

Book of Abstracts

NGSCES 2013

The New Generation of Strongly Correlated Electron Systems

1-5 July 2013

Sestri Levante, Italy

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Università Cattolica del Sacro Cuore



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USEFUL INFORMATIONS

VENUE

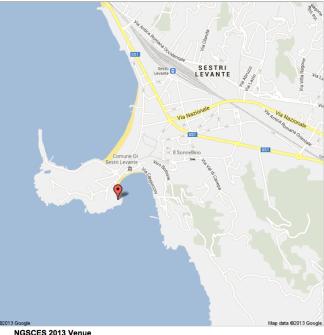
The international conference "The New Generation in Strongly Correlated Electron Systems 2013", NGSCES 2013 will take place in Sestri Levante, Italy, 1th–5th July 2013, at:

Fondazione Mediaterraneo,

Convento dell'Annunziata, Via Portobello, 16039 Sestri Levante, Italy. <u>Google maps</u>

HOW TO GET THERE

FROM THE RAILWAY STATION: Go straight on up to the end of Via Roma, turn left up to Piazza St. Antonio. Turn right in the direction of the seaside and then go straight on up to the promenade, turn left and go straight on up to Piazza Matteotti, in front of a big white church. Leave it on your right and go on the way to the "Baia del Silenzio". Here you can find Fondazione Mediaterraneo.



Convento dell'Annunziata, Via Portobello, 16039 Sestri Levante, Italy

REGISTRATION AND WELCOME APERITIF

The registration is open from **17:00** of **Sunday 30th of June**, at the conference venue. After **18:00**, an **aperitif** with a small buffet will be served on the terrace by the sea at the conference venue (Convento dell'Annunziata).

ORGANIZERS organizers2013@conference.ngsces.org

<u>Claudio Giannetti</u> (I-Lamp and Università Cattolica, Brescia, Italy) <u>Luca de' Medici</u> (ESPCI – ParisTech) <u>Johannes Bauer</u> (Harvard University, Cambridge, USA) Dmytro Inosov (MPI Stuttgart, Germany)

EXCURSION TO "5 TERRE"

The entire afternoon of Wednesday 3rd of June will be left free to visit and enjoy the local natural and artistic treasures. We strongly suggest to take your time to visit the "Cinque Terre", UNESCO World Heritage. You can arrange your own tour through the villages or hiking along the "Via dell'Amore", a 10 miles stunning path along the steep coastline. The best way to start your tour is to take a train from Sestri Levante and stop in one of the villages (Monterosso, Vernazza, Corniglia, Manarola and Riomaggiore). You can find the train timetable on the <u>italian railways website</u>. Trains are leaving from Sestri (direction La Spezia) at 12:58, 13:26, 13:46, 14:19, 14:44, 14:50, 15:18, 15:45, 16:18,...A daily ticket (Cinque Terre CARD) is available. The travel is approximately 30-40 min long. Useful links: Lonely Planet, National Park Cinque Terre, Touristic Website

dinner in Varnazza

After having enjoyed the outstanding natural beauties of the "5 Terre" we will meet at 19:30 in Vernazza. We will have dinner all together at 20:00 on the terrace of the <u>Restaurant Belforte</u>. The menu, at a reduced price of 35 €, will include: octopus salad (starter), trofie al <u>pesto</u> (first dish and regional specialty: a sauce based on basil, pine nuts, olive oil and parmesan), daily fish cooked at the local way (second dish), sweet/cake and wine.

	Sunday 30th June	Monday 1st July	Tuesday 2nd July	Wednesday 3rd July	Thursday 4th July	Friday 5th July
8.45		Welcome speech				
		COLD ATOMS	CORRELATED MATERIALS	ENGINEERED CORRELATIONS	CORRELATED MATERIALS	NON-EQUILIBRIUM
		Chair: Roberta Citro	Chair: Massimo Capone	Chair: Andrey Mishchenko	Chair: Alessandro Toschi	Chair: Fabrizio Carbone
00:60		Kollath (Lecture)	Eremin (Lecture)	Sangiovanni (Invited)	Gull (Invited)	Eckstein (Lecture)
06:30		Schneider (Invited)	Xu	Shen (Invited)	Eberlein	Mansart
10:00		Lev Vidmar	Brouet (Invited)	Peters	Benfatto	Cilento
10:30		Coffee Break	Coffee Break	Coffee Break	Garcia-Garcia	Coffee Break
		COLD ATOMS	CORRELATED MATERIALS	ENGINEERED CORRELATIONS Coffee Break	Coffee Break	NON-EQUILIBRIUM
		Chair: Roberta Citro	Chair: Massimo Capone	Chair: T Domanski		Chair: Fabrizio Carbone
11:00		Kollath (Invited)	Giovannetti (Invited)	Garcia-Barriocanal (Invited)	SPECIAL METHOD SESSION	Eckstein (Invited)
11:30		Fallani (Invited)	Mirri	Quintela	Chair: Nils Bluemer	Kaiser (Invited)
12:00		Sotnikov	Fanfarillo	Koga	Ganahl Granath	Andergassen
12:30		Lunch and beach	Lunch and beach		Rohringer Taranto	CLOSING
					Rost	
					Lunch	
		POSTER PRESENTATION	CORRELATED MATERIALS		CORRELATED MATERIALS	
		Chair: Organizers	Chair: Lilia Boeri		Chair:	
15:00		Poster	Eremin (Invited)		Weng	
15:30		flash	Yamase	FREE EXCURSION	Kratochvilova	
16:00		presentations	Mravlje (Invited)	TO CINQUE TERRE	Mitchell	
16:30		Coffee Break	Coffee Break		Coffee Break	
		CORRELATED MATERIALS	ENGINEERED CORRELATIONS		NON-EQUILIBRIUM	
		Chair: Luca Tocchio	Chair: Tae Won Noh		Chair: J Miller	
17:00		Comin (Invited)	Shen (Lecture)		Kaiser (Lecture)	
17:30		Orth	Bergeal (Invited)		Fausti (Invited)	
18:00	WELCOME	Ralko	Bareille		Rettig	
18:30	RECEPTION	POSTER SESSION - APERITIF				
20:00			CONFERENCE DINNER	MEETING AT VERNAZZA		

PROGRAM AT A GLANCE

Monday, July 1st

8:45-9:00 Opening

- 9:00 Session 1: Correlation effects with Ultracold Atoms (Chair: Roberta Citro)
 - 9:00 9:30 "Strong correlations in ultracold atomic gases" Invited Lecture Corinna Kollath (University of Bonn, Germany)
 - 9:30 10:00 *"Negative absolute temperatures for mobile particles" Invited Talk* **Ulrich Schneider** (Ludwig-Maximilian University, Munich, Germany)
 - 10:00 10:30 "Sudden expansion of interacting bosons in optical lattices: the role of integrability and dimensionality"

Lev Vidmar (Ludwig-Maximilian University, Munich, Germany)

10:30 - 11:00 COFFEE BREAK

11:00 Session 2: Correlation effects with Ultracold Atoms (Chair: Roberta Citro)

- 11:00 11:30 "Correlation dynamics of ultracold bosons in optical lattices" Invited Talk **Corinna Kollath** (University of Bonn, Germany)
- 11:30 12:00 "Quantum simulation with ultracold two-electron Fermi gases" Invited Talk Leonardo Fallani (LENS, Florence, Italy)
- 12:00 12:30 "Quantum magnetism of mass-imbalanced fermionic mixtures" Andrii Sotnikov (University of Frankfurt, Germany)
- 12:30 15:00 LUNCH BREAK

15:00 Session 3: Poster presentations

15:00 – 16:30 Flash presentations (about 2 min)

16:30 - 17:00 COFFEE BREAK

17:00 Session 4: Correlated materials

(Chair: Luca Tocchio)

17:00 – 17:30 "Novel correlated physics in iridium-based oxides: the special case of Na₂IrO₃" – Invited talk

Riccardo Comin (University of British Columbia, Vancouver, Canada)

17:30 – 18:00 "Emergent critical phase and Ricci flow in a 2D frustrated Heisenberg model"

Peter Philipp Orth (Karlsruhe Institute of Technology, Germany)

18:00 – 18:30 *"Statistical Transmutation in Doped Quantum Dimer Models"* Arnaud Ralko (Néel Institute, Grenoble, France)

18:30 – 20:00 POSTER SESSION WITH APERITIF

Tuesday, July 2nd

9:00 Session 5: Iron based superconductors

- 9:10 9:40 *"Magnetism in iron-based superconductors: interplay of magnetic, orbital and structural transitions" Invited Lecture* Ilya Eremin (Ruhr-University, Bochum, Germany)
- 9:40 10:10 *"Electronic Band Structure of BaCo₂As₂: A Fully Doped Ferropnictide Analog with Reduced Electronic Correlations"* Nan Xu (Paul Scherrer Institute)

(Chair: M. Capone)

10:10 – 10:40 "ARPES studies of the electronic structure of iron superconductors" – Invited talk

Veronique Brouet (Laboratoire de Physique des Solides, Orsay, France)

10:40 - 11:00 COFFEE BREAK

11:00 Session 6: Iron based superconductors

- 11:00 11:30 "Correlation effects and competing orders in iron-based superconductors" Invited talk
 - Gianluca Giovannetti (CNR-IOM & SISSA, Trieste, Italy)
- 11:30 12:00 "Optical investigation of Ba(Fe_{1-x}Co_x)₂As₂ detwinned by tunable uniaxial applied pressure"
 Chiara Mirri (ETH Zurich, Switzerland)
- 12:00 12:30 "Hall Effect in pnictides" Laura Fanfarillo (ICMM-CSIC Madrid Spain)
- 12:30 15:00 LUNCH BREAK

15:00 Session 7: Iron based superconductors

- 15:00 15:30 *"Magnetism in iron-based superconductors: interplay of magnetic, orbital, and structural transitions" Invited Talk* Ilya Eremin (Ruhr-University, Bochum, Germany)
- 15:30 16:00 "Superconductivity from orbital nematic fluctuations in iron pnictides " **Hiroyuki Yamase** (National Institute for Materials Science)
- 16:00 16:30 *"New insights to incoherent metals" Invited Talk* Jernej Mravlje (Ecole Polytechnique, France)
- 16:30 17:00 COFFEE BREAK

17:00 Session 8: Engineered correlations

- 17:10 17:40 "Watching Correlated Electrons Move in Artificial Quantum Materials and Interfaces using Photoemission Spectroscopy" – Invited Lecture **Kyle Shen** (Cornell University, Ithaca, USA)
- 17:40 18:10 "Two-dimensional superconductivity induced by high-mobility carrier doping in LaTiO₃/SrTiO₃ heterostructures " – Invited Talk **Nicolas Bergeal** (ESPCI ParisTech, France)
- 18:10 18:40 "A two-dimensional electron gas with hexagonal electronic structure at the (111) surface of KTaO₃"
 Cédric Bareille (CSNSM Université Paris-Sud)

20:00 CONFERENCE DINNER

Wednesday, July 3rd

9:00 Session 9: Engineered correlations

- 9:10 9:40 *"Electronic correlation and geometry: what do we learn from oxide heterostructures?" Invited Talk* Giorgio Sangiovanni (Würzburg University, Germany)
- 9:40 10:10 "Watching Correlated Electrons Move in Artificial Quantum Materials and Interfaces using Photoemission Spectroscopy" – Invited Talk **Kyle Shen** (Cornell University, Ithaca, USA)

(Chair: A. Mishchenko)

(Chair: Lilia Boeri)

(Chair: Tae Won Noh)

(Chair: M. Capone)

10:10 – 10:40 "Strong correlation physics in f-electron superlattices" **Robert Peters** (Kyoto University, Japan)

10:40 - 11:00 COFFEE BREAK

11:00 Session 10: Engineered correlations

(Chair: T. Domanski)

11:10 – 11:40 "Electronic phase diagram of electrostatically doped $La_2CuO_{4+\delta}$ " – Invited Talk

Javier Garcia-Barriocanal (Universidad Complutense, Madrid, Spain)

- 11:40 12:10 *"Structural and Thermoelectric Properties of CrN Thin Films"* **Camilo X. G. Quintela** (University of Santiago de Compostela, Spain)
- 12:10 12:40 "Transport properties through a quantum dot coupled to normal and superconducting leads"

Akihisa Koga (Tokyo Institute of Technology, Japan)

FREE EXCURSION TO "5 TERRE"

19:30 Meeting in Vernazza and dinner at "*Ristorante Belforte*"

Thursday, July 4th

9:00	Session 11:	Correlated materials, superconductivity	(Chair: A. Toschi)
	9:00 – 9:30	"Energetics of Superconductivity in the Two Dime	nsional Hubbard Model" -
		Invited Talk	

Emanuel Gull (University of Michigan, Ann Arbor, USA)

- 9:30 10:00 "Superconductivity and effective interactions in the Hubbard model" Andreas Eberlein (MPI for Solid State Research, Stuttgart, Germany)
- 10:00 10:30 "Superconductor-insulator transition at strong disorder: unconventional superfluid response and glassy physics" Lara Benfatto (Sapienza University of Rome, Italy)
- 10:30 11:00 "Restoring phase coherence in one dimensional superconductivity by power-law hopping"

Antonio M. Garcia-Garcia (Cambridge University and University of Lisbon)

11:00 – 11:30 COFFEE BREAK

11:30	Special ses	sion: Methods for correlated materials	(Chair: Nils Bluemer)
	11:40 – 12:00	ncy quantum impurity	
	12:00 – 12:20	"Quasi continuous-time impurity solver for dynamic linear scaling in the inverse temperature" Daniel C. Rost (Johannes Gutenberg-University, N	-
	10.00 10.40	"Efficient impurity achier using Matrix Draduat Stat	~~"

- 12:20 12:40 "Efficient impurity solver using Matrix Product States" Martin Ganahl (Institute for theoretical physics, TU Graz, Austria)
- 12:40 13:00 "One-particle irreducible functional approach a new route to diagrammatic extensions of DMFT" Georg Rohringer (Vienna University of Technology, Austria)
- 13:00 13:20 *"From infinite to d dimensions: combining dynamical mean field theory and functional renormalization group"* **Ciro Taranto** (TU Wien, Austria)

13:30 - 15:00 LUNCH BREAK

15:00 Session 12: Correlated materials, Kondo and heavy fermion physics

- 15:00 15:30 "Correlated topological orders in Kondo insulators YbB₆ and YbB₁₂" Hongming Weng (The Institute of Physics, Chinese Academy of Sciences)
- 15:30 16:00 "Ambient Pressure Superconductivity in the Antiferromagnetic Compound Ce₂PtIn₈"

Marie Kratochvilova (Charles University, Prague, Czech Republik)

- 16:00 16:30 "Non-Fermi liquid physics in a two-impurity Kondo quantum box device " Andrew Mitchell (University of Oxford, UK)
- 16:30 17:00 COFFEE BREAK

17:00 Session 13: Non-equilibrium physics

- 17:10 17:40 "Control of Nonlinear Dynamics in Complex Matter by Ultrafast Optics" Invited Lecture Stefan Kaiser (Max Planck Hamburg, Germany)
- 17:40 18:10 "New time-domain approaches to strongly correlated electron systems" Invited Talk

Daniele Fausti (University of Trieste, Italy)

18:10 – 18:40 "Time- and angle-resolved photoemission spectroscopy of the CDW material RTe3" Laurenz Rettig (University of Duisburg Essen, Germany)

Friday, July 5th

9:00 Session 14: Non-equilibrium physics

- 9:10 9:40 "Numerical methods many-particle systems out of equilibrium: Impurity solvers for non-equilibrium Dynamical mean field theory" - Invited Lecture Martin Eckstein (Max Planck Hamburg)
- 9:40 10:10 "Coupling of a high-energy excitation to superconducting quasiparticles in a cuprate from coherent charge fluctuation spectroscopy." Barbara Mansart (EPFL Lausanne, Switzerland)
- 10:10 10:40 "The elusive mottness underlying the phase diagram of cuprates unveiled on the ultrafast timescale."

