ARW Workshop
Properties and Applications of Thermoelectric Materials
September 20 - 26, 2008

Hvar 2008 Workshop & Conference
September 20th - September 30th
Hvar, Croatia

Conference on Concepts in Electron Correlation
September 24 - 30, 2008

Program
Abstracts

Institute of Physics, Zagreb
Scope of the workshop

The workshop will focus on thermoelectric effects in the following systems.

i) Novel intermetallic compounds with correlated electrons.

ii) Nanoscale fabricated heterostructures with strongly correlated electrons.

The charge, spin and energy transport in these complex systems is quite anomalous and any attempt to explain the thermoelectric response confronts difficult experimental and theoretical questions. The workshop will review new materials and examine mechanisms that could lead to new thermoelectric and magnetocaloric devices with an enhanced figure-of-merit.

The main topic is the heat, charge and spin transport in strongly correlated systems, and the final objective is to acquire the basic knowledge about the relevant quantum degrees of freedom, which is required to achieve the control and engineer new thermoelectric and magneto-caloric materials with specific quantum mechanical properties. The scientific advances in this field could have important technological implications.

Format

This workshop will devote ample time to discussions. There are 2-3 one-hour lectures in the morning, with unlimited discussion time. Every afternoon session starts in the poster room, for discussions, and continues with two more lectures. The poster room is adjacent to the lecture room and posters will be on the boards during the whole workshop. The powerpoint presentations given by the lecturers will be printed out and also put on the boards, giving the participants the possibility for additional questioning. The after-dinner talks should provide a general overview of the field. The presentations will be available on the web site of the meeting.
## Organization

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**J. Sarrao**  
Los Alamos, USA
Programme of the Workshop

NATO ARW Workshop on Correlated Thermoelectric Materials

Sunday, September 21

Morning session

8:00 Veljko Zlatić, Zagreb, Croatia
Opening of the workshop

8:10 Toshiro Takabatake, Hiroshima University, Japan
Thermoelectrics of Kondo semiconductors and clathrates

9:10 S. Kamran Behnia, Ecole Normal Superier, Paris, France
Nernst effect and the thermomagnetic figure of merit in light- and heavy-electron semi-metals

10:10 coffee break

10:40 S. Dariusz Kaczorowski, Institute of Solid State Physics, Wroclaw, Poland
Rare-earth-based half-Heusler compounds as prospective materials for thermoelectric applications

11:40 Peijie Sun, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
Enhanced Thermoelectricity in the Correlated Semiconductor FeSb₂

Lunch & afternoon break

Afternoon session

16:00 Poster session and additional questioning time for the mornings talks

17:00 Karsten Held, TU Wien, Austria
Pudding mold type band as the origin of large thermopower in LiRh₂O₄

18:00 Richard Hlubina, Bratislava, Slovakia
Optimal thermoelectric materials: beyond the Mahan-Sofo approach

18:45 Veljko Zlatić, Zagreb, Croatia
Multiple energy scales of strongly correlated electrons revealed by the thermoelectric transport data
Monday, September 22

**Morning session**

8:00 **Brian Maple**, UCSD, USA  
Strongly correlated electron phenomena in filled skutterudites

9:00 **Gabi Kotliar**, Rutgers, USA  
Applied physics on strong correlation

10:00 coffee break

10:30 **Jim Freericks**, Georgetown University, Washington D.C., USA  
Thermoelectric response of correlated multilayers

11:30 **Antonio Pereira Gonçalves**, Instituto Tecnologico e Nuclear, Sacavem, Portugal  
New approaches to thermoelectric materials

_Lunch & afternoon break_

**Afternoon session**

16:00 Poster session and additional questioning time for the mornings talks

17:00 **Peter Rogl**, Vienna, Austria  
Thermoelectric Clathrates - Structure - Property Relations

18:00 **Rene Monnier**, ETH, Zurich, Switzerland  
Effects of the crystal field splitting on the thermal transport of correlated electrons

18:45 **Vinh Hung Tran**, Institute for Solid State Physics, Wroclaw, Poland  
Thermoelectric properties of non-fermi liquid systems

_Dinner break_

21:00 After-dinner discussion  
**Sriram Shastry**, University of California, Santa Cruz, USA  
Frequency dependent thermoelectric response - new insights in old problems

Tuesday, September 23

**Morning session**

8:00 **Sadamichi Maekawa**, Tohoku University, Sendai, Japan  
Thermal Current, Spin Current and Charge Current in Strongly Correlated Materials

9:00 **Brian Sales**, Oak Ridge National Lab, USA  
A Critical Overview of Recent Approaches to Improved Thermoelectric Materials
10:00 coffee break

10:30 **Claude Godart**, Paris, France
Role of structures on thermal conductivity in thermoelectric materials

11:30 **Niels Oeschler**, Max Planck Institute, Dresden, Germany
Low-temperature thermoelectric power of strongly correlated f-electron systems

*Lunch & afternoon break*

**Afternoon session**

16:00 Poster session and additional questioning time for the mornings talks

17:00 **Gerd Czycholl**, University of Bremen, Germany
Influence of impurities and crystal field effects on the thermopower of heavy-fermion systems

18:00 **Andreas Ruegg**, ETH, Zurich, Switzerland
Role of multiple subband renormalization in the electronic transport of correlated oxide

18:30 **Hand Zenia**, Georgetown University, Washington, DC, USA
Dynamical mean-field application to thermal transport in correlated heterostructures

*Workshop dinner*

**Wednesday, September 24**

**Morning session**

8:00 **Ernst Bauer**, Technical University, Vienna, Austria
Novel thermoelectric materials

9:00 **Massimo Rontani**, CNR-INFM Research Center, Modena, Italy
Thermoelectric properties of metal/excitonic insulator interfaces

10:00 coffee break

10:30 **Bernard Coqblin**, Universite Paris-Sud, France
Thermoelectric power and thermal transport of anomalous rare-earth Kondo compounds

11:30 **Sriram Shastry**, University of California, Santa Cruz, USA
Thermal and thermoelectric transport in correlated systems: A new perspective

*Lunch & afternoon break*

**Afternoon session**

16:00 Poster session and additional questioning time for the mornings talks

17:00 **Krzysztof Gofryk**, Institute for Transuranium Elements, Karlsruhe, Germany
Thermoelectric power of transuranium-based unconventional superconductors
17:30 Karen Michaeli, Weizmann Institute of Science, Rehovot, Israel
Particle-hole asymmetry in transverse transport phenomena such as Hall and Nernst

18:00 Jose I.Espeso, Universidad de Cantabria, Santander, Spain
When simple alloys turn into complicated

Dinner break

21:00 After-dinner discussion
Zach Fisk, University of California, Riverside, USA
What can we learn from the past?

Thursday, September 25

Morning session

8:00 Zach Fisk, University of California, Riverside, USA
Taking what we learn from the rare earth intermetallics into transition metal materials

9:00 Gertrud Zwicknagl, University Braunschweig, Germany
Quasiparticles and magnetization dynamics of Yb-based heavy-fermion compounds

10:00 coffee break

10:30 Silke Buehler-Paschen, Technical University, Vienna, Austria
Strongly correlated cage compounds: New thermoelectrics

11:15 Sergei Kruchinin, Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine
Thermoelectricity in double-barrier structure with the resonant tunneling

12:00 The ARW program ends. Closing remarks by Alex Hewson.

Lunch & afternoon break

The Conference on Correleted Electrons continues in the afternoon.
Conference on Concepts in Electron Correlation

September 24th - 30th 2008

Scope of the conference

The conference will deal with strongly correlated electron systems. The emphasis will be on the unifying concepts which pertain to most, if not all, electron systems with short range screened Coulomb interactions. These materials exhibit various remarkable anomalies and pose many difficult experimental and theoretical questions. Bringing together some of the most active experimental and theoretical physicists working in the field of electron correlation, we would like to achieve the following:

- To review the most interesting results relevant for strongly correlated systems.
- To focus both on the similarities and differences between various correlated systems.
- To review and discuss the main concepts used in the studies of electron correlation.
- To examine how close the experiments and theory come together, and to guess what comes next.

The aim of the meeting is not so much to offer the ‘present day solution’ of various anomalies observed in strongly correlated systems but, rather, to characterize and describe the anomalies, so as to find a common element in the experimental results.

So far, Hvar meetings were ‘discussions dominated’ and we would like to continue that way. We are planning six talks in the two morning sessions and four talks in the afternoon session. The lecturers are not supposed to present just the regular invited talks, but emphasize plans, possibilities, open problems, and the opportunities for new research in condensed matter physics.

In our view, an important aspect of such a meeting is that in addition to usual lectures, we have informal discussions, dealing with controversial issues and providing the opportunity to young people to ask additional question. The poster session will play an important role. The posters will be on the poster boards in the room adjacent to the lecture hall for the whole meeting, and we would like to have a regular meeting of all the participants at the ‘poster session’, every day one hour before the afternoon session.

