10 T at low temperatures. The data collected at the SANS-I diffractometer at the Paul Scherrer Institute (PSI) in Switzerland clearly confirmed the presence of two phase transitions occurring at $B_{C1} \approx 2$ T and $B_{C2} \approx 6$ T. We found that both phase transitions are nearly isotropic with respect to the field direction. We also found minor variations in the propagation vector of the spiral both as a function of temperature and magnetic field. The absence of long-range order for the unsaturated component of the spin in the high-field spin-nematic phase was established from the absence of Bragg scattering in the SANS diffraction patterns.

Nils Wentzell

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Frequency structures in the 1PI vertex with fRGdyn

We present the implementation and the first results obtained with fRGdyn, a general purpose code aimed at the integration of the fRG flow equations at the one-loop truncation level for a wide class of physical systems. The main feature of fRGdyn is the treatment of the full frequency dependence of the one particle irreducible (1PI) vertex, which was hardly addressed in previous studies. We demonstrate the potential of our code by showing several results for the

single impurity Anderson model. This way we unveil the nontrivial frequency structures that arise in the 1PI vertex, and we interpret them diagrammatically. We show that fRGdyn has the potential of becoming a flexible tool available to everybody who wants to tackle physical problems in fRG fully maintaining the vertex frequency dependence.