Federico Cilento (ELETTRA Trieste, Italy)

10:40 - 11:00 COFFEE BREAK

11:00 Session 15: Non-equilibrium physics

- 11:00 11:30 "Ultrafast melting of long-range order in the Hubbard model" Invited Talk Martin Eckstein (Max Planck Hamburg, Germany)
- 11:30 12:00 "Transient superconductivity in optically modulated YBCO"- Invited Talk Stefan Kaiser (Max Planck Hamburg, Germany
- 12:00 12:30 "Magnetic field effects on the finite-frequency noise and AC conductance of a Kondo quantum dot out of equilibrium" Sabine Andergassen (University of Vienna, Austria)

CLOSING 12:30

(Chair: F. Carbone)

(Chair: F. Carbone)

(Chair: John Miller)

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I. Oral Presentations

Two-dimensional superconductivity induced by high-mobility carrier doping in $LaTiO_3/SrTiO_3$ heterostructures - Invited Talk

Nicolas Bergeal¹

¹LPEM- UMR8213/CNRS - ESPCI ParisTech, 10 rue Vauquelin - 75005 Paris, France

Transition metal oxides display a great variety of quantum electronic behaviours where correlations often play an important role. The achievement of high quality epitaxial interfaces involving such materials gives a unique opportunity to engineer artificial materials where new electronic orders take place. It has been shown that a two-dimensional electron gas 2DEG could form at the interface of two insulators such as LaAlO₃ and SrTiO₃ [1], or LaTiO₃ (a Mott insulator) and SrTiO₃ [2]. We present low temperature transport and magneto-transport measurements up to 45 T on LaTiO₃/SrTiO₃ heterostructures. We showed that a superconducting two-dimensional electron gas is formed at the LaTiO₃/SrTiO₃ interface whose properties can be modulated by field effect using a metallic gate on the back of the substrate [3,4]. The gas consists of two types of carriers: a majority of low-mobility carriers always present, and a few high-mobility ones that can be injected by electrostatic doping. The calculation of the electrons responsible for superconductivity set at the edge of the gas whose extension can be tuned by field effect [4].

- [1] N. Reyren et al., Science **317**, 1196 (2007)
- [2] A. Ohtomo et al., *Nature* **419**, 378 (2002)
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ARPES studies of the electronic structure of iron superconductors - Invited Talk

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In march 2008, a new family of superconductors was discovered. They are all based on square planes of Fe linked by pnictogens (As, P,...) or chalcogenides (Se, Te,...). It raised tremendous interest in the community because superconductivity in Fe-based compounds at such high temperatures was completely unexpected. As for the cuprates, many related compounds are magnetic, suggesting the possibility of exotic superconducting pairing through magnetic fluctuations. However, a major difference with cuprates is that Fe superconductors are multiband systems, with at least there different Fe bands crossing the Fermi level to form small hole and electron pockets. The role of correlations in this complicated electronic structure is actively debated. Angle Resolved Photoemission is a technique of choice to image the electronic structure of a system and evaluate the strength of correlations. I will review the main results emerging from these studies: structure of the Fermi Surface (nature of the orbitals forming the different hole and electron pockets, nesting between them), strength of correlations in different families of iron pnictides and for different bands. Particular attention will be given to the study of the transitions to magnetic and superconducting states.

Novel correlated physics in iridium-based oxides: the special case of Na_2IrO_3 - Invited Talk

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5*d*-based transition metal oxides represent a novel class of materials which attracted a growing interest in the last decade for giving rise to unconventional states of matter. In particular, a few members from the family of iridates, so far the most investigated, have been proposed to be the realization of an unconventional spin-orbit assisted Mott-Hubbard physics. To test this proposal, we have studied the newest addition to the iridate family, sodium iridate (Na₂IrO₃), by ARPES, optics, and band structure calculations in the local-density approximation (LDA). ARPES on potassium-doped surfaces and optics turn out to be in remarkable agreement and return an insulating gap $\Delta \simeq 340$ meV, while the LDA analysis shows an unprecedented finding: without spin-orbit coupling (SOC) the system would be metallic, but with SOC density functional theory predicts an insulating behavior. Further analysis then shows how the correct gap magnitude can only be reproduced with the addition of a Hubbard U=3eV. This establishes Na₂IrO₃ as a novel type of Mott-like correlated insulator in which Coulomb and relativistic effects (SOC) have to be treated on an equal footing.

R. Comin et al. Na₂IrO₃ as a Novel Relativistic Mott Insulator with a 340 meV Gap. *Phys. Rev. Lett.* **109**, 266406 (2012)

Numerical methods many-particle systems out of equilibrium: Impurity solvers for non-equilibrium Dynamical mean field theory - Invited Lecture

Martin Eckstein¹

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Dynamical mean-field theory (DMFT) for non-equilibrium is a promising approach to study models for correlated electrons in higher dimensions. Within DMFT, a lattice problem is mapped to a single-impurity problem. The latter is still a formidable numerical task, which is an interesting problem in its own right, e.g., for studying transport through quantum dots. In this lecture, I review some of the numerical approaches that have been considered as impurity solvers for non-equilibrium DMFT, including diagrammatic weak-and strong-coupling approaches, Quantum Monte Carlo, and exact wave-function based methods (Krylov).

Ultrafast melting of long-range order in the Hubbard model - Invited Talk

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When the antiferromagnetic phase in the Hubbard model is strongly perturbed, by means of an interaction quench or a strong laser pulse, one can induce a melting of the long-range order (LRO). On the shortest timescale the dynamics of this process is not governed by the final thermal equilibrium state the system is approaching: Even when the excitation density exceeds the energy that would be needed to heat the system above the Neel temperature, LRO can either survive for very long times, or melt rapidly, and the crossover between these regimes is marked by a non-thermal critical point with a diverging timescale.

N. Tsuji, M. Eckstein, Ph. Werner, *Phys. Rev. Lett.* **110**, 136404 (2013).
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Magnetism in iron-based superconductors: interplay of magnetic, orbital, and structural transitions - Invited Talk

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Recent discovery of superconductivity in the iron-based layered pnictides with \mathbf{T}_c ranging between 26 and 56K generated enormous interest in the physics of these materials. In my talk I discuss the peculiarities of selection of the stripe magnetic order and the formation of the spin nematic Ising state in the unfolded BZ within itinerant description. We show that the stripe magnetic order is generally preempted by an Ising-nematic order, which breaks C_4 lattice symmetry but preserves O(3) spin-rotational symmetry. This leads to a rich phase diagram as function of doping, pressure, and elastic moduli, displaying split magnetic and nematic tricritical points. The nematic transition may instantly bring the system to the verge of a magnetic transition, or it may occur first, being followed by a magnetic transition at a lower temperature. In the latter case, the preemptive nematic transition is accompanied by either a jump or a rapid increase of the magnetic correlation length, triggering a pseudogap behavior associated with magnetic precursors. Furthermore, due to the distinct orbital character of each Fermi pocket, the nematic transition also induces orbital order. We compare our results to various experiments, showing that they correctly address the changes in the character of the magnetostructural transition across the phase diagrams of different compounds, as well as the relationship between the orthorhombic and magnetic order parameters. Next we analyze the evolution of the spin excitations from the parent antiferromagnetic phase to the superconducting phase and address in particular the coexistence phase of antiferromagnetism and superconductivity.

Quantum simulation with ultracold two-electron Fermi gases - Invited Talk

Leonardo Fallani¹

 1 Dipartimento di Fisica e di Astronomia & LENS Università di Firenze

We will report on recent experiments performed at LENS with ultracold degenerate ¹⁷³Yb Fermi gases. Thanks to their electronic structure, two-electron atoms such as ytterbium offer novel possibilities (over commonly-used alkali atoms) for advanced quantum simulations. In particular, ¹⁷³Yb Fermi gases are characterized by a large nuclear spin and highly-symmetric atom-atom interactions, which result in the possibility of performing quantum simulation of systems with intrinsic SU(N) symmetry, beyond the spin-1/2 case of electronic systems. We will report on the optical manipulation and detection of the atomic spin and on the first experimental results recently obtained with repulsively-interacting ¹⁷³Yb atoms trapped in optical lattices.

New time-domain approaches to strongly correlated electron systems - Invited Talk

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The role played by phonons and high energy excitation of electronic origin in Cuprates superconductivity is still controversial. The interconnections between low energy vibrations and the high energy electronic response are intimately connected to the formation of the superconducting phases in the Cuprates and are still heavily debated. We show here the possibility of exploiting time domain optical spectroscopy to establish a direct link between vibrational modes and electronic charge excitations in two paradigmatic cases, the parent compound La_2CuO_4 and the optimally doped YBCO.

Electronic phase diagram of electrostatically doped $La_2CuO_{4+\delta}$ - Invited Talk

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 2 School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA

In this contribution I will show our recent results on Electronic Double Layer (EDL) techniques applied to the study of high T_C cuprates. The EDL configuration, which employs ionic liquids as gate dielectrics, has succeeded in achieving unprecedented charge transfers, of the order of 10^{15} carriers/cm². This large accumulation and depletion of carriers allowed us to explore the phase diagram of La₂CuO_{4+ δ} ultra-thin films in a continuous fashion, avoiding the presence of miscibility gaps characteristic of bulk samples.

I will focus on the physics of the superconductor to insulator transition (SIT) of high quality samples produced by ozone assisted Molecular Beam Epitaxy. The electronic transport measurements suggest the possibility that this is a quantum phase transition and the magneto-transport experiment highlights the role of electron-electron interactions in the SIT due to the proximity of the Mott-insulating state.

Correlation effects and competing orders in iron-based superconductors - Invited Talk

Gianluca Giovannetti¹

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In copper oxides and iron-based materials high-temperature superconductivity is achieved by suppressing the antiferromagnetic state of the parent compounds upon chemical doping. However the undoped parent compound of copper-oxide is an antiferromagnetic Mott insulator while in iron-based compounds is a metal with a commensurate spin density wave. Performing slave-spin mean-field theory calculations we show that iron superconductors (FeSe, LaOFeAs, BaFe₂As₂) display a behavior of mobile and localized electrons coexisting as a consequence of a sizable Hund's exchange coupling. The Hund's rule simultaneously reduces the quasi particle weights and increases the critical value of the electronic interaction U for the Mott transition. The inter-orbital charge correlations are suppressed and the different orbitals decouple with each other behaving as a collection of independent single bands. The electronic interaction strengths in the d orbitals are controlled by the individual orbital population, which gives a distance from a Mott Insulating state on the hole-doped side and determines a coherent metallic state on the electron-doped side. The phase diagram of iron superconductors is controlled then by a Mott insulating state which would occur in a material with a very large hole-doping, while the parent compound is not close to a Mott state despite the commensurate filling. The nature of the quantum phase transition in iron-based materials, where long-range magnetic order vanishes as a function of the charge, is of key relevance, because continuous transitions are expected to favour superconductivity, due to strong fluctuations. Using constrained density functional calculations we show these materials turn out to be remarkably close to a quantum tricritical point. This work is financed by ERC-FP7 through the Starting Grant SUPERBAD (Grant

This work is financed by ERC-FP7 through the Starting Grant SUPERBAD (Grant Agreement 240524).

Energetics of Superconductivity in the Two Dimensional Hubbard Model - Invited Talk

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Recently developed numerical methods have enabled the explicit construction of the

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superconducting state of the Hubbard model of strongly correlated electrons in parameter regimes where the model also exhibits a pseudogap and a Mott insulating phase. $d_{x^2-y^2}$ symmetry superconductivity is found to occur in proximity to the Mott insulator, but separated from it by a pseudogapped non-superconducting phase. The superconducting transition temperature and order parameter amplitude are found to be maximal at the onset of the normal-state pseudogap. The emergence of superconductivity from the normal state pseudogap leads to a decrease in the excitation gap. All of these features are consistent with the observed behavior of the copper-oxide superconductors.

Control of Nonlinear Dynamics in Complex Matter by Ultrafast Optics - Invited Lecture

Stefan Kaiser¹

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The development of versatile and powerful ultrafast-laser systems ranging from THz to XUV sources opened up new frontiers in the research of strongly correlated electron systems. They allow investigating non-linear dynamics in complex condensed matter, as well as their control with strong THz frequency transients. Light induced superconductivity, control of magnetism by nonlinear phononics, coherent control of Mott insulators and Charge Density Wave states are among the intriguing new phenomena becoming available to experimentalists in the field of condensed matter.

The lecture will present the concept of time-resolved optical experiments and highlight their application in complex matter systems. Both, essential device developments and basic experimental techniques will be discussed that are used to investigate the nonequilibrium dynamics of matter. Then the concepts and methods behind the idea of non-linear control of the dynamics with strong THz fields are introduced and explained on various examples.