We are also planning to have the print-out of all the invited talks (in powerpoint or other format) and we would post these presentations on the boards adjacent to the posters. The meeting will have its web site from which all the presentations will be available. The facilities for video conferencing and real time participation will be provided.
## Organization

### Directors

<table>
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### Program committee

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<td>E. Bauer</td>
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### Advisory Board

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<tr>
<td>P. W. Anderson</td>
<td>Princeton, USA</td>
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<td>P. Coleman</td>
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Conference Programme

Conference on Concepts in Electron Correlation

Thursday, September 25

15:00 Conference registration

15:50 Veljko Zlatić, Institute of physics, Zagreb
Opening of the Conference on Concepts in Electron Correlation

**Afternoon session:** Heavy fermion superconductivity

16:00 Brian Maple, University of California, San Diego, USA
Unconventional superconductivity in novel d- and f-electron materials

16:40 Meigan Aronson, Brookhaven NL and Stony Brook University, NY, USA
Different Routes to Quantum Criticality in Strongly Correlated Electron Materials

17:20 Joe D. Thompson, Los Alamos National Laboratory, USA
Magnetism and Unconventional Superconductivity in CeMn5 Heavy-Fermion Compounds

18:00 Sriram Shastry, University of California, Santa Cruz, USA
Superconductivity in a strongly correlated model system: A numerical study

18:30 Jozef Spalek, Jagiellonian University, Krakow, Poland
Fulde-Ferrell-Larkin-Ovchinnikov superconducting state of paired quasiparticles with the spin dependent masses

21:00 Workshop farewell party and conference welcome party

Friday, September 26

**Morning session:** New superconductors

8:15 Brian Sales, Oak Ridge National Laboratory, USA
Recent Results from Oak Ridge National Laboratory on the Layered Iron Arsenide Superconductors with Tc=55K

8:55 Zlatko Tesanovic, John Hopkins University, Baltimore, USA
Multiband effects in FeAs superconductors

9:35 Jorge Hirsch, UC San Diego, La Jolla, USA
Spin Meissner Effect in Superconductors and the Origin of the Meissner Effect

10:15 coffee break
Quantum dots and confined Kondo effect

10:45 Theo Costi, Research Centre Juelich, Juelich, Germany
Kondo decoherence: from ab-initio calculations to model Hamiltonians and beyond

11:25 Christoph Stampfer, ETH, Zurich, Switzerland
Graphene Quantum dots

12:05 David Logan, Oxford University, Oxford, UK
Kondo effects in multilevel quantum dots

Lunch & afternoon break

16:00 Poster session and additional questioning time for the mornings talks

Afternoon session: Quantum criticality

17:00 Philipp Gegenwart, Goettingen University, Germany Quantum
Criticality in Heavy Fermion Metals

17:40 Kai Grube, Forschungszentrum Karlsruhe, Germany
Thermal expansion and magnetostriction measurements of CeCu_{6-x}Au_{x} single crystals

18:10 Christoph Meingast, Forschungszentrum Karlsruhe, Germany
Thermal expansion and specific heat of MnSi: evidence for quantum critical behavior

18:40 Guido Donath, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
Dimensional Crossover of Quantum Critical Behavior in CeCoIn_{5}

Dinner break

21:00 After-dinner discussion
Gabi Kotliar, Rutgers University, USA
Computational material science

Saturday, September 27

Morning session: Cuprate superconductors

8:15 Abhay Pasupathy, Princeton University, USA
Visualizing pair formation on the atomic scale in high-Tc superconductors

8:55 Peter Johnson, Brookhaven National Laboratory, Upton, New York, USA
A Re-examination of the pseudo-gap regime of High Tc-Superconductivity

9:35 Erik van Heumen, University of Geneva, Switzerland
Optics clues to pairing glues in the cuprates

10:15 coffee break

10:45 Peter Prelovsek, University of Ljubljana, Slovenia
Spectral functions and high-energy kink in cuprates
11:25 **Carlo Di Castro**, Universita di Roma La Sapienza, Italy
Phase diagram of Coulomb frustrated electronic systems

12:05 **Adolfo Avella**, Universita degli Studi di Salerno, Italy
Underdoped cuprate phenomenology in the two-dimensional Hubbard model within the Composite Operator Method

*Lunch & afternoon break*

16:30 Poster session + discussions (tea/coffee)

**Afternoon session**: Cold atoms and optical lattices

17:00 **Henning Moritz**, Federal Institute of Technology, Zurich, Switzerland
Strongly correlated fermionic gases in optical lattices

17:40 **Corinna Kollath**, Ecole Polytechnique, Palaiseau Cedex, France
Strong correlations in quantum gases

18:20 **Walter Hofstetter**, J.W. Goethe-Universitaet, Frankfurt/Main, Germany
Strong correlations and inhomogeneity in optical lattices

*Dinner break*

21:00 After-dinner discussion
**Jorge Hirsch**
High-temperature superconductivity - what can be expected in the future?

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**Sunday, September 28**

**Morning session**: Heavy fermions, normal state properties

8:15 **Zachary Fisk**, University of California Irvine, USA
Kondo scale in the dense Kondo Lattice

8:55 **N. Peter Armitage**, Johns Hopkins University, Baltimore, USA
Towards the Lifshitz point in elemental bismuth: Light electrons gone heavy at the metal-insulator transition?

9:35 **Peter Oppeneer**, Uppsala University, Sweden
Calculated electronic structure properties of URu2Si2 and Ce-115 materials

10:15 coffee break

10:45 **Andrzej M. Oles**, Max-Planck-Institut FKF, Stuttgart, Germany
Modelling of phase transitions in the RVO3 perovskites

11:25 **Thomas Pruschke**, University of Goettingen, Germany
Competing interactions and magnetic order in correlated electron systems

12:05 **Alex Hewson**, Imperial College, London
Renormalisation group approaches to strong correlation behaviour.

*Lunch & afternoon break*
16:00 Posters, coffee, discussions

Afternoon session

17:00 Erio Tosatti, SISSA, Trieste, Italy
Two Dimensional Triangular Lattice Mott-Hubbard Insulators in Real Life: Sn/Si(111), Sn/Ge(111) and Other Surfaces

17:40 Philipp Hansmann, Max Planck Institute, Stuttgart, Germany
LaNiO$_3$/LaAlO$_3$ heterostructures: A LDA+DMFT analysis

18:20 Didier Poilblanc, C.N.R.S. & Universite de Toulouse, France
The physics of doped Quantum Dimer Models

20:00 Conference dinner

Monday, September 29

Morning session: Low-dimensional systems

8:15 Thierry Giamarchi, University of Geneva, Switzerland
Spin ladders, BEC, Luttinger liquids and beyond

8:55 Leonardo Degiorgi, ETH, Zurich, Switzerland
Infrared and Raman study of the charge-density-wave ground state

9:35 Holger Fehske, Ernst-Moritz-Arndt-Universitat, Greifswald, Germany
Luttinger, Peierls or Mott? Quantum phase transitions in 1D strongly correlated electron-phonon systems

10:15 coffee break

10:45 Janez Bonca, J. Stefan Insitute, Ljubljana, Slovenia
Optical and spectral properties of the t-J Holstein model

11:25 Frithjof Anders, Bremen University, Germany
Steady-state currents through nano-devices: a scattering-states numerical renormalization group approach to open quantum systems

12:05 To be announced

Lunch & afternoon break

16:00 Posters, coffee, discussions

Afternoon session: Magnetic oxides

17:00 Echur Sampathkumaran, Tata Institute of Fundamental Research, Mumbai, India
Geometrical frustrated magnetism in spin-chain oxides crystallizing in K$_4$CdCl$_6$-type rhombohedral structure

17:40 Peter Littlewood, University of Cambridge, Cambridge, UK
Electronic soft matter in manganites

18:20 Kalobaran Maiti, Tata Institute of Fundamental Research, Mumbai, India
Electron spectroscopic study of correlated transition metal oxides

Dinner break
21:00 After-dinner discussion

Peter Littlewood
Perspectives in SCES

Tuesday, September 30

Morning session

8:15 Laszlo Borda, Universitaet Bonn, Germany
Spin and charge correlations around a magnetic impurity

8:55 Gleb Finkelstein, Duke University, Durham, USA
Carbon nanotube quantum dots: SU(4) Kondo and the mixed valence regimes

9:35 Armando Aligia, Centro Atomico Bariloche, Argentina
Kondo effect in transport through Aharonov-Bohm-Casher interferometers

10:15 coffee break

10:45 Siddharth Shanker Saxena, University of Cambridge, UK
Superconducting Properties of Graphite Intercalates

11:25 Klaus Becker, Technische Hochschule Dresden, Germany
On the theory of high-temperature superconductors

12:05 Michele Fabrizio, International School for Advanced Studies, Trieste, Italy
Strongly correlated superconductivity arising in a pseudo-gap metal

Lunch & afternoon break

Afternoon session

16:00 Igor Sega, Institut J. Stefan, Slovenia
Omega/T scaling in the dynamical spin response of high-temperature superconductors

16:40 Fred Zawadowski, Budapest, Hungary
On the applicability of bosonization and the Anderson-Yuval methods in quantum impurity problems

17:20 To be announced

18:00 Conference summary
Abstracts
Anomalous mixed-state thermal conductivity in URu$_2$Si$_2$

Hiroto Adachi, Manfred Sigrist

Theoretische Physik, ETH-Hönggerberg, Zurich 8093, Switzerland

Submitted : 02-09-2008

Keywords : semi-metal, electron-hole compensation, mixed-state thermal conductivity

URu$_2$Si$_2$ is an unique heavy fermion superconductor because it possesses the hidden-order phase with the critical temperature $T_h = 17.5K$. The superconducting phase ($T_c = 1.5K$) is embedded in the hidden-order phase. Recent experiments have clarified that this superconducting phase shows several intriguing properties. In this study, we focus on the anomalous mixed-state thermal conductivity recently observed in URu$_2$Si$_2$. We will discuss how the peculiar electronic structure in the hidden-order phase leads to a new type of mixed-state thermal transport.

Kondo effect in transport through Aharonov-Bohm and Aharonov-Casher interferometers

Armando Aligia
Centro Atomico Bariloche, E. Bustillo 9500, Bariloche 8400, Argentina
Submitted : 11-09-2008

In this talk, I will start with a basic explanation of the Anderson model and the Kondo effect, and its manifestations in the physics of nanodevices, such as quantum dots and impurities or groups of impurities on noble-metal surfaces, including the "quantum mirage", and comparison with experiment.

I will explain briefly a simple way to extend the Hubbard model to include Rashba spin-orbit coupling that correctly describes Aharonov-Bohm and Aharonov-Casher phases in a ring under applied magnetic and electric fields. When the ring is connected to conducting leads, I will present a formalism that is able to describe both, Kondo and interference in the Kondo regime, the spin-orbit coupling reduces strongly the conductance from the unitary limit. This effect in combination with the magnetic flux, can be used to produce spin polarized carriers.
Steady-state currents through nano-devices: a scattering-states numerical renormalization group approach to open quantum systems

Frithjof Anders
Institut für Theoretische Physik, Universität Bremen, P.O. Box 330 440, D-28334 Bremen, Germany
Submitted: 13-4-2008
Keywords: Non-equilibirum, quantum-dot, steady-state currents

We propose a numerical renormalization group (NRG) approach to steady-state currents through nano-devices[1]. A discretization of the scattering-states continuum ensures the correct boundary condition for an open quantum system. We introduce two degenerate Wilson chains for current carrying left and right-moving electrons reflecting time-reversal symmetry in the absence of a finite bias $V$. We employ the time-dependent NRG[2] to evolve the known steady-state density operator for a non-interacting junction into the density operator of the fully interacting nano-device at finite bias. We calculate the temperature dependent current as function of $V$ and applied external magnetic field using a recently developed algorithm for non-equilibrium spectral functions[3].

Towards the Lifshitz point in elemental bismuth: Light electrons gone heavy at the metal-insulator transition? 1

N. Peter Armitage
The Johns Hopkins University, Dept. of Physics, 3400 N. Charles St., Baltimore, MD 21218, USA
Submitted: 15-09-2008

I present a detailed pressure and temperature-dependent optical study of single-crystal bismuth using infrared reflectivity and ellipsometry. In the ambient pressure optical conductivity, an anomalous temperature dependent mid-infrared absorption feature is observed. An extended Drude model analysis reveals that it can be connected to a sharp upturn in the scattering rate, the frequency of which exactly tracks the strongly temperature dependent plasmon frequency. We interpret this absorption and increased scattering as direct optical evidence for a charge carrier interaction with a collective mode of purely electronic origin, here electron-plasmon scattering. The observation of a “plasmaron” as such is made possible by the exceptional properties of semi-metal bismuth, but it is also likely relevant to the low energy transport and thermodynamic properties of other semi-metals, like graphite and graphene. As a function of pressure, we observe massive changes in bismuth’s optical and infrared conductivity as the material approaches a Lifshitz-like metal/insulator transition in which the charge density approaches zero. This study shows the anomalous effects of interactions in a low carrier density system and particularly one such as this one in which Galilean invariance is broken.

1 Done in collaboration with:
Riccardo Tediosi (1), Enrico Giannini (1), Laszlo Forro (2), Dirk van der Marel (1)
(1) University de Geneve
(2) Ecole Polytechnique Federale de Lausanne
Different Routes to Quantum Criticality in Strongly Correlated Electron Systems

M. C. Aronson, M. C. Bennett, M. S. Kim, Y. Janssen, K. S. Park

1 Brookhaven National Laboratory, Upton NY 11973 USA
2 Stony Brook University, Stony Brook, NY 11937 USA

Submitted : 04-09-2008

Keywords : quantum criticality, strong correlations, heavy electron compounds

The vanishing of magnetic order at a quantum critical point (QCP) is a central feature of virtually all classes of correlated electron systems, and may be accompanied by unconventional ordered states such as superconductivity, and by anomalous critical scattering. Some of the most detailed studies have focused on f-electron heavy electron compounds, and here the picture has emerged that magnetic order requires the formation of moments, provided by the divergence of the quasiparticle mass at the QCP. We combine specific heat, magnetization, and electrical resistivity measurements on the new compound Yb$_3$Pt$_4$ to argue that alternative routes to quantum criticality are also possible. The weakly first order antiferromagnetic transition in Yb$_3$Pt$_4$ can be tuned by field to a critical end point, which is extended to a quantum critical point at 1.62 T. Both the ordered and paramagnetic phases are Fermi liquids at low temperatures, but the quasiparticle mass does not diverge at the QCP. Instead, a divergence of the zero temperature susceptibility and the quasiparticle scattering is observed, controlled by a zero field fixed point and not the nearby QCP. We suggest that like Stoner ferromagnets, and itinerant antiferromagnets, Yb$_3$Pt$_4$ is the first example of a heavy electron systems where magnetic order occurs at the QCP due to increasingly strong quasiparticle interactions.

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This work was supported by the U. S. National Science Foundation DMR-0405961
Underdoped cuprate phenomenology in the 2D Hubbard model within the Composite Operator Method

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Università degli Studi di Salerno, I-84081 Baronissi (SA), Italy
Submitted : 11-09-2008

Keywords : Underdoped Cuprates, Hubbard Model, Composite Operator Method (COM)

The two-dimensional Hubbard model is studied within the Composite Operator Method (COM) with the self-energy computed in the Self-Consistent Born Approximation (SCBA) [1]. COM describes interacting electrons in terms of the new elementary excitations that appear in the system owing to strong correlations; residual interactions among these excitations are treated within the SCBA. On decreasing the doping (from overdoped to underdoped region), anomalous features develop in the spectral function $A(k, \omega)$, the Fermi surface, the momentum distribution function $n(k)$, the dispersion, and the density of states $N(\omega)$ in the intermediate coupling regime ($U = 8$) at low temperatures ($T = 0.01 \div 0.02$). At high doping ($n = 0.7$), the system resembles an ordinary weakly-interacting metal (Fig. 1 (left)). At low doping ($n = 0.92$), a pseudogap opens, hot and cold spots appear and non-Fermi-liquid features develop (Fig. 1 (right)). This behavior, together with the presence of kinks in the calculated electronic dispersion, is in agreement with the ARPES data for high-$T_c$ cuprates superconductors.

Figure 1: Spectral function at the chemical potential $A(k, \omega = 0)$ as a function of momentum $k$ for $U = 8$, (top left) $n = 0.7$ and $T = 0.01$ (top right) $n = 0.92$ and $T = 0.02$. Spectral function $A(k, \omega)$ along principal directions ($\Gamma = (0, 0) \rightarrow M = (\pi, \pi)$, $M \rightarrow X = (\pi, 0)$, $X \rightarrow Y = (0, \pi)$ and $Y \rightarrow \Gamma$) for $U = 8$, (bottom left) $n = 0.70$ and $T = 0.01$ (bottom right) $n = 0.92$ and $T = 0.02$.

Understanding the energy scales relevant for the valence transition in YbInCu$_4$

I. Aviani$^1$, M. Očko$^1$, D. Starešinić$^1$, K. Biljaković$^1$, J. Hemberger$^2$, A. Loidl$^2$, J. L. Sarrao$^3$

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Valence transition in YbInCu$_4$ is interesting from both technological and fundamental aspect. A large magnetic entropy change at the transition could be used in thermomagnetic devices. In addition, the transition temperature $T_V$ can be tuned by doping. Knowing the relevant energy scales is crucial for understanding and modeling the transition.

Our measurements and the data analysis of specific heat, magnetic susceptibility, electrical resistance and thermopower of the Y-doped YbInCu$_4$ show that the low-temperature properties of the local moment phase can be explained by the CF effects but with a modified CF scheme, so that the Kondo interaction is very week.

Our results support the Falicov-Kimball scenario for the onset of the valence transition. In this picture, the Fermi level $E_F$ is placed just below the dip in the DOS, and the hole delocalization at the transition pushes the $E_F$ deeper in the DOS where the density of states is higher. This suddenly sets up the Kondo interaction (with high characteristic temperature $T_K^{\text{FE}} = 400$ K) which screens the Yb moments. A new equilibrium itinerant hole concentration (and Yb valence) is fixed by the equilibrium between the Kondo condensation energy gain and the magnetic entropy lose due to the quenching of the Yb$^{3+}$ moments. The valence fluctuating (VF) phase is stabilized when about 15% of holes are delocalized.