One research highlight, inducing perfect coherent transport in underdoped cuprate superconductors far above T_c , will be discussed in detail in the separate talk.

Transient superconductivity in optically modulated $YBa_2Cu_3O_{6+x}$ - Invited Talk

Stefan Kaiser¹

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We recently discovered that photo-stimulation with femtosecond mid-infrared pulses induces a non-equilibrium state in YBa₂Cu₃O_{6+x}, which shows properties characteristic of a superconductor for temperatures as high as 300 K [1]. The parent, undoped compounds of high-T_c cuprates are antiferromagnetic Mott insulators, whose physical properties are strongly modified upon doping the Cu-O planes with a few percent charge carriers. One region of their phase diagram which has attracted much attention is the so-called pseudogap phase [2,3], found below a characteristic temperature T^{*} in moderately-doped materials. The origin of this gapped, but non-superconducting state has been attributed to a variety of microscopic phenomena, ranging from a precursor superconducting state with pre-formed Cooper pairs without phase coherence, to a scenario where electronic correlations compete with superconductivity [4]. Here, we show how phase coherence can be established in underdoped $YBa_2Cu_3O_{6+x}$ for temperatures far above T_c , throughout the pseudogap region. High intensity optical pulses at THz frequencies are used to dynamically modulate the crystallographic structure, inducing a transient superconducting state, which is evidenced by the appearance of a Josephson plasma edge in the *c*-axis reflectivity and a divergent imaginary optical conductivity at low frequency [1]. THz time-domain spectroscopy allows us to fully characterize not only the optical properties of the dynamically modulated state but also its time evolution after driving the phonon mode and its decay back to the ground state. We discuss here key parameters for possible scenarios and mechanisms. In particular, we show in detail how this transient state appears to be inhomogeneous, with transient optical properties that can be well reproduced using an effective medium model. That also allows us to describe how the state is established and how the induced coherent coupling dephases after the driving pulse is gone.

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[3] D. N. Basov and T. Timusk. *Electrodynamics of high-Tc superconductors*. Rev. Mod. Phys. 77, 721 (2005).

[4] A. Dubroka, M. Rössle, K. W. Kim, et al., Evidence of a Precursor Superconducting Phase at Temperatures as High as 180 K in $RBa_2Cu_3O_{7-\delta}$ (R = Y, Gd, Eu) Superconducting Crystals from Infared Spectroscopy. Phys. Rev. Lett. 106, 047006 (2011).

Correlation dynamics of ultracold bosons in optical lattices - Invited Talk

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Atomic gases cooled to Nanokelvin temperatures are a new exciting tool to study a broad range of quantum phenomena. In particular, an outstanding degree of control over the fundamental parameters, such as interaction strength, spin composition, or dimensionality has been achieved. This has facilitated access to strongly correlated quantum many body physics in exceptionally clean samples. For example, artificial periodic structures for the atomic gas can be created using laser light to mimic condensed matter systems. Further, the outstanding tunability of cold gases allows to rapidly change the system parameters or to induce a coupling to an environment and to observe the subsequent quantum evolution. This ability poses new challenges for the understanding of quantum dynamics in correlated many-body systems. I will report on recent progress on investigating bosonic gases in optical lattices subjected to time-dependent parameter changes or coupling to an dissipative environment. We focus on the induced correlation dynamics.

New insights to incoherent metals - Invited Talk

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In correlated metals, the Fermi liquid response is observed below low frequencies and temperatures. The Fermi liquid coherence scales in transition-metal oxides range from a Kelvin until 100 Kelvin or so. I will argue that these trends can be understood well within dynamical mean-field theory calculations, with the filling of the atom as the main control parameter. I will stress the influence of the Hund's rule coupling and discuss in which aspects the metals in which correlations arise due to the Hund's rule coupling differ from those in which they originate from a proximity to a Mott insulator. As concrete examples, I will discuss molybdates, vanadates and ruthenates. Above the Fermi liquid temperature, the crossover to incoherent regime occurs. The resistivity and the thermopower of a doped Mott insulator and of a Hund's metal will be discussed.

Electronic correlation and geometry: what do we learn from oxide heterostructures? - Invited Talk

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Layered oxide heterostructures and surfaces of transition-metal oxides give us access to confined electron liquids, which, by dint of the amazing progresses in growing techniques, can be engineered with tunable properties. Playing around "with novel low-dimensional electron systems is a dream not only for new-generation device chasers but also for condensed matter theorists. The presence of strongly correlated d-electrons is by far the most fascinating aspect. $LaVO_3/SrTiO_3$ heterostructures are a perfect example of that: a mobile two-dimensional electron liquid is formed at the n-type TiO₂|LaO interface involving Ti and V d-carriers. As I will discuss in the first part of my talk, $LaVO_3/SrTiO_3$ is for this reason very promising for photovoltaics applications.[1] Experimentally it has been shown that, upon changing the number of grown monolayers in heterostructures containing d-electrons, metal-insulator transitions can be induced. In the second part of my talk I will therefore show to what extent our theories are currently able to describe the interplay between geometry and many-body effects. This has particularly fascinating perspectives if we think of becoming able to design new topological insulators containing strongly interacting electrons. In a model calculation we have shown that electron-electron interactions can be indeed exploited to access topological states dominated by quantum many-body fluctuations. [2]

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Negative absolute temperatures for mobile particles -Invited Talk

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Absolute temperature, that is the fundamental temperature scale in thermodynamics, is usually bound to be positive. Under special conditions, however, negative temperatures - where high-energy states are more occupied than low-energy states - are also possible. In this talk, I will present a negative temperature state for motional degrees of freedom: By tailoring the Bose-Hubbard Hamiltonian we experimentally created an attractively interacting ensemble of ultracold bosons, which is stable against collapse for arbitrary atom numbers. In this negative temperature state, the quasi-momentum distribution develops sharp peaks at the upper band edge, revealing thermal equilibrium and bosonic coherence over several lattice sites. Negative temperatures imply negative pressures and open up new parameter regimes for cold atoms, enabling fundamentally new many-body states and counterintuitive effects such as Carnot engines above unity efficiency.

Watching Correlated Electrons Move in Artificial Quantum Materials and Interfaces using Photoemission Spectroscopy - Invited Talk

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Our ability to control electronic properties at the interfaces between materials has had enormous scientific and technological implications. Extending this idea beyond the familiar semiconductors, we can now use materials which possess inherently strong quantum many-body interactions as our building blocks to create artificial heterostructures and interfaces. For example, metallic, magnetic and even superconducting states have been realized at the interface between two insulators. I will describe some of our recent work in creating and exploring emergent electronic and magnetic phases which arise in these new ärtificial quantum materialsüsing a combination of oxide molecular beam epitaxy and high-resolution angle-resolved photoemission spectroscopy (ARPES) to investigate the electronic structure and many-body interactions which determine their properties. I will describe some of our work using this tool, including work on oxide superlattices of $([LaMnO_3]_{2n}/[SrMnO_3]_n)$, comprised of alternating LaMnO₃ and SrMnO₃ blocks, which can be tuned by changing the separation between interfaces from a 3D ferromagnetic metal, to a 2D polaron liquid, and finally to a pseudogapped ferromagnetic insulator. I will also describe some of our recent work on a dimensional crossover in ultrathin $LaNiO_3$ films change from a correlated Fermi liquid to an insulator as the film thickness is reduced below 3 unit cells.

Magnetic field effects on the finite-frequency noise and ac conductance of a Kondo quantum dot out of equilibrium -Talk

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We present analytic results for the finite-frequency current noise and the nonequilibrium ac conductance for a Kondo quantum dot in presence of a magnetic field. We determine the line shape close to resonances and show that while all resonances in the ac conductance are broadened by the transverse spin relaxation rate, the noise at finite field additionally involves the longitudinal rate as well as sharp kinks resulting in singular derivatives. Our results provide a consistent theoretical description of recent experimental data for the emission noise at zero magnetic field, and we propose the extension to finite field for which we present a detailed prediction.

A two-dimensional electron gas with hexagonal electronic structure at the (111) surface of KTaO₃ - Talk

<u>Cédric Bareille</u>¹, F. Fortuna¹, T. C. Rödel², F. Bertran³, M. Gabay⁴, A. Taleb-Ibrahimi³, P. Le Fèvre³, M. Bibes, A. Barthélémy⁵, T. Maroutian⁵, P. Lecoeur⁵, M. J. Rozenberg⁴, A. F. Santander-Syro¹

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Transition-metal oxides (TMOs) are correlated-electron systems presenting remarkable properties, such as high-temperature superconductivity or multi-ferroic behaviour. The realization of two-dimensional electron gases (2DEGs) at surfaces or interfaces of TMOs, a field of current active research, is crucial for harnessing the functionalities of these materials in view of future applications. From a fundamental point of view, these 2DEGs offer the possibility to explore new physics emerging from the combined effects of electron correlations and low-dimensional confinement. In this framework, the theoretical study of correlated electrons confined in exotic lattice symmetries, like the graphene-like 2D honeycomb lattice, has been recently receiving a lot of attention. Based on our recent results showing that 2DEGs can be directly obtained at the surface of TMOs [1, 2], here we create a 2DEG at the (111) surface of KTaO₃, an insulator with a strong spin-orbit coupling. Using angle-resolved photoemission, we directly observe that the confined states form a hexagonal network of quasi-1D ëlectron gutters", an electronic structure wholly novel with respect to all known oxide-based

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2DEGs. These findings demonstrate that the Fermi Sea of the oxide-based 2DEGs can be dramatically modified by properly choosing the cleaving plane of the perovskite crystal, suggesting new routes to craft exotic low-dimensional states in correlated oxides.

- [1] A. F. Santander-Syro et al., Nature 469, 189-193 (2011).
- [2] A. F. Santander-Syro *et al. Phys. Rev. B* 86, 121107(R) (2012).

Superconductor-insulator transition at strong disorder: unconventional superfluid response and glassy physics -Talk

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In the last few years there has been a resurgence of interest in the superconductorinsulator transition (SIT) induced by strong disorder in conventional superconductors [1]. Indeed, the improvement of the experimental tecniques, as e.g. scanning tunneling microscopy, offered a new perspective on the characteristics of the superconducting state near the SIT, which can even share similarities with the behavior of unconventional high-temperature superconductors. A typical example is provided by the spontaneous emergence of spatial inhomogeneity of the local density-of-state on nanometer scales, with a persistence of gap-like features even above the critical temperature (the so-called pseudogap). These finding stimulated a new theoretical investigation on some long-standing issues, as e.g. the validity of the bosonic vs fermionic picture of the SIT, and on new ones, as the emergence of a glassy-like behavior of the system. In this talk I will try to make a short overview of the experimental and theoretical state-of-the art in this field, and I will briefly discuss some recent results we obtained for the unconventional superfluid response [2] and the spatial order-parameter distribution [3] at strong disorder.

M. V. Feigelman *et al.*, Annals of Physics **325**, 1368 (2010) and references therein.
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The elusive mottness underlying the phase diagram of cuprates unveiled on the ultrafast timescale - Talk

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- ⁶ Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan
- ⁷ School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA
- ⁸ Department of Physics and Astronomy, University of British Columbia, Vancouver, BC V6T 1Z1, Canada
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The puzzling story of correlated materials still misses the critical understanding of the direct role played by the short-range electronic correlations in determining the physical properties throughout the doping (p) - temperature (T) phase diagrams. For example, in hole-doped copper-oxides a universal pseudogap state emerges as both doping and temperature decrease, and is precursor of the high-temperature superconductivity. At equilibrium, the interplay between the electronic correlations and the charge, spin and lattice degrees of freedom makes this elusive state of matter prone to instabilities towards new broken-symmetry phases. Therefore, the cause-effect relationship between shortrange correlations and long range orders in the pseudogap state and its role in the onset of high-temperature superconductivity are still unknown. Here we demonstrate that the phase diagram of cuprates is dominated by short-range correlations. Consequently, longrange orders originate from instabilities of this correlated ground state. To prove these results we adopt a non-equilibrium approach based on the use of ultrashort light pulses to artificially create, in different prototypical families of superconducting copper oxides, a non-equilibrium electronic distribution dominated by anti-nodal quasiparticles, resulting decoupled from the lattice on the sub-ps timescale. Taking ultrafast (~ 100 fs) snapshots of the electronic scattering time τ we show that it transiently increases, as a direct effect of electronic correlations, until a quasi-equilibrium nodal distribution is recovered. The onset temperature of this anomaly in the lifetime of antinodal excitations scales with doping and coincides with the ubiquitous pseudogap region. In a more general scenario, this non-equilibrium approach to the study of the electronic correlations in real materials is the counterpart of experiments in ultracold gases trapped in ideal optical lattices, in which novel many-body properties and Mott insulating phases can be identified and studied by optically tuning the occupation distribution and the Coulomb repulsion U.

Superconductivity and effective interactions in the Hubbard model - Talk

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We study the superconducting ground state of the two-dimensional Hubbard model at weak coupling using the functional renormalization group within a purely fermionic setting. The effective Nambu two-particle vertex is parametrized in terms of bosonexchange interactions in the particle-hole and particle-particle channels, providing an efficient description of its singular dependence on momenta and frequencies. We compute the momentum dependence of the two-particle vertex on one-loop level and determine the d-wave superconducting gap as a function of the interaction, the next-nearest neighbor hopping and the fermionic density. Our results suggest the existence of an optimal value of the next-nearest neighbor hopping for pairing.

Efficient impurity solver using Matrix Product States - Talk

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We propose an efficient extension to a recently developed expansion technique for spectral functions using Matrix Product States and Chebyshev polynomials. Chebyshev moments are postprocessed with linear prediction, giving significant improvement of spectral resolution at quasi no cost. We benchmark the method on the exactly solvable resonant level model. By analyzing the single impurity anderson model, we show that the method is also capable of resolving sharp resonaces (within certain parameter regions). We also propose a modi

fication of the usual technique by expanding $exp(-\tau H)$ instead of H, opening the possibility of using established methods for time evolution of Matrix Product States for direct calculation of spectral functions. We apply the method as impurity solver within the Dynamical Mean Field Theory, and present results for the Hubbard Model on the infinite-dimensional Bethe lattice.