In the simplest picture, we assume the Kondo condensation energy $E_K$ is proportional to the product of the concentration $x^{3+}$ of the Yb$^{3+}$ ions and the concentration of delocalized itinerant holes $1 - x^{3+}$, $E_K = T_K^{\text{FE}} x^{3+} (1 - x^{3+})$. If we neglect the entropy of the fermion liquid, the entropy change at the transition is roughly $T_V x^{3+} \ln(4)$. By equating these two expressions we obtain the valence change at the transition $1 - x^{3+} = T_V \ln(4) / T_K^{\text{FE}} = 42$ K $\ln(4) / 400$ K $= 0.15$, that is the experimentally observed value.

$^1$This work is supported by the Croatian Ministry of Science, Education and Sports project No. 035-0352827-2841 and the ECOM COST Action P16
Tunneling and polaron states in a metal-molecule-metal junction

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Submitted : 14-09-2008

Keywords : phonon assisted tunneling, inelastic tunneling spectroscopy, single site polarons

We study a simple model for the electron tunneling through an insulating barrier. The tunneling can be elastic and/or inelastic, ie. assisted by phonon or some other excitations. The model has been already studied in a number papers and it can be applied to measurements like (i) electron tunneling in metal-metal oxide-metal junction, (ii) tunneling through double-barrier heterostructure, (iii) single molecule conductivity, (iv) inelastic tunneling spectroscopy, (v) phonon spectroscopy, etc. Inelastic processes can be observed as spikes in the I-V curve. In this work we discuss possibility of the electron capture in the localized polaronic states within the insulating barrier. This inelastic process seem to be neglected or overlooked in previous theoretical studies of the model.
Are Ge-based skutterudites promising thermoelectrica? Ground state properties, electronic and thermal transport 1

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Submitted: 15-09-2008

Keywords: Skutterudites, superconductivity, thermoelectrics

Cage-forming compounds such as zeolithes, fullerenes, clathrates or skutterudites have proven to be not only of scientific but also of significant technological interest. The ability of these materials to accommodate guest filler species provides a wide range of varying physical and chemical properties. The majority of cage forming elements of skutterudites is essentially based on volatile and/or toxic pnictogens (P, As, Sb). We report on the previously discovered skutterudites MPt4Ge12 (M = Ba, Sr, La, Pr, Eu, Th, U) [1, 2, 3, 4] as the first members of a new class of skutterudites, based on a framework, entirely formed by Ge-atoms. A variety of bulk properties as well as band structure calculations allows understanding of superconductivity, magnetic behaviour. Electronic and thermal transport of these systems are discussed in terms of the temperature dependent electrical resistivity, thermal conductivity and Seebeck effect.


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Microscopic approach to high-temperature superconductors

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Submitted : 21-08-2008

Starting from the $t$-$J$ model, microscopic properties of high-temperature superconductors will be discussed in the superconducting and in the pseudogap phase at moderate hole doping. Our theoretical approach (PRM) is based on a stepwise elimination of high-energy transitions using unitary transformations. For both phases, one arrives at renormalized 'free' Hamiltonians for correlated electrons. For the superconducting phase, the order parameter turns out to have $d$-wave symmetry with a correlation length of a few lattice constants. Also, the spectral function from angle-resolved photoemission spectroscopy (ARPES) along the Fermi surface is in good agreement with experiment. For the pseudogap phase, our analytical results show well-defined excitation peaks around $\omega = 0$ near the nodal direction which become strongly suppressed around the antinodal point. The origin of the pseudogap can be traced back to a suppression of spectral weight from incoherent excitations in a small $\omega$-range around the Fermi energy.
Nernst effect as a probe of correlated electrons

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The Nernst effect, the generation of a transverse magnetic field by a longitudinal thermal gradient, has emerged as a powerful probe of electronic interactions. As originally discovered in the context of research on cuprates, it has proved to be a very sensitive probe of superconducting fluctuations. Our recent studies of the Nernst effect in an amorphous thin film of a conventional superconductor, could resolve superconducting fluctuations in a wide temperature window, exceeding well above both $T_c$ and $H_c2$. However, superconducting fluctuations are not the unique source for a Nernst signal. Recently giant Nernst signals were detected in Heavy-Fermion semi-metals, such as the hidden-order state of URu$_2$Si$_2$ or the mysterious ordered state of PeFe$_4$P$_{12}$. Moreover, studies of the thermoelectric response near the quantum critical point in CeCoIn$_5$ have documented a direct link between a large Nernst signal and a small Fermi energy. Even elemental bismuth, the system in which Nernst and Ettingshausen discovered their effects, has become a subject of renewed attention thanks to recent studies of the Nernst effect. The origin of the giant quantum oscillations in the Nernst response across the quantum limit, as well as the unexpected anomalies observed beyond this limit, remain open questions.
Optical and spectral properties of the t-J Holstein model

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Keywords: t-J-Holstein model, spectral functions, optical conductivity

We develop an efficient numerical method for the description of a single-hole motion in the antiferromagnetic background. The method is free of finite-size effects and allows calculation of physical properties at an arbitrary wavevector. Methodical increase of the functional space leads to results that are valid in the thermodynamic limit. In the case of the t-J model we found good agreement with cumulant expansion, exact-diagonalization approaches on finite lattices as well as self-consistent Born approximations. The method allows a straightforward addition of other inelastic degrees of freedom, such as lattice effects. Our results for spectral functions as well as quasiparticle weight of the t-J-Holstein model are in agreement with diagrammatic Monte Carlo method. Calculated spectral functions in Fig (a) in the strong coupling limit reproduce well the waterfall structure seen in ARPES spectra on Ca2−xNaxCuO2Cl2.

We also compute the charge stiffness and optical conductivity of the t-J Holstein model, Fig (b). Coherent hole motion is most strongly influenced by the electron-phonon coupling within the physically relevant regime of the exchange interaction. Optical conductivity in the crossover to the strong coupling regime shows a two-peak structure. The low-frequency peak represents the excitation of the first string state, while the higher-frequency peak corresponds to the mid infrared band, broadened and renormalized by phonon excitations. Results are in agreement with recent optical measurements.

We furthermore extend the existing method to computation of the bipolaron. We discuss the shape of the magnetic bipolaron and the condition for the formation of the bound state.

Figure 1: (a) Intensity plots of $A_k(\omega)$ for the TJHH model ($J/t = 0.4$, $t'/t = -0.34$, $t''/t = 0.23$ and $t = 0.375$ meV.) at different values of electron-phonon coupling strength $\lambda$ and phonon frequency $\omega_0/t = 0.2$ and (b) $\sigma_{xx}$ for the t-J-Holstein model.
Spin and charge correlations around a magnetic impurity

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Keywords: Kondo problem, screening cloud

We study the Kondo model—a magnetic impurity coupled to a one-dimensional wire via exchange coupling—by using Wilson’s numerical renormalization group technique. By applying an approach similar to which was used to compute the two-impurity problem we managed to improve the poor spatial resolution of the numerical renormalization group method. In this way we have calculated the impurity-spin conduction-electron-spin correlation function which is a measure of the Kondo compensation cloud whose existence has been a long-standing problem in solid-state physics.

We also show that the long distance charge density oscillations in a metal induced by a weakly coupled spin-1/2 magnetic impurity exhibiting the Kondo effect are given, at zero temperature, by a universal function $F(r/\xi_K)$ where $r$ is the distance from the impurity and $\xi_K$, the Kondo screening cloud size $= v_F/T_K$, where $v_F$ is the Fermi velocity and $T_K$ is the Kondo temperature.

In addition to those, we present results on the prototype of the underscreened models, the $S = 1$ single channel Kondo model. We demonstrate that the singular dynamics of the underscreened Kondo model modifies essentially the spin correlations as compared to the fully screened case: In contrast to the spin-$\frac{1}{2}$ model, its powerlaw decay obtains now only logarithmic corrections for $x > \xi_K$, and its long-distance tail is thus more pronounced than in the fully screened case. We demonstrate that this numerically observed tail of the "underscreening cloud" is in agreement with the expectations of an effective ferromagnetic spin-$\frac{1}{2}$ Kondo model describing the scattering off the residual magnetic moment.
Low temperature properties of Kondo lattices

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Keywords : Kondo effect, slave-boson, energy scales

We study the low-temperature properties of a periodic Anderson model using the slave-boson formalism. For a singular density of conduction states (DOS), we generalize the single-impurity result of Withoff and Fradkin: the strong coupling fixed point becomes irrelevant if the DOS vanishes at the Fermi level $E_F$. However, for $E_F$ close enough to the singularity, and close to half-filling, the Kondo temperature, $T_K$, can become much smaller than the characteristic Fermi liquid scale. At $T = 0$, a meta-magnetic transition occurs at the critical magnetic field $H_c \approx (k_B/\mu_B)T_K$. Our results provide a qualitative explanation for the anomalies observed in the low temperature behavior of the intermetallic compounds with Yb, Ce, and Eu ions.
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September 20 - 26, 2008 Hvar, Croatia

Thermoelectric power and thermal transport of anomalous rare-earth Kondo compounds

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The thermoelectric power and the thermal conductivity have been well studied experimentally and theoretically in Cerium, Ytterbium or other anomalous rare-earth systems. Very large values of the thermoelectric power have been observed in compounds such as CeAl₃, CeCu₂Si₂ or YbCu₂Si₂. The thermoelectric power of Cerium compounds has been studied theoretically, within the Coqblin-Schrieffer (CS) Hamiltonian with a crystalline field (CF) splitting Δ, at high [1] and low [2] temperatures compared to the Kondo temperature Tₖ, and shows a peak at a temperature corresponding to typically Δ/3 and another one at Tₖ/2.

Pressure has a strong effect on Cerium systems and, according to the well known Doniach diagram, it yields an increase of the Kondo coupling. A good example is provided by the change under pressure from an antiferromagnetic ordering to a non magnetic heavy fermion behavior, as observed for example in CeRu₂Ge₂ [3]. On the other hand, the effect of hydrogenation is more complicate and presents different behaviors. A classical case is provided by compounds where hydrogenation yields an increase of the lattice parameters, opposite to the effect of pressure. Such a “negative” pressure is invoked in the case of CeRuSi and hydrogenation changes the moderate heavy fermion compound CeRuSi to the antiferromagnet CeRuSiH which has a smaller electronic specific heat constant [4]. A brief discussion of the different behaviors due to the hydrogenation in Cerium compounds is also presented here.

On the other hand, the thermal conductivity of anomalous rare-earth Kondo compounds has been also studied theoretically within the same model with the CS Hamiltonian and CF effects [5]. The magnetic part Wₘₐₜ of the thermal resistivity, taken as the difference between the inverse of the thermal conductivity of the Kondo compound and that of an equivalent non magnetic compound, has been obtained in several Ce, Pr, Tm and Yb compounds and a LogT-dependence of the product WₘₐₜT has been observed at sufficiently high temperatures in these compounds, in good agreement with theory and in a way similar to the magnetic part of the electrical resistivity [6].

We present finally a discussion of the transport properties and the resulting figure of merit in strongly correlated electron systems.

Kondo Proximity Effect: How Does a Metal Penetrate Into a Mott Insulator?

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Keywords: Proximity effect, Heterostructures, Mott Insulators

We consider a heterostructure of a metal and a paramagnetic Mott insulator using an adaptation of dynamical mean-field theory to describe inhomogeneous correlated systems [1, 2, 3]. The metal can penetrate into the insulator via the Kondo effect [3]. We investigate the scaling properties of the metal-insulator interface close to the critical point of the Mott insulator. At criticality, the quasiparticle weight decays as $1/x^2$ with distance $x$ from the metal within our mean-field theory. Our numerical results (using the numerical renormalization group as an impurity solver) show that the prefactor of this power law is extremely small, implying that the Mott insulator is \textit{de facto} impenetrable to the metal. We discuss extensions of our approach to deal with charge reconstruction at interfaces.

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Kondo decoherence: from ab-initio calculations to many-body Hamiltonians and beyond ...

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Keywords: Decoherence, realistic description of Kondo impurities, transport

Understanding decoherence, the process by which a quantum system loses phase coherence by getting entangled with its environment, is important in the context of quantum computation. Here we show how decoherence, induced by dilute magnetic impurities and studied via weak antilocalization, can be harnessed to resolve a longstanding question concerning the classic Kondo systems of Fe impurities in the noble metals gold [1] and silver: which Kondo-type model yields a realistic description of the relevant multiple bands, spin and orbital degrees of freedom? In order to answer this question we follow a three-pronged strategy: (i), we perform spin-resolved density functional theory calculations that suggest an \( n = 3 \) channel fully screened (\( S = 3/2 \)) Kondo model, (ii), we solve this model for dynamic and transport properties using the numerical renormalization group method [2] within the complete basis set [3] and full density matrix approach [4], and, (iii), we compare the predictions to previous and new measurements of both the resistivity and decoherence rate in quasi 1-dimensional wires. We also compare the experimental data to \( n = 1 \) and \( n = 2 \) channel fully screened Kondo models (underscreened and overscreened models were previously shown to be incompatible with the data [5]). Excellent agreement is found for \( n = 3 \) with a single Kondo scale for both the resistivity and decoherence rate. This contrasts to previous comparisons [5] for an \( n = 1 \) fully screened Kondo model which could fit either the resistivity or the decoherence rate with a given Kondo scale, but not both. Our results set a new benchmark for the level of quantitative understanding attainable for the Kondo effect in real materials.

Influence of disorder on the thermopower of heavy-fermion materials
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Submitted: 12-09-2008

The influence of substitutional disorder on the transport properties of heavy-fermion systems is investigated. The dynamical mean-field theory treatment of the periodic Anderson model PAM has been combined with the coherent potential approximation for disordered systems to obtain a suitable treatment for the disordered PAM. Considering two distinct local environments of a binary alloy $A_cB_{1-c}$ with arbitrary concentration $c$, we explore two types of disorder: on the $f$ site and on the ligand sites. The temperature and concentration dependence of the thermoelectric power is calculated. The characteristic concentration dependence as well as the order of magnitude of the thermopower are reproduced for metallic heavy-fermion systems and for Kondo insulators. In particular, sign changes of the Seebeck coefficient as function of temperature and concentration are observed.
Infrared and Raman study of the charge-density-wave ground state

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Keywords : charge-density-wave, optical properties, pressure dependence

The question of the relationship between the effective dimensionality of a physical system and the symmetry of its ground state is an important issue in order to figure out the relevant mechanism driving materials into peculiar charge ordering. In this respect, the rare-earth polychalcogenides RTeₙ (where R is the rare earth element and n=2, 2.5, 3) have recently attracted great interest because of their low dimensionality. Among the RTeₙ families are members that variously host large commensurate distortions, ordered and disordered vacancy structures, and Fermi surface driven charge-density-wave (CDW). They supply furthermore a playground to study the interplay between CDW state, peculiar magnetic order and eventually pressure induced superconductivity. Optical spectroscopic methods (infrared reflectivity and Raman scattering) were applied as a function of both temperature and external pressure, in order to address the complete excitation spectrum in these CDW materials. We establish the energy scale of the single particle excitation across the CDW gap and find that the CDW collective state gaps a large portion of the Fermi surface. The CDW gap decreases upon compressing the lattice (both with chemical and applied pressure, Fig. 1). The suppression of the CDW gap leads to a release of additional charge carriers, manifested by the shift of weight from the gap feature into the metallic component of the optical response (inset Fig. 1). Furthermore based on the observation of a power law behavior in the optical conductivity, we suggest that interactions and Umklapp processes may play a role in the onset of the CDW broken symmetry ground state. We discuss our optical conductivity at high frequencies with respect to predictions based on the Tomonaga-Luttinger liquid scenario. We will moreover present our Raman scattering experiments as a function of chemical and applied pressure. The observed spectra display five peaks (Fig. 2), four of which we can assign to Aₑg Raman active phonon modes by comparing their frequencies to those obtained from a first principles calculation. The latter also produces the Kohn anomaly in the phonon dispersion, eventually responsible for the formation of the CDW condensate. Furthermore, distorting the lattice along the displacements of the soft phonon, modes of B₁g symmetry become Raman active in our experimental geometry. Our Raman scattering results give clear cut evidence for a coupling between the CDW condensate and the lattice vibrational modes.
Figure 1: Single particle peak energy $\omega_{SP}$ (i.e., the CDW gap) as a function of the lattice constant $a$ for LaTe$_2$, CeTe$_3$ and the RTe$_3$ series. Inset: single particle peak energy $\omega_{SP}$ versus plasma frequency $\omega_p$ for LaTe$_2$, as a function of pressure. Pressure is here an implicit variable.

Figure 2: Raman scattering spectra for the rare-earth tri-tellurides series RTe$_3$ ($R =$ La, Ce, Pr, Nd, Sm, Gd and Dy) at ambient pressure (a), and for LaTe$_3$ (b) and CeTe$_3$ (c) both for increasing (continuous line) and decreasing (dashed line) pressure. All spectra have been shifted for clarity. The pressure dependence of all modes is fully reversible. All modes slightly disperse (thin dotted lines as guides to the eye) and disappear upon compressing the lattice. The inset in Fig. 2b shows the polarization dependence of the Raman spectra of LaTe$_3$ for parallel incident and scattered light polarizations and at different orientations of the incident polarization. The origin of the angle scale is arbitrary.
Dimensional Crossover of Quantum Critical Behavior in CeIn$_5$

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CeMIn$_5$ ($M$ = Co, Rh) compounds are of great current interest due to their interplay of magnetism, superconductivity and non-Fermi-liquid behavior. In order to classify quantum criticality in these systems, we use low-temperature thermal expansion and the Grüneisen ratio $\Gamma$ of thermal expansion to specific heat. We compare these thermodynamic properties with theoretical predictions for an antiferromagnetic quantum critical point (QCP) [1]. CeCoIn$_5$ displays a field-induced QCP which almost coincides with the upper critical field of unconventional superconductivity [2]. At the field-tuned quantum phase transition ($H_{QCP} = 5$T), a crossover scale $T^* \approx 0.3$K is observed, separating $\alpha(T)/T \sim T^{-1}$ ($T > T^*$) from a weaker $T^{-1/2}$ divergence ($T < T^*$). We ascribe this change to a crossover from 2D to 3D critical fluctuations which may go along with a change from unconventional to conventional quantum criticality. The effect of disorder on quantum criticality, which is studied in CeCoIn$_{5-x}$Sn$_x$ ($0 \leq x \leq 0.18$), shifts $T^*$ to higher temperatures [3].