Restoring phase coherence in one dimensional superconductivity by power-law hopping - Talk

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A central result in one-dimensional (1D) superconductivity is that even at zero temperature quantum fluctuations destroy phase coherence. Here we put forward a mechanism which can restore phase coherence: power-law hopping. We study a 1D attractive-U Hubbard model with power-law hopping by Abelian bosonization and density-matrix renormalization group (DMRG) techniques. The parameter that controls the hopping decay acts as the effective, non-integer spatial dimensionality deff. We show analytically that for any $d_{eff}>1$ at zero temperature, power-law hopping suppresses fluctuations and induces phase coherence, namely, long-range superconducting order. A detailed DMRG analysis fully supports these findings. These results are also of direct relevance to quantum magnetism as our model can be mapped onto a spin-chain with power-law decaying couplings, which can be studied experimentally by cold ion-trap techniques.

Distributional Exact Diagonalization; a real frequency quantum impurity solver - Talk

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I will present a quantum impurity solver that is based on exact diagonalization of a representative distribution of finite size Anderson models. Operationally the method is close to the standard (Caffarel-Krauth) ED formalism but where the observation that a continuum of Anderson models can give almost equally good fits to the impurity-bath Green's function on imaginary frequencies is used to generate a distribution of such. In this way a practically continuous real frequency self energy can be calculated as a sample average. We find results in good agreement with DMRG for the local spectral function (DOS) and self energy for the paramagnetic Hubbard model within DMFT both in the metallic and insulating states. The method is naturally parallelizable which opens for doing direct real frequency calculations (without any analytic continuation) on multi-orbital models with arbitrary local interactions. Preliminary results are presented in *PRB* **86**, 115111 (2012).

Hall Effect in pnictides - Talk

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The multiband character of pnictide systems complicates the analysis of transport experiments data, since in these systems the contribution of carriers having hole and electron character is unavoidably mixed. The experiments on Hall transport highlighted several anomalies both concerning the order of magnitude of the Hall coefficient R_H and its temperature/doping dependence [1,2]. For example, within a semiclassical Boltzmann-like approach, R_H is expected to be almost zero in slightly doped compounds, while from experiments it is found to have a large absolute value with a strong temperature dependence. We present a theoretical investigation of Hall transport taking into account the multiband character of pnictides. The analysis of an effective two-band model with dominant interband interaction, reveals an unconventional scenario, beyond the Boltzmann theory, where the quasiparticle currents dressed by vertex corrections acquire the character of the majority carriers. This leads to a larger (positive or negative) Hall coefficient than what expected on the basis of the carrier balance, with a marked temperature dependence [3]. Moreover in order to deeply understand the orbitals role in transport phenomena, we consider the analysis of Hall transport within a more microscopic multiorbital language.

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[2] L. Fang, H. Luo, P. Cheng, Z. Wang, Y. Jia, G. Mu, B. Shen, I.I. Mazin, L. Shan, C. Ren, and H-H. Wen, *Phys. Rev. B* 80, 140508(R) (2009).

[3] L. Fanfarillo, E. Cappelluti, C. Castellani, L. Benfatto, *Phys. Rev. Lett.* **109**, 096402 (2012).

Transport properties through a quantum dot coupled to normal and superconducting leads - Talk

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Recently electron transport through nanofabrications has attracted much interest. One of the simplest systems is a quantum dot with discrete energy levels, which gives us a stage to study fundamental quantum physics. The quantum dot system coupled to the normal and superconducting leads is one of the interesting systems to study how the Kondo screening and the Andreev reflections affect transport properties. In fact, the Kondo-enhanced Andreev transport has been discussed in the InAs quantum dot contacted with the normal and superconducting electrodes. These nontrivial aspects related to the interplay between the Coulomb interactions and proximity-induced on-dot pairing have been discussed by various theoretical approaches. However, some analytical approaches introduce a sort of the nontrivial mean-field to discuss the nonequilibrium phenomena beyond the lower-order calculations and/or to satisfy the current conservation through the quantum dot, which may not be controllable in the strong coupling region. Therefore, the unbiased and robust method for nonequilibrium properties is desired to discuss the transient phenomena and steady state of quantum many-body systems. To this end, we make use of the continuous-time quantum Monte Carlo (CTQMC) method based on the Keldysh formalism. Here we extend the CTQMC method in the continuous-time auxiliary field formulation to treat the superconducting state in the Nambu formalism. By applying the method to the Anderson impurity model, we calculate the particle number, double occupancy, pairing correlations and currents. We then discuss the transient phenomena and steady state in the quantum dot system.

Ambient Pressure Superconductivity in the Antiferromagnetic Compound Ce_2PtIn_8 - Talk

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The family of $\operatorname{Ce}_n T_m \operatorname{In}_{3n+2m}$ (n = 1, 2; m = 1; T = transition metal) heavy fermion compounds are known to be on the verge of a magnetic to non-magnetic quantum critical point (QCP) [1]. In the vicinity of the materials $\hat{a} \in \mathbb{C}^{\sim}$ QCP an unconventional superconducting state has been reported which attracted much of the attention in the past decades. However, this family of compounds is interesting for some other reason. The compounds crystallize in the tetragonal $Ho_n Co_m Ga_{3n+2m}$ structures which provide the possibility to tune the structural dimensionality from more 2D to 3D ($127 \rightarrow 115 \rightarrow$ 218) [1]. This makes them ideal candidates to investigate the influence of the parameter "dimensionality" with respect to quantum criticality [2]. Here, we report on Ce_2PtIn_8 which is the only compound within the family showing both superconductivity and magnetic ordering at ambient pressure. Except the $CePt_3Si$ compound [3], there is not known any other cerium based material revealing both phenomena. In the specific heat, resistivity and ac susceptibility two magnetic transitions are observed; the compound orders antiferromagnetically below $T_N = 2.1$ K and further cooling reveals another, order-to-order transition at $T_m = 2$ K. The transitions merge at 4 T and split again in higher magnetic fields. Finally, superconductivity emerges at $T_C = 0.39$ K. Application of hydrostatic pressure leads to formation of a superconducting dome with $T_{C}^{max} = 0.7$ K at 1 GPa. The magnetic field-pressure-temperature phase diagram will be discussed in the context of superconductivity and magnetism evolution in related compounds.

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- [2] J. Custers et al., Nature Mat. 11, 189 (2012).
- [3] E. Bauer et al., *Phys. Rev. Lett.* **92**, 027003 (2004).

Coupling of a high-energy excitation to superconducting quasiparticles in a cuprate from coherent charge fluctuation spectroscopy - Talk

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Despite their obvious physical difference, from a mathematical (or purely formal) point of view, magnetism and superconductivity are closely linked phenomena. Coherent charge and pairing fluctuations can be described in terms of precession of pseudospins operators, first introduced by Anderson, and behaving as spin1/2 operators [1]. In our experiment, a polarized ultrafast laser pulse excites the superconductor through the Impulsive Stimulated Raman Scattering (ISRS) effect [2]. The coherent oscillations of the Cooper pairs condensate are detected via delayed supercontinuum pulses and enable a new technique, Coherent Charge Fluctuation Spectroscopy (CCFS), to distinguish the electronic excitations that couple to the superconducting quasiparticles [3]. This is of pivotal importance for cuprates, as the applicability of conventional pairing theories,

based on retarded interactions between electrons mediated by low energy glue bosons, has been doubted and a completely different framework has been proposed involving non retarded interactions associated with high-energy electronic scales. We found that the superconducting condensate oscillations resonate at the typical scale of Mott physics (2.6 eV), implying a substantial contribution of non retarded interactions to the pairing, as in unconventional (non Migdal Eliashberg) theories.

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- [2] R. Merlin, Solid State Comm. 102, 207 (1997).
- [3] B. Mansart et al., Proc. Natl. Acad. Sci. 110, 4539-4544 (2013).

Non-Fermi liquid physics in a two-impurity Kondo quantum box device - Talk

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The two-impurity Kondo model is a classic paradigm, capturing in its simplest form the competition between Kondo screening and local singlet formation — the same essential physics governing the analogous propensity for heavy fermion behaviour or magnetic ordering in lattice systems. When the screening channels are strictly independent, the model supports a delicate non-Fermi liquid quantum critical point, which should be accessible in a quantum box device. We examine this system theoretically, showing in particular that application of dot and box gate voltages yield a rich range of physics, from fine-tuned two-impurity Kondo criticality in the Coulomb blockade regime, to robust two-channel behaviour via the Matveev mechanism at the box charge-degeneracy point.

Optical investigation of $Ba(Fe_{1-x}Co_x)_2As_2$ detwinned by tunable uniaxial applied pressure - Talk

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The iron-pnictide superconductors are excellent materials in order to study the competition between structural, magnetic and superconducting phases. These materials in the underdoped regime undergo an antiferromagnetic transition into a broken-symmetry ground state at T_N which is always preceded by or coincident with a tetragonal-toorthorhombic structural distortion at $T_s \geq T_N$. The in-plane anisotropy of the orthorhombic phase is masked by the formation of twin domains. By applying uniaxial pressure one can fully detwin the materials and induce single-domain specimen. Here we investigate the optical conductivity of $Ba(Fe_{1-x}Co_x)_2As_2$, for x = 0 and 2.5%, under in-situ tunable uniaxial pressure across their structural and magnetic transitions with electromagnetic radiation polarized along the in-plane a- and b-axes. We reveal the pressure and temperature dependence of the anisotropic charge dynamics, which extends to high temperature and from the far infrared up to high frequencies. Our results show the important role played by the nematic susceptibility as well as the electronic nature of the structural transition. We thus provide clear-cut evidence for an analogy between the electronic anisotropy in iron-pnictides and the magnetization in ferromagnets induced by the applied pressure and the external magnetic field, respectively.

Emergent critical phase and Ricci flow in a 2D frustrated Heisenberg model - Talk

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We introduce a two-dimensional frustrated Heisenberg antiferromagnet on interpenetrating honeycomb and triangular lattices [1]. Classically the two sublattices decouple, and örder from disorder "drives them into a coplanar state. Applying Friedan's geometric approach to nonlinear sigma models, we obtain the scaling of the spin-stiffnesses governed by the Ricci flow of a 4D metric tensor. At low temperatures, the relative phase between the spins on the two sublattices is described by a six-state clock model with an emergent critical phase and two Berezinskii-Kosterlitz-Thouless (BKT) phase transitions.

[1] Peter P. Orth, Premala Chandra, Piers Coleman, and Jörg Schmalian, *Phys. Rev. Lett.* **109**, 237205 (2012).

Strong correlation physics in f-electron superlattices - Talk

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In the last years, remarkable progress in the fabrication of artificial interfaces and heterostructures, which are made of strongly correlated materials, took place, opening a new field in material design. Quite recently artificially layered heavy fermion materials, i.e. $CeIn_3/LaIn_3$ and $CeCoIn_5/YbCoIn_5$ superlattices, have been created.¹⁻³ These materials are made of a periodic arrangement of f-electron layers and of normal-metal layers. We theoretically analyze such f-electron superlattices by using real space dynamical mean field theory. We will focus on two things: the influence of the Kondo-effect of the f-electrons and the formation of magnetically long-range ordered states. Within the superlattices structure the Kondo effect of the f-electrons extends also into neighboring layers, in which no f-electrons are present. Due to constructive or destructive interference depending on the superlattice geometry the Kondo effect can be enhanced or even completely suppressed in the neighboring layers. Furthermore, also magnetic order can be observed. Here, it is important to notice that due to the RKKY interaction different

layers are magnetically coupled to each other, and that the coupling strength between the layers depend on the superlattice structure.

Structural and Thermoelectric Properties of CrN Thin Films - Talk

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The thermoelectric properties of CrN has recently attracted considerable interest due to its fairly low resistivity ρ and large thermoelectric power S. Moreover, the presence of an unknown type of disorder scattering decreases its thermal conductivity with respect to other transition metal nitrides. Here we describe our efforts to increase the thermoelectric power factor $PF = S^2/\rho$ through the fabrication of thin-films. For such purpose, epitaxial CrN (001) thin films were grown by reactive dc magnetron sputtering on MgO (001) substrates. The influence of thickness and thermal annealing in NH₃ on film composition and thermoelectric properties was studied. By tuning these parameters, we were able to increase PF by more than one order of magnitude with respect to the optimized bulk material, reaching 15 μ Wcm⁻¹K⁻² at room temperature.

Statistical Transmutation in Doped Quantum Dimer Models - Talk

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Quantum Dimer Models (QDM) arise as low energy effective models for frustrated magnets. Some of these models have proven successful in generating a scenario for exotic spin liquid phases with deconfined spinons. Doping, i.e. the introduction of mobile holes, has been considered within the QDM framework and partially studied. A fundamental issue is the possible existence of a superconducting phase in such systems and its properties. For this purpose, the question of the statistics of the mobile holes (or "holons") shall be addressed first. We prove a general &tatistical transmutation&ymmetry of such doped QDM by using composite operators of dimers and holes: the energy spectrum is invariant under a simultaneous change of statistics (i.e., bosonic into fermionic or vice versa) of the holes and of the signs of all the dimer resonance loops. This exact transformation enables to define duality equivalence classes (or families) of doped QDM, and provides the analytic framework to analyze dynamical statistical transmutations. We discuss various possible superconducting phase originating from the condensation of (bosonic) charge-e holons is examined. We also investigate the doping of the triangular quantum dimer model with special focus on the topological Z_2 dimer liquid. Finally, we show that doping leads to four (instead of two for the square lattice) inequivalent families of Hamiltonians. Competition between phase separation, superfluidity, supersolidity, and fermionic phases is investigated in the four families.

- [1] Phys. Rev. Lett. **109**, 016403 (2012)
- [2] arxiv:1210.1270, accepted in Phys. Rev. B (2013)

Time- and angle-resolved photoemission spectroscopy of the CDW material RTe_3 - Talk

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The charge density wave (CDW) formation in the family of rare-earth tritellurides RTe₃ presents an excellent model system to study the effects of charge and lattice order and broken symmetry in a low-dimensional material. As revealed by angle-resolved photo emission spectroscopy (ARPES), energy gaps open in the electronic bands below the CDW transition temperature, leading to the suppression of large areas of the Fermi surface (FS). Time-resolved spectroscopies can provide complementary information on the dynamics of the electronic structure after photoexcitation and on the underlying processes like electron-electron or electron-phonon interaction. Here, we use femtosecond (fs) time-resolved ARPES (trARPES) which provides insight into the ultrafast dynamics of the electronic structure linked to collective excitations of the charge ordered state. The time-resolved Fermi surface mapping using a novel position-sensitive time-of-flight spectrometer reveals the ultrafast collapse of the CDW energy gap using strong excitation fluences $F > 0.5 \text{ mJ/cm}^2$. Furthermore, the momentum-dependent analysis of the transient occupied and unoccupied band dispersion allows for a direct measure of the time-dependent order parameter and allows to identify a modification of the CDW nesting condition on a femtosecond time scale. At low excitation fluences $F < 0.5 \text{ mJ/cm}^2$, we observe the coherent excitation of the CDW amplitude mode at a frequency of f =2.2 THz, which modulates the CDW order parameter magnitude. We show its coherent control in a pump-pump-probe experiment, demonstrating the collective nature of the amplitude mode.