When simple alloys turn into complicated

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Keywords : Ce alloys, incommensurate structures

In some cases, simple metallic alloys, whose magnetic behaviour is supposed to be well-known and, thus, they are not subject of further studies, might surprise us revealing anomalous behaviours that point towards a more complicated magnetic ground state.

This is the case of CeGe, a binary Ce-based alloy that was already studied in the 60’s, and reported as a simple antiferromagnet [1], being this consideration accepted until recent times [2]. However, a careful study of this alloy has evinced that the magnetic ground state of this alloy must be more complex.

In the present work we will show experimental results that clearly prove that the magnetic structure of CeGe at low temperatures must be incommensurate. These results include microscopic probes, such as neutron diffraction or muon spectroscopy, and macroscopic measurements, among which the transport properties (electrical resistivity and thermoelectric power) are specially relevant, as they exhibit an anomalous behaviour at the Néel temperature that is indicative of a gap opening at the magnetic superzone.

Strongly correlated superconductivity arising in a pseudo-gap metal

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Keywords: Mott transition, Superconductivity, Kondo effect

We solve a simple two-orbital Hubbard model with an antiferromagnetic on-site exchange in the limit of infinite coordination lattices by means of dynamical mean field theory (DMFT). The model has a phase diagram that is surprisingly similar to cuprates, including pseudo-gap and Fermi-liquid normal phases, and a superconducting one. With the help of the numerical renormalization group solution of the two-orbital Anderson impurity model onto which the lattice model is mapped by DMFT, we uncover the mechanism that allows a pseudo-gap phase to develop a large superconducting gap. We find that the Fermi liquid phase, the pseudo-gap phase and the superconducting one are all legitimate outcomes of an unstable phase that exists only at high temperature, above $T_c$ as well as above the pseudo-gap and the Fermi liquid coherence temperatures, which is accessible by DMFT as a metastable phase only because one can prevent any symmetry breaking.
Luttinger, Peierls or Mott? Quantum phase transitions in 1D strongly correlated electron-phonon systems

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Submitted: 29-05-2008

Keywords: quantum phase transitions, 1D electron-phonon systems, numerical approaches

The challenge of understanding metal-insulator and insulator-insulator quantum phase transitions 1D has stimulated intense work on generic microscopic models of interacting electrons and phonons. Combining Lanczos diagonalization with Chebyshev moment expansion and density matrix renormalisation group techniques we present unbiased results for ground-state and spectral properties of the Holstein-Hubbard model at half-filling. For the spinless fermion case, we identify four distinct regimes of the phase diagram, corresponding to an attractive or repulsive Luttinger liquid at weak electron-phonon (EP) coupling, and an band-insulator or polaronic superlattice at strong coupling. Electron and phonon spectra reveal substantially different physics in these regimes and beyond indicate that the size of the phonon frequency significantly affects the nature of the Peierls transition. For the spinful case, with respect to the metal the the electron-electron interaction favours a Mott insulating state, whereas the EP interaction tends to establish a Peierls state with true CDW long-range order. While polaronic features emerge only at strong EP couplings, pronounced phonon signatures, such as multi-quantum bound states, can be found in the Mott insulating regime as well. In order to corroborate the Mott to Peierls transition scenario, we determine the spin and one- and two-particle charge excitation gaps and comment on the possibility of an intervening metallic phase in the weak-coupling regime.
SU(4) Kondo Effect in Carbon Nanotube Quantum Dots: Kondo Effect without Charge Quantization

Gleb Finkelstein
Duke University Submitted: 14-09-2008
Keywords : Kondo effect, quantum dot

Carbon nanotubes present an ideal system for investigating quantum electronic transport at the nanoscale. In our nanotube quantum dots, we can control the contact transparency and thereby can tune the electronic conductance from the well-developed Coulomb blockade to the Kondo regime. We work with high quality nanotubes, where quantum-mechanical orbitals are doubly-degenerate, forming four-electron “shells”. For electrons tunneling within the nanotube, the orbital quantum number is preserved and the tunneling Hamiltonian possesses SU(4) symmetry. We present our observations of the SU(4) Kondo effect for one, two, and three electrons in a shell. Surprisingly, as the contacts are made more transparent and the charge quantization is completely suppressed, we still observe the SU(4) Kondo effect. This behavior is different from the SU(2) Kondo effect which is destroyed by charge fluctuations. The hallmark of the new transport regime is the surprising lack of single-electron features at low temperature, which are uncovered as the temperature is raised. Recent numerical calculations demonstrate a very good agreement with our measurements.
The Kondo Scale in the dense Kondo lattice

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A characteristic of dense Kondo lattices is the so-called coherence temperature $T^*$ below which the system condenses into a low resistance ground state for which a description in terms of Bloch states is appropriate. We argue that $T^*$ corresponds to the temperature at which the Rln2 entropy of the Kondo ion is developed and empirically show that this temperature is determined by nearest neighbor RKKY coupling of the Kondo ions.

\footnote{This work has been done in collaboration with Yi-feng Yang, D. Pines, J. D. Thompson, and H. Lee. Support from NSF-DMR-0710492 is gratefully acknowledged.}
Thermal electricity in strongly correlated multilayers

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Keywords: Thermoelectric transport, multilayered nanostructures

In designing novel thermoelectric devices, much effort has been spent on investigating how to improve the properties of bulk devices. Here, we focus on examining multilayered nanostructures for two reasons: (i) they allow one to “quantum engineer” the electronic structure of the device and (ii) the nanoscale interfaces should provide localization to phonon transport. We show, via an explicit example of a metal–Mott-insulator–metal device, how one can get large thermoelectric response from nanoengineering two materials that have no thermoelectric response in the bulk. This work implies that by using multilayered systems, one has the potential to create interesting thermoelectric devices out of materials that might not have been considered as viable thermoelectrics in the past.

Our formal development includes a number of elements. We describe how to perform (all electronic) calculations of transport in multilayered nanostructures composed of metallic and strongly correlated components. We use the inhomogeneous dynamical mean-field theory formalism to approach the problem and we give examples of solutions for both the Falicov-Kimball model and the Hubbard model. We show how one can derive the linear response transport of charge and heat through such a device and also discuss the roles of electronic charge reconstruction and vertex corrections.

We end with a brief discussion of what happens in a metal–Mott-insulator–metal sandwich when the Mott insulator is described by the Hubbard model, which has Fermi liquid behavior for small interaction strength. At low temperatures, the system can become conducting with what is anticipated to be highly nonlinear behavior.

This work was supported by the National Science Foundation under grant No. DMR-0705266. Recent work on this problem includes the formalism for thermal transport \cite{1}, electronic charge reconstruction of a Mott insulator \cite{2}, and the thermoelectric response of a metal–Mott-insulator–metal sandwich \cite{3}.

\begin{figure}[h]
\centering
\includegraphics{figure1.png}
\caption{Figure of merit of a metal–Mott-insulator–metal device as a function of temperature for different chemical potential mismatches (from Ref. \cite{3})}
\end{figure}

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Quantum criticality in heavy-fermion systems

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Submitted : 11-09-2008

Quantum criticality in f-electron based heavy-fermion systems arises from the competition of the on-site Kondo with the inter-site exchange interaction. The essential question is how the heavy quasiparticles evolve if these materials are tuned from the paramagnetic into the antiferromagnetically ordered state. The traditional picture describes a spin-density-wave transition at which the quasiparticles retain their itinerant character. Unconventional quantum criticality, which qualitatively differs from the predictions of standard theory, may arise due to a destruction of Kondo screening. The latter may lead to a decomposition of the heavy quasiparticles into conduction electrons and local magnetic moments. I will report a comparative low-temperature study on different quantum critical heavy fermion metals with particular focus on YbRh$_2$Si$_2$. 
Spin ladders, BEC, Luttinger liquids and beyond

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Submitted: 14-09-2008

Effects of interactions change drastically with dimension. In particular, in one dimension, the canonical description of interacting systems, namely the Fermi liquid theory, is replaced by the so-called Luttinger liquid, with drastically different properties. Hunting for Luttinger liquids, despite the ever growing number of one dimensional systems, is a very challenging task. I will review the important properties of such systems, and will show how recently examined spin ladder system offer a unique opportunity to test for such a Luttinger liquid physics. I will also show how these systems present the challenge of going from the one dimensional world, where spins behave essentially as fermions, to the three dimensional one where they behave essentially as bosons and can lead to Bose-Einstein condensation.
Role of structures on thermal conductivity in thermoelectric materials

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The figure of merit $ZT = \sigma S^2 T/\kappa$ ($S$ the Seebeck coefficient, $\sigma$ and $\kappa$ the electrical and thermal conductivity respectively) is an essential element of the efficiency of a thermoelectric material for applications, which convert heat to electricity or, conversely, electric current to cooling. From the expression of the power factor $\sigma S^2 T$ it was deduced that a highly degenerated semiconductor is necessary. In order to reduce the lattice part of the thermal conductivity, various mechanisms, mainly related to the structure of the materials, have been tested in new thermoelectric materials and have been the topics of different reviews. This include cage-like materials, effects of vacancies, solid solutions, complex structures (cluster, tunnel, . . .), nano-structured systems. We plan to review structural aspects in the modern thermoelectric materials and include results of the very last years in such view. Moreover, as micro- and nano-composites seem to be promising to increase $ZT$ in large size samples, we will also briefly discuss the interest of spark plasma sintering technique to preserve the micro- or nano- structure in highly densified samples.
Thermoelectric properties of transuranium-based unconventional superconductors

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Keywords: transuranium intermetallics, strong electronic correlations, superconductivity

Transuranium intermetallics show a large variety of exotic behaviors that in most cases come from 5f–ligand hybridization. Physical phenomena like long–range magnetic ordering, heavy–fermion ground state, and/or "non-Fermi liquid" behavior raised a great interest to the study of physical properties of these systems. Recently, this interest was even increased with the discovery of unconventional superconductivity in PuCoGa\textsubscript{5}, PuRhGa\textsubscript{5}, and very recently in NpPd\textsubscript{5}Al\textsubscript{2}. It has been found that these phases present d–wave superconductivity ($T_c \sim 5\text{–}18$ K) and heavy-fermions features ($\gamma \sim 100\text{–}200$ mJ/mol K\textsuperscript{2}) that may be at the origin of the superconductivity. To shade more light on the physical properties in these intermetallics we have examined thermoelectrical properties of PuCoGa\textsubscript{5} and NpPd\textsubscript{5}Al\textsubscript{2}. For both compounds, the Seebeck coefficient shows negative values in the whole temperature range. At $T_c$ the thermopower exhibits a sharp transition to a zero value as expected for superconducting state. The overall shape and the magnitude of the Seebeck coefficient observed for NpPd\textsubscript{5}Al\textsubscript{2} and PuCoGa\textsubscript{5} ($|S| \sim 20\text{–}30$ $\mu$V/K) is characteristic of systems with strong electronic correlations. The experimental data were analyzed in terms of phenomenological models and compared to those reported in the literature for similar materials.
New approaches to thermoelectric materials

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Submitted : 01-09-2008

Keywords : thermoelectric power, conducting glasses, Te films

A deeper understanding of the parameters that affect the dimensionless figure of merit, the development of new concepts (such as the so-called phonon-glass/electron crystal) and the use of new synthesis techniques has recently led to new systems with better thermoelectric performances. Here we present part of the work that has been recently performed in our groups in order to get new and improved thermoelectric systems. Special emphasis will be done on the possibility of electrical conducting glasses and doped tellurium films representing new families of enhanced thermoelectrical materials. In particular, results will be presented and discussed on Cu\textsubscript{4}Ge\textsubscript{y}Te\textsubscript{2} general composition glasses and on bismuth doped tellurium films.
Thermal expansion and magnetostriction measurements of CeCu$_{6-x}$Au$_x$ single crystals

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Submitted: 11-09-2008

Keywords: heavy-fermion systems, thermal expansion, quantum phase transitions

The archetypical heavy-fermion compound CeCu$_{6-x}$Au$_x$ is one of the best investigated examples of a magnetic Quantum Critical Point (QCP). It can easily be tuned across the onset of antiferromagnetic order by changing its volume $V$ either by alloying with Au or applying pressure. Due to the instability at the QCP the entropy $S$ shows at finite temperatures a maximum as a function of $V$. This renders the thermal expansion $\alpha \propto \partial S/\partial V$ very sensitive to the quantum critical behavior at the QCP. We have performed low-temperature thermal expansion and magnetostriction measurements at the critical Au content $x_c = 0.1$ and, close to $x_c$ in the antiferromagnetic phase, at $x = 0.15$. The measurements show strong deviations from the Fermi liquid behavior visible in the divergence of $\alpha/T$ and the Grüneisen parameter $\Gamma$ for $T \to 0$. We will report on the scaling behavior of $\alpha$ and $\Gamma$, the change of the anisotropic pressure and strain dependences of the characteristic energy scales, and the influence of magnetic fields on the critical behavior.
Superconductivity, Magnetism and Charge Density Waves in Rare-Earth Tritellurides under Pressure


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Submitted: 14-09-2008

Keywords: charge density waves, superconductivity, high pressure

The quasi-2D rare-earth tritelluride compounds $R$Te$_3$ ($R$=La-Nd, Sm, and Gd-Tm) have lately received significant attention as the first system in which nominal square-planar symmetry is broken by the formation of a unidirectional charge density wave (CDW). Furthermore, the CDW transition temperatures of these compounds display striking systematics across the rare-earth series. However, prior to the work detailed in this poster, there appear to have been no high-pressure transport studies of rare-earth tritellurides in order to investigate the possibility of pressure-induced superconductivity in these compounds.

We performed a series of high pressure electrical resistivity measurements on single crystals of CeTe$_3$ and TbTe$_3$. Measurements in a nearly hydrostatic piston-cylinder cell reached a maximum pressure of 22.8 kbar while two further measurements in a Bridgman anvil cell reached a maximum pressure of 152 kbar. The antiferromagnetic ordering temperature of CeTe$_3$ displays a dramatic increase with pressure. In TbTe$_3$ we find, to our knowledge, the first example of superconductivity in a rare-earth tritelluride.

Figure 1: (a) Pressure dependence of the transition temperatures for CeTe$_3$. inset: near 45 kbar, the room temperature resistivity displays an abrupt drop, possibly indicating a structural phase transition. (b) Pressure dependence of the transition temperatures of the phases observed in TbTe$_3$. At 22.8 kbar, charge density wave, antiferromagnetic and superconducting order all appear upon progressively cooling the sample.

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LaNiO$_3$/LaAlO$_3$ heterostructures: A LDA+DMFT analysis

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Submitted: 2008-30-08

Keywords: strong correlations, heterostructures, superconductivity

The discovery of high temperature superconductivity in cuprates [1] initiated the quest for finding related transition metal oxides with comparable or even higher transition temperatures. The family of nickel oxides have been subject to investigation for some time in order to find similarities and differences to isoelectronic cuprate structures [2]. The emerging possibilities to synthesize transition metal oxide heterostructures open new opportunities in this respect. We investigate the LaNiO$_3$/LaAlO$_3$ heterostructure [3]. In the threevalent Ni$^{3+}$ the two Nickel $e_g$ states $|x^2 - y^2\rangle$ and $|3z^2 - r^2\rangle$ are occupied by one electron. Our analysis was performed with the local density approximation (LDA) and its combination with dynamical mean field theory (LDA+DMFT) [4]. The quasi 2D-character of the system may suggest, that the $|3z^2 - r^2\rangle$ states—which barely overlap in the $xy$-plane—play only a negligible role. However, this is not true since the hopping processes from the $|3z^2 - r^2\rangle$ to the highly mobile $|x^2 - y^2\rangle$ states are by no means small. In this way additional mobility is given to the $|3z^2 - r^2\rangle$ states, which enriches the physical features of the system. The interaction effects in the Nickel $e_g$ states were treated within a two band model at quarter filling. The effective Hamiltonian for this system reads

\[ H_{eff.} = \sum_{ij\mu\sigma} t_{ij\mu\sigma} c_{i\mu\sigma}^\dagger c_{j\mu\sigma} + \sum_{i\sigma} n_{i\sigma} n_{i\sigma}^\dagger + \sum_{i\neq j\sigma\sigma'} (V - \delta_{\sigma,\sigma'} J) n_{i\sigma} n_{j\sigma'}^\dagger, \]  

(1)

where $c_{i\mu\sigma}$ ($c_{i\mu\sigma}^\dagger$) annihilates (creates) an electron on Ni site $i$, in orbital $l$ with spin $\sigma$, $n_{i\sigma} = c_{i\mu\sigma}^\dagger c_{i\mu\sigma}$, $\delta_{\sigma,\sigma'}$ denotes the Kronecker symbol, U and V represent the intra-orbital and inter-orbital repulsion respectively and $J$ is the Hund exchange term. Hamiltonian (1) was then solved by means of the DMFT using a Hirsh Fye Quantum Monte Calro impurity solver. The results for the paramagnetic/high-temperature phase show that both bands remain metallic and contribute to the Fermi surface, unless the Coulomb interaction is turned to unrealistically large values. For investigating possible ordering tendencies at low temperatures the exchange parameters of an effective Kugel-Khomskii-like spin-orbital-model [5] were derived within an effective two site calculation. The results indicate the presence of strong antiferromagnetic fluctuations which might drive the heterostructure on the insulating side of the metal insulator transition at low temperatures. Such antiferromagnetic fluctuations are also considered to be essential for high temperature superconductivity.