One-particle irreducible functional approach - a new route to diagrammatic extensions of DMFT - Talk

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We present a new approach[1] for including non-local electronic correlations on all length-scales beyond the local correlations of dynamical mean-field theory. It is based on the generating functional for one-particle irreducible (1PI) local vertex functions. This formalism allows us to unify aspects of the dynamical vertex approximation (D\GammaA), which is based on two-particle irreducible local vertices[2], and the dual fermion scheme (DF), which considers one-particle reducible vertices. In particular, the new method includes one-particle reducible contributions from the three- and more-particle vertices in the dual fermion approach, as well as specific diagrams not included in the ladder version of D\GammaA. To demonstrate the applicability and physical content of the 1PI approach, we compare the diagrammatics of 1PI, DF and D\GammaA, as well as the numerical results of these approaches for the half-filled Hubbard model in two dimensions.

[1] G. Rohringer, A. Toschi, H. Hafermann, K. Held, V. I. Anisimov, A. A. Katanin, arXiv:1301.7546.

[2] G. Rohringer, A. Valli, and A. Toschi, Phys. Rev. B 86, 125114 (2012).

Quasi continuous-time impurity solver for dynamical mean-field theory with linear scaling in the inverse temperature - Talk

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The dynamical mean-field theory (DMFT) is a powerful method describing correlated electron systems. The limitations of DMFT are mainly set by the impurity solver, e.g. due to exponential scaling with system size or bias due to discretization errors. Many of these limitations were overcome with the recent development of diagrammatic Monte Carlo impurity solvers. However, this methods scale cubic in the inverse temperature β and low temperature physics are hardly accessible. Recently, Khatami et al. proposed a linear in β Quantum Monte Carlo approach, that solves the impurity problem by a mapping on a finite bath, similar to exact diagonalization (ED) and renormalization group schemes, but introduces Trotter discretization errors. We enhanced this approach

and present a unbiased linear in β solver, which can solve much larger clusters than current ED solver. [Preprint: arXiv:1303.2004]

Quantum magnetism of mass-imbalanced fermionic mixtures - Talk

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We study magnetic phases of two-component mixtures of ultracold fermions with repulsive interactions in optical lattices in the presence of hopping and population imbalance by means of dynamical mean-field theory (DMFT). According to our analysis, massimbalanced mixtures have important advantages over balanced systems in thermodynamic characteristics that are relevant for obtaining and detecting quantum magnetism in optical lattices. It is shown that mixtures with both imbalances present can have easyaxis antiferromagnetic, ferrimagnetic, charge-density wave, canted-antiferromagnetic order or be unordered depending on parameters of the system. We study the resulting phase diagram in detail and investigate the stability of the phases to thermal fluctuations. We also perform a quantitative analysis for a gas confined in a harmonic trap, by applying the local density approximation and a real-space generalization of DMFT.

From infinite to d dimensions: combining dynamical mean field theory and functional renormalization group - Talk

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During the last decade dynamical mean field theory (DMFT) and functional renormalizaton group (fRG) approaches have been used to study interacting Fermi systems. On one side, DMFT provides a non-perturbative description of the local physics. Limitations arise in situations where spatial fluctuations play an important role, as in low dimensional or (quantum) critical systems. On the other side, fRG is a powerful tool to study systems involving a wide range of relevant energy scales and of competing instabilities, as the cuprate or pnictide high-temperature superconductors. At the same time, its application is restricted to the weak-coupling regime. We propose the combination of these complementary methods in DMF²RG to describe both the local physics and the non-local correlations. Starting from the DMFT local self energy and two-particle vertex, the RG equations yield the gradual evolution from the effective impurity model in infinite dimensions to the considered lattice model in the physical dimension. Thereby the momentum-dependence of the self energy and two-particle vertex is obtained. We present first results for the application to the two-dimensional Hubbard model at halffilling.

Sudden expansion of interacting bosons in optical lattices: the role of integrability and dimensionality - Talk

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Recently, an increased effort has been devoted to understand out-of-equilibrium effects in interacting quantum many-body systems, in particular to explore and establish the possible links between equilibrium and nonequilibrium properties. In the field of optical lattices, recent experiments have shown the possibility of measuring the expansion velocity of an initially trapped system, which after the sudden release of the trap expands in an empty lattice [1]. Recent theoretical studies of interacting fermions have indicated that the measurement of expansion velocity may provide information about the initial state [2]. In our work, we show that measuring the expansion velocity of an initially trapped gas of interacting bosons allows one to distinguish between a superfluid and a Mott insulating state in the initial ground state in one dimension. We perform time-dependent DMRG calculations of the Bose-Hubbard model in a harmonic trap and a box trap. We derive a state diagram of a trapped system as a function of Coulomb repulsion and density from the expansion velocity. The resulting diagram is consistent with the state diagram obtained by measuring equilibrium properties such as local density distribution, local density fluctuations and on-site compressibility [3,4].

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- [2] Langer et al., Phys. Rev. A 85, 043618 (2012)
- [3] Rigol et al, *Phys. Rev. A* **79**, 053605 (2009)
- [4] Kollath et al., Phys. Rev. A 69, 031601(R) (2004)

Correlated topological orders in Kondo insulators \mathbf{YbB}_6 and \mathbf{YbB}_{12} - Talk

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The electronic structures of two Kondo insulators YbB₆ and YbB₁₂ have been studied by using the local density approximation (LDA)+Gutzwiller method incorporating Green's function scheme. Similar as the typical mixed valence material SmB₆, we find that YbB₆ has non-trivial Z_2 topology, indicating that YbB₆ is another three dimensional topological insulator with strong correlation effect. However, YbB₁₂ is a normal Kondo insulator since at X point of Brillouin zone it has band inversion twice and its (001) surface states are trivial. The surface state of YbB₆ differs from that of SmB₆ by having opposite spin-momentum locking effect, which is due to the opposite effective spin-orbit coupling in j=7/2 and j=5/2 f-orbitals.

Electronic Band Structure of BaCo₂As₂: A Fully Doped Ferrophictide Analog with Reduced Electronic Correlations - Talk

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We report an investigation with angle-resolved photoemission spectroscopy of the Fermi surface and electronic band structure of BaCo₂As₂. Although its quasinesting-free Fermi surface differs drastically from that of its Fe-pnictide cousins, we show that the BaCo₂As₂ system can be used as an approximation to the bare unoccupied band structure of the related BaFe_{2-x}Co_xAs₂ and Ba_{1+x}K_xFe₂As₂ compounds. However, our experimental results, in agreement with dynamical-mean-field-theory calculations, indicate that electronic correlations are much less important in BaCo₂As₂ than in the ferropnictides. Our findings suggest that this effect is due to the increased filling of the electronic 3d shell in the presence of significant Hund's exchange coupling.

Superconductivity from orbital nematic fluctuations in iron pnictides - Talk

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We address the question how superconductivity can arise from nematic fluctuations in the context of iron pnictides, by employing an effective two-band model which possesses an orbital nematic instability. We solve the linearized Eliashberg equations and take also the renormalization factor into account. We find that low-energy, long-wavelength

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nematic fluctuations give rise to strong-coupling superconductivity, with transition temperatures comparable to those typically found in the pnictides. Furthermore, the nematic superconductivity is rather robust against repulsive Coulomb interactions and can co-exist with the nematic order.

II. Poster Presentations - Monday

Hunds metallicity in iron-based superconductors

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Combining density-functional theory and dynamical mean-field theory we investigate the ground-state of iron-based superconductors. Focusing on iron chalcogenide materials, namely FeSe, KFe₂Se₂ and K₂Fe₄Se₅, we show that, although having large substantial mass enhancements and scattering rates, these materials are not close to a Mott Metal-To-Insulator transition. However, increasing interaction parameters in a physically reasonable range does lead to enhanced orbital differentiation. In that sense, strong electronic correlations in these materials arise due to the Hund's rule coupling and not predominantly from Coulomb parameters U. We will also discuss the perovskite pnictides, where the blocking layer is built up by other transition-metal oxide materials like vanadium oxide. There, we find that the system can be viewed as two Hund's correlated electron fluids in the same material, one in the iron plane and on in the blocking layer. Inclusion of correlation effects also resolves the problem of reconciling the experimental properties with electronic structure calculations.

Solution of the Periodic Anderson Model by means of a continued fraction algorithm.

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The semi-phenomenological continued fraction method, previously applied to the Hubbard model [1], was adapted to the Periodic Anderson Model (PAM) with momentum independent hybridization. The method applies to the various paramagnetic phases that can be modeled with the PAM by varying the filling [2]: the Kondo regime including the Kondo insulator, the charge transfer regime including the Mott insulator. The partial fillings are determined self-consistently. We have developed a numerical code with a local self energy, allowing to compare our results with the ones derived by the Dynamical Mean Field Theory (DMFT) [1]. The scenario previously applied to CeFePO in comparison to ARPES [3] will be discussed in detail. We show that realistic kinetic energy input (one body part of PAM) has important feedback on the quasiparticle spectrum, notably through the appearance of renormalized van Hove singularities. The rapidity in terms of computer time, the ease of changing model parameters and generating ARPES intensity plots including matrix element effects, makes the new code a useful strategic tool being midway between microscopic theory and experiment.

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Charge order in the Falicov-Kimball model - a dual fermion approach

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In this contribution we study charge ordering in the Falicov-Kimball model within the dynamical mean field theory (DMFT) and its recently developed dual fermion extension, which allows for the systematic diagrammatic description of the spatial corrections to the DMFT solution. We focus on the critical properties of the model and compare various levels of approximations. The Falicov-Kimball model is particularly well suited to this purpose as the reducible n-point vertices entering a dual fermion calculation can be constructed analytically from the exactly solvable DMFT limit. We show that an inclusion of the non-local spatial correlations allows to describe the temperature dependent charge gap in the excitation spectra and to reduce the values of the critical temperatures in the strongly correlated regime to the exactly known values. It is also shown that in 2 dimensions such a framework allows to obtain critical exponents different from the mean-field values, a behavior expected for the Falicov-Kimball model.

Legget modes in Fe-based superconductors as a probe of Time Reversal Symmetry Breaking

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In the last years the discovery of superconductivity in iron-based superconductors renewed the interest on unconventional superconducting (SC) mechanisms that can lead to higher critical temperatures than conventional phonon-assisted superconductivity. A fundamental question associated to the unconventional nature of pairing is how it can affect the behavior of the SC amplitude and phase collective modes, which in turn can influence the observable physical quantities giving indirect information on the nature of the underlying SC state. For example, SC fluctuations above Tc influence the way resistivity drops to zero above Tc (the so-called paraconductivity), while well-defined phase collective modes below Tc can be probed by Raman spectroscopy. A beautiful example has been given by the observation in MgB₂ of the Legget mode [1], which corresponds to relative density (phase) fluctuations of the condensate in the various bands. Since also pnictides show a multiband structure, the natural question arises on the existence and observability of Legget-like modes in these systems as well. Here I will show that in the case of pnictides, where interband interactions mediated by spin fluctuations are believed to dominate, the nature of the collective modes changes drastically with respect to MgB₂. While generally in two-bands like models the Legget mode is absent, it can appear instead in three-bands models in correspondence of a Time-Reversal-Symmetry-Breaking (TRSB) transition to a s + is, that has been recently proposed to occur in strongly hole-doped Ba_{1-x}K_xFe₂As₂ [2,3]. In particular I'll show that there exists a wide range of temperatures where the Legget mode lies well below the treshold of quasiparticle excitations, making it undamped and easily accessible by Raman spectroscopy [4]. This prediction can be tested against the experiments to prove the existence or not of a TRSB transition in pnictides.

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Subradiance localization in the open 3D Anderson-Dicke model

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Anderson localization is a paradigmatic coherence effect in disordered systems, often analyzed in the absence of dissipation. Here we consider the case of coherent dissipation, occuring for open system with coupling to a common decay channel. This dissipation induces cooperative Dicke super- and subradiance and an effective long range coupling, expected to destroy Anderson localization. We are thus in presence of two competing effects, i.e localization driven by disorder and delocalization driven by dissipative opening. Here we show that in an open 3D Anderson model, subradiance enables the system to preserve signatures of a localization transition. We demonstrate the existence of a subradiant localized regime, emerging from the interplay of opening and disorder, in which subradiant states are hybrid and localized, while superradiant states are extended. We also provide analytical predictions for this regime, confirmed by numerical simulations.

Electron-phonon superconductivity in APt_3P compounds: from weak to strong coupling

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We study the newly-discovered Pt phosphides APt_3P (A=Sr, Ca, La) [1] using firstprinciples calculations and Migdal-Eliashberg theory. Given the remarkable agreement with the experiment, we exclude the charge-density wave scenario proposed by previous first-principles calculations, and give conclusive answers concerning the superconducting state in these materials. The pairing increases from La to Ca and Sr due to changes in the electronphonon matrix elements and low frequency phonons. Although we find that all three compounds are well described by conventional s-wave superconductivity and spin orbit coupling of Pt plays a marginal role, we show that it could be possible to tune the structure from centrosymmetric to non centrosymmetric opening new perspectives towards the understanding of unconventional superconductivity.

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Exotic spin orders driven by orbital fluctuations in the Kugel-Khomskii spin-orbital model

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We study zero temperature phase diagrams of the spin-orbital Kugel-Khomskii model in two- and three-dimensional (2D and 3D) versions [1,2] realized by K_2CuF_4 and KCuF₃ respectively. The model contains Heisenberg interactions between spins S = 1/2coupled with e_q orbitals described by pseudo-spins T = 1/2. The orbital interactions are intrinsically frustrated even on a square lattice so the model exhibits different types of orders as its parameters, crystal field splitting E_z and Hund's exchange $\eta = J_H/U$, are varied. The model is solved on square lattices using cluster mean field theory. We find that in addition to the antiferromagnetic (AF), ferromagnetic (FM) and valence-bond phases known before [3], the model exhibits configurations with exotic magnetic order, i.e. with: (i) nearest-neighbor (NN) spins being perpendicular and second NN being AF in ab plane(s), both in the 2D [1] and 3D [2] cases; (ii) NN spins having non-trivial angle along the c axis interpolating between AF and FM; (*iii*) spins forming AF stripes in the ab planes in the 3D case [2]; All these spin orders go beyond the Heisenberg physics and emerge from the entangled spin-orbital fluctuations. We prove it by deriving effective spin Hamiltonians for these phases by perturbative expansions in the orbitals. For the phase (i) we show that virtual orbital flips in the ground state get dressed with singlets of density controlled by E_z [1]. We argue that such configurations can be found experimentally near the AF-FM transition in some oxides by applying (chemical) pressure or strong magnetic field.

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New ferronematic order in underdoped cuprates

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We study a model for low doped cuprates where doped holes form magnetic vortices and, due to short-range interaction, aggregate into stripe segments which are composed of vortex-antivortex pairs. Since a vortex in a XY spin system in two dimensions can be mapped to a 2D topological charge, whose sign depends on the winding number of the vortex, we can treat each pair as an electric dipole. We argue that a state with macroscopic polarization is stabilized, which we call a ferronematic. This state can be characterized as a charge nematic which, due to the net polarization, breaks inversion symmetry and also exhibits an incommensurate spin modulation. We find that incommensurability and macroscopic polarization are directly related and thus they can represent a reasonable order parameter to describe this broken symmetry state. We show that our calculation can reproduce the doping dependent spin structure factor of lanthanum cuprates in excellent agreement with experiments. As a further step a Monte Carlo analysis provides information on the temperature and doping evolution of these complex phases as well as on the thermodynamic phase transitions.

Crystalline electric field effects in Ce_2RhIn_8 , $CePt_2In_7$ and Ce_2PtIn_8

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The group of heavy-fermion tetragonal compounds based on the CeIn₃ common structural unit became of great importance after the discovery of unconventional superconductivity in them a decade ago. However this phenomenon is still not satisfactorily explained. An important piece of this complicated puzzle is the study of crystalline electric field (CEF). It is speculated, that the interplay between the low temperature CEF levels and the Kondo f-s hybridization creates spin fluctuations relevant to the superconducting condensate [1]. Detailed studies of the CEF have been done only on the HoCoGa₅ structure type (so called 115) compounds [2] whereas CEF parameters for related structures are missing or studied only by indirect methods. In this work, we present CEF excitations of the heavy fermion superconductors Ce₂RhIn₈, CePt₂In₇ and Ce₂PtIn₈ obtained by inelastic neutron scattering. All these compounds order antiferromagnetically at low temperatures. Ce₂RhIn₈ and CePt₂In₇ become superconducting under applied pressure while Ce₂PtIn₈ undergoes a superconducting transition at ambient pressure at 0.4 K. We discuss the relationship between the evolution of T_C and broadening of CEF excitations due to the Kondo hybridization and also compare the results with the well known 115 compounds.

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Friedel Oscillations in Strongly Correlated Fermionic Systems

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We studied how electronic correlations alter the Friedel Oscillations (FO) in manybody lattice model using the Dynamical Mean Field Theory (DMFT). We solved the fermionic Hubbard model in a one-dimensional lattice with a finite number of sites and using either periodic or open boundary conditions. As a test model we used a phenomenological model for the self-energy [1], satisfying the Luttinger theorem, to account for the electronic correlations. It has been observed that the change in the interaction parameter affects the amplitude and period of FO. Next we extended the studies to two and three dimensional lattice systems. We have further used the self-energy obtained within the Hubbard I approximation and the DMFT to analyse the effect of correlations seen in FO.

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Slow quench of one-dimensional Bose gases

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We investigate the response of a Bosonic gas subjected to a slow parameter change. We focus on the analysis of the response of a Lieb-Liniger Bose gas within a bosonization analysis and compare our results with numerical results obtained for the Bose-Hubbard model taking its continuum limit for different limiting regimes. In a certain regime of parameters, we find unconventional decay of stretched exponential form for the singleparticle correlation function. This is very unconventional for a one-dimensional system in which typically an algebraic decay occurs within a Luttinger liquid theory. We discuss experimental signatures of such findings in the context of cold atoms systems.

Evidence for a Peierls phase-transition in a three-dimensional multiple charge-density waves solid

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We studied the ultrafast photoinduced charge-density-wave to metal phase transition in a complex solid, namely $Lu_5Ir_4Si_{10}$. After melting the charge ordering using infrared laser pulses, the consequent charge redistribution is probed with fs time resolution through the spectral weight analysis of the transient optical response over a broad energy range [1]. The time-dependent spectral weight reveals a signature of the CDW melting and the time-scale of this photo-induced phase transition. This new kind of analysis allows us to show that the charge order remains preserved until the lattice distorts sufficiently to induce the phase transition. These results are completed by ab-initio modeling of the electronic band structure, identifying the orbitals involved in the CDW and the electronic transitions leading to the photo-induced melting of the charge order. This allows us to reveal the Peierls origin of multiple CDW in this three-dimensional solid.

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Temperature dependent electron-phonon coupling in a high T_c cuprate probed by femtosecond X-ray diffraction

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The strength of the electron-phonon coupling parameter and its evolution throughout a solid's phase diagram often determines phenomena such as superconductivity, charge and spin-density waves. Its experimental determination relies on the ability to distinguish thermally activated phonons from those emitted by conduction band electrons, which can be achieved in an elegant way by ultrafast techniques. Separating the electronic from the out-of-equilibrium lattice subsystems, we probed their re-equilibration by monitoring the transient lattice temperature through femtosecond X-ray diffraction in $La_{2-x}Sr_xCuO_4$ single crystals with x=0.1 and 0.21. The temperature dependence of the electron-phonon coupling is obtained experimentally and shows similar trends to what is expected from the ab-initio calculated shape of the electronic density-of-states near the Fermi energy. This study evidences the important role of band effects in the electron-lattice interaction in solids, in particular in superconductors.

Quantum Critical Phenomena in $Ce_nT_mIn_{3n+2m}$ Heavy Fermion Compounds

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A plethora of puzzling phenomena in condensed matter originates from the rivalry of ground states. In heavy Fermion (HF) compounds the magnetic ground state, enforced by the intersite Rudermann-Kittel-Kasuya-Yoshida interaction, competes with the paramagnetic one where the Kondo effect prevails. On the verge of this ground state flip critical quantum fluctuations lead to aberrant behavior from expected Fermi liquid theory and exotic phases like unconventional superconducting or nematic ones. The standard model of HF physics is based on Dioniach's Kondo lattice hypothesis, where transition of magnetic to non-magnetic order depends on a single parameter J, the hybridization strength. Recently we proposed an extension of this model by a second parameter G accounting for the degree of quantum fluctuations of the local moments to unify the existing quantum critical scenarios, the spin density wave and the Kondo breakdown scenario [J. Custers et al. Nature Mat. 11, 189 (2012)]. However, what has been systematically neglected in the discussion of quantum criticality is the emergence of exotic phases. The focus of this presentation is the HF family of $Ce_n T_m In_{3n+2m}$ (n =1, 2; m = 1; T = transition metal) materials. In these materials the dimensionality (parameter G) can be subsequently changed from 2D to 3D and hence allow testing the principles of the global phase diagram of HF compounds. Additionally many show superconductivity. New results on the recently discovered compound Ce_2PtIn_8 where superconductivity emerges out of an antiferromagnetic phase at ambient pressure and Ce₂PdIn₈, an ambient pressure superconductor will be presented.

Tracking the dynamics of the pairing glue in a cuprate superconductor with ultrashort laser pulses

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The mechanism explaining the formation of Cooper pairs in high- T_c superconductors has not reached any final consensus. A pairing mechanism involving the coupling with phonons or excitations of electronic origin, or a cooperative contribution of both these bosonic degrees of freedom has been proposed to trigger the superconductivity in these compounds. Experiments performed at equilibrium conditions are able to reconstruct the spectrum of the pairing glue but they don't allow to infer any precise information about the relative weight of the electronic and phononic contributions to the glue. We tackle this problem by measuring the optical response of a $Bi_2Sr_2Ca_{0.92}Y_{0.08}Cu_2O_{8+\delta}$ crystal using broadband ultrafast spectroscopy. Exploiting the simultaneous spectral and temporal resolution of this technique, we are able to study the temporal evolution of the dielectric function on a broad energy range and to disentangle unambiguously the electronic and phononic contribution of the glue on the basis of their different temporal dynamics. On the time scale faster than the effective temporal resolution of the experiment and the typical electron-phonon thermalization time, the quasiparticles are already thermalized with the excitations of electronic origin, such as spin fluctuations or loop currents, participating to the glue. The strength of this interaction (λ =1.1) and its spectral distribution fully accounts for the high critical temperature of the system[1]. The non-equilibrium optical response of the same system, recently measured with unprecedentedly high temporal resolution (<10 fs), fully confirms the previous physical scenario and exhibits, on a broad energy range, an additional temporal dynamics occurring on a time scale of few femtoseconds (10 fs). These recent results constitute the direct observation of the relaxation process between electronic carriers and the bosonic excitation of electronic origin. Furthermore they takes on crucial importance for the formulation of a microscopic model aiming to describe the non-equilibrium physics of photoinduced carriers in strongly correlated systems.

[1] S. Dal Conte et al. Disentangling the electronic and phononic glue in a high-T_c superconductor. Science **335** 1600 (2012)

Interplay between the correlations and superconductivity in the Andreev spectroscopy

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A purpose of this presentation is to overview the recent electron transport studies through the strongly correlated quantum dots located between the conducting and superconducting electrodes. In particular, I shall discuss the low energy (sub-gap) regime where the Andreev spectroscopy can quantitatively probe a competition between the on-dot pairing (induced via proximity effect) and the Coulomb repulsion, leading to the Kondo physics. Signatures of their nontrivial interplay have been recently explored both theoretically [1-3] and experimentally [4-6]. Under specific conditions, when the on-dot pairing eventually coexists with the Kondo resonance, there is expected a characteristic zero-bias enhancement in the differential Andreev conductance [7,8]. This fact has been indeed observed experimentally [4]. I will also point out a number of further activities using the multi-dot or multi-electrode configurations, where such interesting phenomena as the quantum interference, Cooper pair splitting and crossed Andreev scattering can be practically realized. [1] A. Oguri, Y. Tanaka, and J. Bauer, Phys. Rev. B 87, 075432 (2013)

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A nonequilibrium Dynamical Mean Field Theory approach based on the Lindblad equation

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In order to apply the Dynamical Mean Field Theory to nonequilibrium steady state situations, an auxiliary impurity problem has to be devised which exhibits dissipative mechanisms and thus enables the time evolution to a stationary state. For this purpose, we have introduced an effective model whereby the impurity is coupled to bath sites which in turn are connected to a Markovian environment [1]. This provides a description of the impurity system within a quantum master equation. A superfermionic representation is used to rewrite the Lindblad equation in a non-hermitian Hamiltonian form. With some modifications, the well-established exact diagonalization methods for sparse hermitian matrices can be adapted to the non-hermitian case, enabling us to address the steady state and the dynamics of this problem. The Single Impurity Anderson model is presented as a test case [2], and results are compared with those from Density-Matrix-Renormalisation-Group-like and cluster-embedding approaches.

E. Arrigoni *et al.*, *Phys. Rev. Lett.* **110**, 086403 (2013)
 A. Dorda *et al.*, in preparation

Proposal for Quantum Optics techniques applied to study out of equilibrium strongly correlated electron systems

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Balance homodyne detection (BHD) is a standard tool in Quantum Optics and Quantum Information used to characterize the quantum states of light. We report on the development of a BHD apparatus working in the pulsed regime and applied, in combination with pump&probe techniques, to characterise the quantum states of ultra-short light pulses after the interaction with photo-excited matter. The development of this technique will provide a new tool for studying strongly correlated electron systems driven out of the equilibrium by the interaction with intense pulses of coherent electromagnetic radiation. Our work constitutes an original experimental framework joining for the first time BHD with ultra-fast time- and frequency-resolved techniques.

Non local correlation effects in the Hubbard model

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There is great effort to incorporate the non local correlations in many body methods to describe the correlated materials better. The degree of includement of non local correlations play an essential role in the physics of high correlated system. At this poster we want to consider the effect of non local correlations on the metal insulator transition especially connected to the change of the critical interaction strength U with the level of non local correlations. From the comparison of some important physical quantities calculated in many body methods which are connected to the metallic and insulatic phase, one can try to understand the effect of non local correlations better. The connection between the apperance of the pseudegap with includement of non local correlations is of great interest. These analysis confirms the need of great effort to investigate more effective ways to include more and more contributions of non local correlations.

Ultrafast relaxation dynamics of a hole in anti-ferromagnetic spin background

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We study a highly excited hole propagating in the antiferromagnetic background modeled by the t-J Hamiltonian on a square lattice. We show that the relaxation consists of two distinct stages. The initial ultrafast stage with the relaxation time $\tau \sim (\hbar/t_0)(J/t_0)^{-2/3}$ (where t_0 is the hopping integral and J is the exchange interaction) is based on generation of string states in the close proximity of the hole. This unusual scaling of τ is obtained by means of comparison of numerical results with a simplified t- J_z model on a Bethe lattice. In the subsequent (much slower) stage local spin excitations are carried away by magnons. The relaxation time on the two–leg ladder system is an order of magnitude longer due to the lack of string excitations. This is further reinforcing the importance of string excitations for the ultrafast relaxation in the two-dimensional system.

Quantum magnetism of ultracold fermions on optical lattices with novel geometries

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Very recently, antiferromagnetic signatures have been reported for ultracold fermions in optical lattices with tunable dimerization [1] (and, alternatively, tunable anisotropy). Using determinantal quantum Monte Carlo, we compute the double occupancy and spin correlation functions in the dimerized half-filled Hubbard model in the whole range of parameters (with lattice varying from honeycomb through simple cubic to isolated dimers), separate the effects of bandwidth change from the non-trivial spin-correlation physics, and determine the optimal parameters for experimental detection.

Using the same methods, we also explore the impact of impurities, i.e., lattice sites with increased interaction or reduced coupling to the normalisites, on the AF correlations at half filling and find interesting magnetization patterns that deviate significantly from corresponding real-space DMFT predictions. The results are expected to be relevant both for cold-atom experiments (e.g. using mirror arrays for lattice generation) and for strongly correlated materials.

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Magnetic Property of the Zinc Pnictides of Europium: ESR Study

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Ternary Eu- and Yb- pnictides with CaAl₂Si₂-type structures have become the subject of particular interest, because they exhibit very promising thermoelectric properties. We have studied the magnetic properties of the $EuZn_2(P, As, Sb)_2$ compounds by ESR (electron spin resonance) method. The ESR has measured for X band in TE102 rectangular cavity in the range from 4.2 to 300 K. Above 150 K we observed the symmetric resonance lines Eu^{2+} with ideal a Lorentzian lineshape. At the temperature decreasing well before the antiferromagnetic (AFM) ordering temperature we have observed an increasing of lineswidth and a decreasing of the resonance fields, which in our case very good described by Landau's theory of magnetic fluctuations. The paramagnetic temperature T_p , of the AFM EuZn₂(P, As, Sb)₂ compounds has the positive sign. We believe such behaviour of T_p is connected with critical spin fluctuation. and the relevant instability of magnetic and crystal structures. The obtained ESR data are interpreted in terms of two band models and of Bloembergen-Rowland's indirect exchange interaction through the electrons of the valence band. We also discuss the issues of stability CaAl₂Si₂-type structures, (similar compounds with the bismuth and nitrogen is unknown), interplay of spin and valence fluctuations (nonmagnetic $4f^6$ and magnetic $4f^7$ states of Eu), the magnetic phase transitions in comparison to the similar ESR date for Rh-Eu pnictides with structure $ThCr_2Si_2$.

Impurities in the Kagome lattice

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Impurities in the Kagome lattice The Kagome lattice is the prototype lattice to study effects of geometric frustration. Both classical and quantum models on this and related lattices are still under debate. For the quantum Heisenberg model the ground state is still not clear. For the quantum Heisenberg model numerical methods such as variational Monte-Carlo (VMC), DMRG and series expansion have been used to clarify the ground state. A conclusive picture was not reached. Within VMC the best state is the Dirac-Spin-Liquid (DSL) state. Close in energy are different types of Valence Bond Crystal(VBC) States and the uniform spin-liquid (USL) state. An interesting point is the impact of impurities to such model-systems: Static impurities are especially in the structurally perfect Kagome compound present, dynamic ones might play a role while formation of the crystal. In this talk I present numerical investigations of the role of impurities to this problem, particularly the t-J and Hubbard model on this lattice. While at half filling the Kagome lattice most likely has a Spin-liquid type of ground state, upon doping valence bond patterns form in the large U limit. The form of the crystal can be understood by a few observed short range effects close to an impurity. The low U limit appears to have a rich phase-diagram including various exotic phases and magentically ordered phases.

Quantum criticality in an extended periodic Anderson model

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We investigate an extended periodic Anderson model in which an additional d-f Coulomb interaction (U_{df}) is taken into account. Three different methods are applied: mean-field theory, variational calculation, and exact diagonalization of finite chains. The variational calculation is performed using the Gutzwiller trial wave function and gives a critical value of U_{df} and two quantum critical points (QCPs), where the valence susceptibility diverges. We derive the critical exponent for the valence susceptibility and examine how the position of the QCP depends on the other parameters of the Hamiltonian. Above the critical value of U_{df} , the Kondo regime is bounded by two first-order transitions in agreement with the mean-field approach. These first-order transitions merge into a triple point at a certain value of U_{df} . For even larger U_{df} , above the triple point, valence skipping occurs. Although the other methods do not result in a critical point, their results are in a fairly good agreement with that of the variational method.

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Evolution of ferromagnetic order in $Yb(Rh_{1-x}Co_x)_2Si_2$ with $x \le 0.27$

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Antiferromagnetic (AFM) order appears in YbRh₂Si₂ at $T_N=70$ mK although strong ferromagnetic fluctuations are observed. The application of chemical pressure x in the series Yb(Rh_{1-x}Co_x)₂Si₂ stabilizes the AFM phase, i.e. T_N increases with increasing x. A second phase transition at $T_L < T_N$ emerges with increasing x and the strength of the ferromagnetic fluctuations raises up to a maximum for x \approx 0.27 [1]. Eventually, in pure YbCo₂Si₂ both phase transitions T_N and T_L are of AFM nature with 4f local moments aligned along the crystallographic *ab*-plane. However, the sample with x = 0.27 reveals only one phase transition at 1.30 K which is surprisingly ferromagnetic with moments parallel to the c-axis [2]. This motivates a deeper investigation of the magnetic properties in Yb(Rh_{1-x}Co_x)₂Si₂ with the magnetic field applied along the c-axis. Here, we present AC-susceptibilty measurements of single crystals with x \leq 0.27 down to a temperature of 25 mK.

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- [2] S. Lausberg *et al.*, arXiv:1210.1345

Shedding light on the pairing mechanism in iron-based superconductors

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Whether superconductivity in iron-pnictides and -chalcogenides stems from local or itinerant effects is a question still debated on. In order to investigate the influence of Fermi surface nesting on the pairing mechanism, we calculate from first-principles calculations the static and dynamic susceptibility of various iron-based compounds. We show that the susceptibility depends sensitively on doping and pressure application and confront our theoretical results with conclusions drawn from experiments. For instance, our results give evidence that pairing through Fermi-nesting mechanisms alone is not sufficient to explain the evolution of the transition temperature with pressure in FeSe.

Magnetic order in $CePd_{1-x}Ni_xAl$

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Quantum critical points (QCPs) occur when second order phase transitions are suppressed to T=0. They cause remarkable universal behaviour even at finite temperatures and have therefore attracted much attention by both experimentalists and theoreticians. The best studied case are transitions into antiferromagnetism. Here, the transition temperature depends on the strength of the spin-spin coupling, which can be tuned by doping, pressure or magnetic field. Recently, it has been suggested that the temperature-coupling phase diagram needs to be supplemented by a third axis, which measures frustration. CePdAl is a promising system to study the influence of frustration on QCPs systematically. It has a hexagonal structure in which the magnetic cerium atoms form a quasi-Kagome lattice in the basal plane. This leads to a partial frustration of the antiferromagnetic coupling so that only two thirds of the cerium spins show long range magnetic order below the Néel temperature T_N . While $T_N=2.7$ K in the pure compound, it can be suppressed by doping with Ni on the Pd site and reaches $T_N=0$ at a Ni concentration of 14%. Here, we present our study on the magnetic order in $CePd_{1-x}Ni_xAl$ with elastic neutron scattering, both in the pure system and for 10% doping. In both samples we have observed short range order additionally to the long range order at the same ordering vector $(0.5 \ 0 \ 0.35)$. The temperature dependence of the short and long range order peaks is investigated in detail, leading to a better understanding of the role of frustration in CePdAl.

Heavy Fermion Ferromagnet YbNi₂: An ESR Study

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The electron spin resonance (ESR) signal below 30 K which was found out in the recently synthesized Kondo lattice YbNi₂ [1] has been attributed to the hybridized electronic states created by the combined effect of the 4f local magnetic moments of Yb³⁺ and conduction electrons in the presence of ferromagnetic (FM) correlations [2-4]. The significant broadening and disappearance of the ESR line at temperatures above 15 K could be explained by the spin-lattice relaxation processes of the Yb³⁺ ions through the first excited Stark doublet with an activation energy of \simeq 75 K. We compare this ESR behavior with the data of our measurements of X-ray diffraction, X-ray absorption, AC/DC susceptibility, and electrical resistivity on the bulk and nanometric samples.

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Valence and geometry controlled Kondo effects in transition metal centered molecules

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We study the impact of strong electronic correlations on the electronic structure of different molecules with 3d transition metal (TM) centers. Specifically, we investigate the series of transition metal benzene sandwiches (TMBz₂) bridging a copper nanocontact as well as TM-TPP and TM-Pc molecules adsorbed on surfaces. To this end we employ a first principles DFT++ method (density functional theory combined with an impurity solver) for calculating the electronic structure and coherent transport properties of nanoscopic conductors that explicitly takes into account the dynamic correlations arising from the strongly interacting 3d shell of the transition metal center. Depending on the chemical valence of the transition metal center, the geometry of the molecule or different ligand groups different flavours of the Kondo effect, like e. g. the orbital Kondo effect, can be observed.

Functional renormalization group study of an eight-band model for the iron arsenides

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We investigate the superconducting pairing instabilities of eight-band models for the iron arsenides. Using a functional renormalization group treatment, we determine how the critical energy scale for superconductivity depends on the model parameters. Most importantly, if we vary the parameters from values corresponding to LaFeAsO to Sm-FeAsO, the pairing scale is strongly enhanced, in accordance with the experimentally found trend. We analyze the reasons for this trend and discuss the relation of our results to those found using five-band models.

Correlated lattice fermions in a spin-dependent random potentials

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Motivated by the new possibilities for experiments with ultracold atoms in optical lattices we explore the thermodynamic properties of correlated lattice fermions in the presence of an external spin-dependent random potential. The corresponding Hubbard model with the local on-site spin-dependent disorder is solved within the dynamical mean-field theory. The spin-dependent disorder is found to drive the magnetic polarization of the system when the total number of fermions is fixed. The magnetic response of the system with finite magnetization differs from that of a system with spin-independent disorder. The spin-dependence of the disorder also affects the metal-insulator transition at half filling.

Coherent Quantum Transport of Charge Density Waves

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The charge density wave (CDW) is a correlated electron-phonon system that can transport electrons en masse, in some cases at temperatures up to 360 K, i.e., well above the temperature of the human body. Recent experiments show oscillations of period h/2e in conductance vs. magnetic flux of charge density wave (CDW) rings above 77 K, revealing macroscopically observable quantum behavior. The time-correlated soliton tunneling model discussed here is based on coherent, Josephson-like tunneling of microscopic quantum solitons of charge 2e. The model interprets the CDW threshold electric field as a Coulomb blockade threshold for soliton pair creation, often much smaller than the classical depinning field but with the same impurity dependence. This picture draws upon the theory of time-correlated single-electron tunneling to interpret CDW dynamics above threshold. Similar to Feynman's derivation of the Josephson current-phase relation for a superconducting tunnel junction, the picture treats the SchrA¶dinger equation as an emergent classical equation to describe the time-evolution of Josephson-coupled order parameters related to soliton dislocation droplets. Vector or time-varying scalar potentials can affect the order parameter phases to enable magnetic quantum interference in CDW rings or lead to interesting behavior in response to oscillatory electric fields. The ability to vary both magnitudes and phases is an aspect important to future applications in quantum computing.

Optical conductivity and ARPES of the Hubbard-Holstein model: equilibrium and pump-probe phenomena

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Angle resolved photoemission spectra (ARPES) [1,2] and optical conductivity (OC) [3,4] of the 2D Hubbard-Holstein and t-J-Holstein models are calculated at equilibrium and compared with experiments at zero and low chemical dopings. The ARPES of underdoped systems reveal either short-living quasiparticles or kink in electronic dispersion, as observed in experiments. The OC at equilibrium shows a three-peak structure in agreement with experimental observations. Time dynamics of the physical properties and OC of the 2D Hubbard-Holstein model is also studied when undoped system is put out of equilibrium by an ultrashort powerful light pulse [5]. At nonzero electron-phonon interaction, lattice and spin subsystems oscillate with the phonon period $T_{ph} = 80$ fs. The decay time of these oscillations is about 150-200 fs, similar to the relaxation time of the charge system. We propose a criterion for observing phononic oscillations in high T_c compounds: the time span of the pumping light pulse has to be shorter than the phonon oscillation period T_{ph} .

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Time and frequency resolved optical spectroscopy on Hg-based high- T_c superconductors

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One of the major challenge in high-Tc superconductivity is the understanding of the appearence below a certain temperature $T^* > T_c$ of a new state called pseudogap state. In order to reveal the mechanism underlying the elusive pseudogap state and investigate the possible relation between the pseudogap state and the superconducting phase, we perform reflectivity measurements with time and spectral resolution on mercurybased cuprates in the normal state, in the pseudogap state and in the superconducting phase. Broadband ultrafast spectroscopy is a powerful tool to investigate the properties of materials driven out of equilibrium by an ultrashort light pulse. Measuring the relaxation dynamics, different processes can be disentangled by their different relaxation time, while the use of a supercontinuum probe pulse allows to study the photoinduced modification of the dielectric function of the system. The data are reproduced by the Extended Drude Model accounting for the opening of an anisotropic gap in the DOS at $T < T^*$. Above T^* the system exhibits a metallic-like behavior with a pump-induced increasing of the electronic scattering rate. In contrast, a striking behavior occurs in the pseudogap state, since the electronic scattering rate transiently decreases within the first hundreds of femtoseconds after the pump excitation. In the superconducting phase, this behaviour is overwhelmed by a pump-induced change of the interband hing-energy optical transitions, that accounts for the reflectivity variation.

The research activity leading to these results is part of the GO FAST (Governing ultrafast the conductivity of correlated materials) project, funded from the European Union Seventh Framework Programme (FP7 2007-2013), under Grant No. 280555.

Investigating the ultrafast optical properties of correlated materials

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One of the frontiers in the physics of correlated materials is the possibility of using ultrashort light pulses to optically manipulate the electron distribution and create non-thermal metastable phases, in view of achieving the ultrafast optical control of the electric, optical and magnetic properties. Here, I develop a technique for femtosecond time-resolved optical pump-probe spectroscopy that allows to take snapshots of the evolution of the dielectric function of correlated materials on the sub-picosecond timescale, after excitation with an infrared short light pulse. The non-equilibrium optical response is probed by supercontinuum light generated by focusing the output beam of a cavitydumped Ti:sapphire oscillator into a photonic crystal fiber. We apply this technique to investigate different families of correlated materials ranging from correlated hightemperature superconductors (Bi2212 and Hg1201 copper oxides) to iridates (Na₂IrO₃), in which the spin-orbit interaction and the Coulomb repulsion between two electrons occupying the same lattice site compete on the same energy scale. We demonstrate that time-resolved optical spectroscopy is a key-technique to disentangle different competing degrees of freedom by their different timescales and spectral responses. The research activity leading to these results is part of the GO FAST (Governing ultrafast the conductivity of correlated materials) project, funded from the European Union Seventh Framework Programme (FP7 2007-2013), under Grant No. 280555.

Construction of a compact and high resolution capacitance dilatometer for measuring the thermal expansion and magnetostriction of correlated metals

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Dilatometry experiments provide an extremely sensitive way to probe phase transitions of correlated metals. We describe the design and construction of a parallel-plate capacitance dilatometer, suitable for measurements at very low-temperatures and high magnetic fields. The design of our cell is identical to the one reported in [1] and is expected to reach a length change resolution of 0.05 Å. The main body of the dilatometer is fabricated from a single block of Oxygen Free High Conductivity copper. Using a piezoelectric rotator, the cell can be rotated *in situ* at low temperatures, inside the vacuum chamber of a dilution refrigerator with a diameter of 40 mm. This will allow for a precise tuning of the magnetic field direction with respect to the crystallographic axes of the sample investigated. We will present calibration results and the first test runs using single crystals of the superconducting ferromagnet UCoGe.

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Investigation of dimensional crossover of the electronic band structures in LaNiO3 ultrathin films using in situ angle resolved photoemission spectroscopy

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Recently, the dimensional crossover of the electronic structure in LaNiO3 (LNO) superlattices and ultrathin films has attracted much attention [1]. Namely, when a two-dimensional (2D) LNO is under tensile strain, the eg orbitals can become reconstructed to form a single $d_{x^2-y^2}$ orbital structure, which is quite similar to that of high-T_c cuprate superconductors [2]. To confirm this prediction, we performed in situ angle-resolved photoemission spectroscopy studies on LNO ultrathin films. We prepared the LNO ultrathin films on SrTiO₃ substrate (+1.7 % tensile misfit strain)

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with varying the film thickness from 1 to 10 unit cells (UC). (1) We investigated three-dimensional (3D) electronic band structure of 10 UC-thick LNO film. The measured 3D electronic band structure can be explained by the DMFT calculations (not by the LDA calculations), indicating that electronic correlation is strong. (2) We observed that the dimensional crossover of the band structure occurs around 3 UC of LNO film. Although a complete eg orbital reconstruction has not been achieved, the eg orbital reconstruction was in the right direction in accordance with the earlier theoretical prediction. (3) We found that the quasi particle peak at Fermi level becomes suppressed in 2D LNO ultrathin films. This could be understood by disorder effects, such as Anderson localization or percolation of insulating channels. Further details will be discussed in presentation.

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An ab-initio approach to electron dynamics and transport properties of the lithium purple bronze $Li_{0.9}Mo_6O_{17}$

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We investigate the electronic structure of the strongly anisotropic quasi lowdimensional purple bronze $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$. Building on all electron ab-initio band structure calculations, we obtain a minimal model in terms of four maximally-localized Wannier orbitals, which turn out to be far from atomic like. The obtained model is comprised of two half-filled strongly dispersing orbitals arranged in chains along the b direction, and two full orbitals in a-c direction, respectively. Within this effective theory we consider electron-electron interactions using the (extended) Variational Cluster Approach as well as Dynamical Mean-Field Theory. We find good agreement with experimental photo emission data [*Phys. Rev. Lett.* **103**, 136401 (2009)], using a moderate on-site interaction strength. Long-range hybridizations between the full and the half-filled orbitals at the Fermi energy seem to be an essential ingredient for the electron dynamics. We furthermore discuss the applicability of an even more minimalistic two-orbitals model. Transport coefficients are obtained within a many-body framework which reproduce trends of the experimentally determined highly anisotropic values for the dc conductivity.

Divergent Precursors of the Mott-Hubbard Transition at the Two-Particle Level

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Amongst plenty other successes, DMFT is able to cover the Mott- Hubbard metal-toinsulator transition (MIT), which is an intrinsic non-perturbative phenomenon. At the MIT the local spin susceptibility diverges, following Curie's law in the insulating phase, whereas the local charge susceptibility remains finite at the transition [1]. However, these divergencies are not the only hallmarks of the MIT at the two-particle level. In fact, the first non-perturbative precursors of the MIT can be identified well inside the metallic phase in the frequency structures of the irreducible vertex functions [2, 3]. The strong enhancements of the irreducible vertex functions, characterising this precursor, stem from local scattering processes and can be traced up to the limit of high temperatures (i.e. the atomic limit).

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Nonequilibrium Dynamics Across an Impurity Quantum Critical Point

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Whether a small quantum mechanical system is able to equilibrate with its environment once an external local perturbation drives it out of thermal equilibrium is a central question which cuts across many different fields of science. Here we consider such a problem for a correlated quantum impurity coupled to a fermionic reservoir and driven out of equilibrium by local quantum quenches such as those recently realized in optical absorption experiments on single quantum dots. We argue that equilibration in this problem is deeply connected to the occurrence of Kondo Effect at low energy and that a highly non trivial dynamical behavior may emerge whenever a local quantum critical point intrudes between a conventional Kondo screened phase and a Kondo unscreened one. We discuss this issue in the context of the Anderson Impurity model coupled to a pseudo-gap reservoir by using a correlated time dependent variational wave function that is able to qualitatively describe this physics.

Towards a first-principles determination of effective Coulomb interactions: Role of inter-shell interactions

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We describe the construction of an effective low-energy model to describe correlated systems in which the hybridization of localised d- and f-states with ligand p-states is non-negligible. Traditional single-shell models have been shown to be unsuitable in describing such systems while a multi-shell treatment is prohibitively expensive. By applying constrained RPA to DFT orbitals, we calculate effective screened Coulomb interactions that take into account inter-shell interactions explicitly and charge-transfer energies from first-principles. This scheme is applied to a variety of systems including transition-metal oxides, rare-earth systems and actinides. For the specific case of UO₂, we compare the spectrum calculated within a configuration interaction framework using these ab initio parameters to photoemission and inverse photoemission data.

Ce and Mn valence states in $CeCu_4Mn_yAl_{1-y}$ studied by x-ray photoemission spectroscopy

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We have recently shown that the $CeCu_4Mn_yAl_{1-y}$ compounds exhibit a transition between the spin-glass (SG) behavior (y=1) and the Kondo system (y=0) [1]. The Mn-Al dilution does not change the crystal structure of the parent compounds, which crystallize in the $CaCu_5$ -type structure. The SG state has been confirmed by the frequency dependence of the ac magnetic susceptibility, the relaxation of the remanent magnetization and the split of the field-cooled and zero-field-cooled dc magnetic susceptibility. The electronic specific heat coefficient is enhanced for all y and increases with the Al content. The effective moment of Mn increases with decreasing the Mn concentration. To clarify the valence state of Ce and Mn in $CeCu_4Mn_uAl_{1-u}$ compounds we have employed the x-ray photoelectron spectroscopy (XPS) technique. The Ce core-level XPS spectra point to a stable trivalent configuration of Ce atoms in all the $CeCu_4Mn_yAl_{1-y}$ compounds, thereby supporting such an assumption made in Ref. [1]. The Mn 2p core-level spectra exhibit a multiple-peak structures, which reflect the different valence states for Mn atoms. The Ce 3d and 4d spectra show the spin-orbit split components $3d_{5/2}$ - $3d_{3/2}$ and $4d_{5/2}$ - $4d_{3/2}$, respectively. The absence of a satellite peak corresponding to the Ce $4f^0$ contribution indicates that cerium is present as a trivalent ion in the compounds studied. In the valence band it is visible that the main broad peak is due to the Mn 3d, Cu 3d and Ce 4f states.

[1] K. Synoradzki et al., J. Phys.: Condens. Matter 24 (2012) 136003

Spin-liquid versus spiral-order phases in the anisotropic triangular lattice

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We study the competition between magnetic and spin-liquid phases in the Hubbard model on the anisotropic triangular lattice, which is described by two hopping parameters t and t' in different spatial directions and is relevant for layered organic chargetransfer salts. By using a variational approach that includes spiral magnetic order, we provide solid evidence that, in the regime t'/t < 1, a spin-liquid phase is stabilized in the strongly-correlated regime and close to the isotropic limit t'/t = 1. In addition, a magnetically ordered spiral state is found, connecting the (collinear) Néel and the (coplanar) 120° phases. This finding suggests the idea that the spin liquid may be considered as an instability emerging from a strongly correlated spiral phase. On the contrary, in the regime t'/t > 1, a spiral magnetic state is found close to the isotropic point, while the system exhibits quasi-1D features for a large enough ratio t'/t. We observe that the pitch vector of the spiral phase obtained from the unrestricted Hartree-Fock approximation is substantially renormalized in presence of electronic correlations. Finally, our results are discussed in the context of organic charge-transfer salts.

Effective crystal field and Fermi surface topology: a comparison of *d*- and *dp*-orbital models

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The effect of electronic correlations to enhance or reduce the effective crystal field in multi-orbital correlated materials can be crucial in determining the topology of the Fermi surface and, hence, the physical properties of these systems. In this respect, recent local density approximation (LDA) plus dynamical mean-field theory (DMFT) studies of Ni-based heterostructure have shown contradicting results, depending on whether the less correlated p orbitals are included or not. We investigate [1] the origin of this problem and identify the key parameters controlling the Fermi surface properties of these systems. A particularly important one is the filling of the identified d-orbitals: in the dp-calculation this is larger so that HundÕs exchange leads to a larger local magnetic moment for the dp-model.

[1] N. Parragh, G. Sangiovanni, P. Hansmann, S. Hummel, K. Held, and A. Toschi, arXiv 1303.2099.

Superconductivity in the non-centrosymmetric half Heusler compound YPtBi

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Noncentrosymmetric superconductors have recently come to the fore as a fruitful playground to study novel superconducting phases. The lack of inversion symmetry, which results in a splitting of the Fermi surface, is predicted to give rise to a mixing of even and odd parity Cooper pair states. We here focus on the half Heusler compound YPtBi that superconducts at $T_c=0.77$ K and is a candidate for topological superconductivity [1]. We have carried out resistivity measurements under pressures up to $p\sim 2.5$ GPa that reveal superconductivity is promoted by pressure. The reduced upper critical field $B_{c2}(T)$ curves collapse onto a single curve, with values that exceed the model values for spin-singlet superconductivity. The B_{c2} data point to an odd-parity component in the superconducting order parameter [2]. μ SR experiments indicate a magnetic penetration depth $(T\rightarrow 0)$ in excess of 0.7 μ m, in agreement with a low H_{c1} value extracted from magnetization measurements [3]. We discuss our results in view of the prediction that YPtBi is possibly a new platform for topological superconductivity.

- [1] N. P. Butch et al., *Phys. Rev. B* 84, 220504(R)(2011)
- [2] T.V. Bay, T. Naka, Y.K. Huang and A. de Visser, Phys. Rev. B 86, 064515 (2012)
- [3] T.V. Bay et al., in preparation.

Two-particle Green's functions calculated by continuous time quantum Monte Carlo simulations

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While dynamical mean field theory (DMFT) has provided fundamental insights into the physics of strongly correlated materials, its approximations break down in low dimensional systems and near second-order phase transitions. Diagrammatic extensions of DMFT like the dynamical vertex approximation (D Γ A) and the dual fermion approach which attempt to tackle this problem have the local two-particle Green function as central ingredient. Besides, this quantity is also needed for vertex corrections to response functions. A state-of-the-art method for solving the DMFT impurity problem is the continuous-time quantum Monte Carlo (CT-QMC) method in its hybridization expansion formulation (CT-HYB). The sheer amount of information encoded in two-particle quantities, however, makes their computation very demanding in this framework. We improve on the naïve measurement by using fast Fourier transformations as well as symmetries of the Hamiltonian and of the vertex. We have implemented this method into the CT-HYB solver [1] using the Krylov method and provide benchmarks and examples for up to seven correlated orbitals.

[1] N. Parragh, *Phys. Rev. B* 86, 155158 (2012)

Nematic quantum critical behaviors in high-temperature superconductors

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In the past decade, there have been a number of experimental signatures pointing towards a nematic quantum phase transition near the superconducting transition in some high-temperature superconductors [1]. The critical nematic fluctuation interacts strongly with the gapless nodal quasiparticles, which plays a crucial role in the study of quantum critical behaviors. By considering this interaction and employing the method introduced in Refs. [2], we find that superconductivity is strongly suppressed at the nematic quantum critical point [3]. In addition, superconducting and nematic order parameters may be decoupled from each other near the nematic quantum critical point, which implies that the superconductivity can coexist with the nematic order homogeneously [3].

[1] E. Fradkin et al., Annu. Rev. Condens. Matter Phys. 1, 153 (2010); E.-A. Kim et al., Phys. Rev. B 77, 184514 (2008).

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[3] G.-Z. Liu, J.-R. Wang, and J. Wang, *Phys. Rev. B* **85**, 174525 (2012); J. Wang and G.-Z. Liu, submitted to *Phys. Rev. B* (2013).

Andreev bound states in correlated Josephson quantum dots

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We investigate the Andreev bound states of quantum dot setups coupled to BCS source and drain leads with gap Δ and phase difference ϕ . We use a computational technique based on the functional renormalization group to treat the local Coulomb interaction U. We show results for the Andreev bound states as a function of the system's parameters and compare them to recent experimental data. By applying a Zeeman field B the energy difference of singlet and triplet spin configurations is tuned. The high flexibility in the implementation and the reduced numerical effort allows to explore the

whole parameter space and to analyze the effects of $0-\pi$ and singlet-triplet quantum phase transitions on the bound states.

Von Neumann entropy spectra and entangled bound states in the anisotropic spin-orbital model

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We investigate the phase diagram and von Neumann entropy spectral function for the one-dimensional anisotropic spin-orbital model. The excitations include one or two bound states, depending on the model parameters, which are characterized by different correlation lengths and by logarithmic scaling of the von Neumann entropy with increasing system size. Surprisingly, finite entanglement entropy is found for the ferromagnetic phase with alternating orbitals when the orbital interactions are more classical and do not obey the SU(2) symmetry. We demonstrate that spin-orbital bound states can be experimentally explored using resonant inelastic x-ray scattering, where entangled states could be easily distinguished from the spin-orbital continuum.