Pudding mold type band as the origin of large thermopower in LiRh$_2$O$_4$\textsuperscript{1}

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Submitted : 13-09-2008

To calculate thermodynamic and transport properties we employ the combination of local density approximation and dynamical mean field theory (LDA+DMFT method.) After briefly introducing this method, we will focus on the newly synthesized mixed-valent spinel LiRh$_2$O$_4$ for which a large thermopower is observed in the metallic cubic phase above 230K \cite{1}. We calculate the Seebeck coefficient by LDA+DMFT; not only LDA+DMFT but also by the less involved Boltzmann equation approach well reproduces the experimental values. A careful analysis of the latter shows unexpectedly that the origin of the large thermopower shares a common root with a very different oxide: Na$_x$CoO$_2$. We also discuss how it is possible to further increase the powerfactor of LiRh$_2$O$_4$ through doping, which makes the material even more promising for technological applications.

\cite{1} Okamoto \textit{et al.} (arXiv:0806.2504)

\textsuperscript{1}In cooperation with R. Arita, K. Kuroki, A. Mlukoyanov, S. Skornyakov, and V. Anisimov
Renormalisation group approach to strong correlation behaviour

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Submitted : 26-02-2008
Keywords : renormalisation, strong correlation

We review results of the renormalised perturbation approach as applied to infinite dimensional Hubbard [1, 2] and Hubbard-Holstein model [3, 4] in the strong correlation regime. From the low lying excitations of a numerical renormalisation group calculation (NRG), using dynamical mean field theory, renormalised parameters for the bandwidth, chemical potential and local quasiparticle interations can be calculated (see 1(a)). The quasiparticle spectra deduced describe well the low energy one-particle spectral densities when compared with the direct NRG calculations. The renormalised parameters when used to calculate the repeated quasiparticle scattering also in excellent agreement with the low energy spin dynamics from a direct NRG calculation (see 1(b)). The approach has been generalised to include an arbitrary magnetic field, and antiferromangetic order in the case of the Hubbard model. We assess the potential of this approach to describe the to give relevant information physics for the calculation of transport properties for models with strong correlation behaviour.

Figure 1: (a) The local quasiparticle interaction $\tilde{U}$ and z-factor (inset) for the Holstein model as a function of the electron-phonon coupling $g$ at half-filling and (b) the imaginary part of the longitudinal and transverse dynamic spin susceptibilities for the infinite dimensional Hubbard model as calculated from the RPT and NRG for $U = 6$ at 5% doping in a magnetic field $h = 0.15$.

Spin Meissner Effect in Superconductors and the Origin of the Meissner Effect

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Keywords: spin current, charge expulsion, hole superconductivity

The expulsion of magnetic flux from the interior of a metal that becomes superconducting (Meissner effect) was discovered experimentally in 1933. Contrary to conventional wisdom, I argue that it is impossible to explain this effect within the accepted framework of London-BCS theory: one would have to assume either violation of Lenz's law, or violation of angular momentum conservation, or both. Instead, I propose that the outward motion of magnetic field lines as a metal goes superconducting reflects and is a consequence of outward motion of electric charge, just like would happen in a classical plasma (Alfven's theorem). According to the theory of hole superconductivity[1], metals become superconducting because they are driven to expel excess negative charge from their interior. This is why high $T_c$ occurs in the highly negatively charged ($CuO_2)^-, B^- and (FeAs)^- planes of cuprates, MgB$_2$ and iron arsenides respectively, and why NIS tunneling spectra are asymmetric, with larger current for a negatively biased sample. How to reconcile the resulting macroscopic charge inhomogeneity with the supposed non-existence of macroscopic electric fields in the interior of superconductors will be discussed in the talk. Charge expulsion is also associated with an expansion of the electronic wavefunction and a decrease in the kinetic energy associated with quantum confinement, consistent with observations[2]. In addition to explaining the Meissner effect, this physics gives rise to a spin-Meissner effect[3]: a macroscopic spin current is predicted to flow near the surface of superconductors in the absence of applied external fields, of magnitude equal (in the appropriate units) to the critical charge current of the superconductor. The orbital angular momentum of each electron in the spin current equals its spin angular momentum. This physics also provides a geometric interpretation of the difference between type I and type II superconductors, and predicts that the macroscopic electric field in the interior of superconductors equals the thermodynamic critical magnetic field $H_c$ or $H_{c1}$ for type I and type II superconductors respectively. These predictions are theoretically and experimentally testable.

Optimal thermoelectric materials: beyond the Mahan-Sofo approach  

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Submitted : 12-09-2008  
Keywords : Boltzmann equation, figure of merit, phonon drag

Much of the current literature on optimal thermoelectrics is based on the Mahan-Sofo (MS) approach [1], according to which the transport coefficients can be expressed as integrals of the transport function $\Sigma_{MS}(\varepsilon)$, where $\Sigma_{MS}(\varepsilon) = \frac{2}{\pi} \sum_{k} v_{k}^{2} \tau_{k} \delta(\varepsilon - \varepsilon_{k})$. The MS approach is based on the standard transport theory formulated in terms of the semi-classical Boltzmann equation. MS made two additional assumptions: (i) the relaxation time approximation was adopted and (ii) the drag effects between electrons and phonons were neglected. The purpose of this talk is to discuss thermoelectric phenomena within the Boltzmann equation approach, but without invoking the additional assumptions (i) and (ii).

In the first part of this talk I will discuss the purely electronic contribution to the figure of merit $ZT$. Considering the simplest variational solution to the Boltzmann equation which goes beyond the relaxation time approximation and which describes both, the heat current and the charge current [2], I will show that the role of the MS function $\Sigma_{MS}(\varepsilon)$ is played by the function $\Sigma(\varepsilon) = \frac{2}{\pi} \sum_{k} v_{k}^{2} \tau_{k} \delta(\varepsilon - \varepsilon_{k})$ that does not contain the relaxation time $\tau_{k}$ of the electrons. After presenting a simple physical explanation of the optimal shape of the function $\Sigma(\varepsilon)$ I will consider several special cases. First I will show that a nondegenerate doped semiconductor whose chemical potential is sufficiently far from the band edge represents an (electronically) ideal thermoelectric material. Then I discuss several metallic systems with a structure in $\Sigma(\varepsilon)$ close to $\mu$ caused by band-structure effects: weak hybridization with a set of localized levels, van Hove singularities in layered systems, and resonant interlayer tunneling in layered systems. I will argue that none of these systems leads to a promising thermoelectric material.

In the rest of this talk I will present preliminary results of a study of the coupled system of electrons and phonons. I will consider the simplest variational solution to the coupled Boltzmann equations for the electrons and phonons [2] and I derive a full formula for the figure of merit of such a system. In order to concentrate on novel effects, I then specialize to a particle-hole symmetric system and discuss under what conditions it can exhibit a large figure of merit. Relation of such an approach with the recent experimental results on silicon nanowires [3] will be discussed.


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Resistivity and Hall Measurements on the Clathrate-System $\text{Ba}_8\text{Ni}_4\text{Ge}_{42}$

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Keywords: Clathrate, Hall, Resistivity

Clathrate compounds possess low thermal conductivity making this group of materials an excellent candidate for thermoelectric applications. The low thermal conductivity originates in the weak bonding of so-called guest atoms inside the host atom cages. This results in low frequency, localized (“rattler”) vibration modes which couple to the lattice modes by resonantly scattering the acoustic mode (heat carrying) phonons of the host framework. Hereby, thermal conductivity is lowered. In general normal semiconducting materials like Si and Ge have a reasonably high power factors ($PF = S^2/\rho$, $S$ is thermopower and $\rho$ the electrical resistivity). The strategy is to synthesize a suitable semiconducting clathrate. A promising candidate is $\text{Ba}_8\text{Ni}_4\text{Ge}_{42}$ [1]. Here we report on resistivity and Hall measurements on polycrystalline $\text{Ba}_8\text{Ni}_4\text{Ge}_{42}$. Preparation took place at the MPI CPIS. The sample was annealed, ground to powder and pressed to a pill from which a bar of size 228 mm$^3$ was cut. Previous $\text{Ba}_8\text{Ni}_4\text{Ge}_{42}$ samples have shown aging symptoms. The resistivity drastically changed after keeping the sample under air for several weeks [3]. In order to avoid oxidation the sample was kept and even contacted under Argon atmosphere. Only for a short period it was on air when the sample was placed into the dewar. Measurements were performed on a commercial Quantum Design PPMS. The temperature range reaches from 400K down to 2K and the maximum applicable field is 9T. Hall measurements were conducted in field sweep and temperature sweep mode.

Figure (1a) shows the temperature dependent resistivity measured in zero field. Resistivity increases with decreasing temperature as expected for a semiconducting material. Field sweeps at several temperatures yield a linear behaviour of the Hall resistivity from which we determined the Hall constant (slope a the fit). In figure (1b) the temperature dependence of the Hall constant is depicted below 20K. The Hall constant amounts to $9 \cdot 10^{-9}$m$^3$/C at room temperature. Upon lowering $T$ the Hall constant $R_H$ starts to increase slightly and exhibits a maximum at around 7K. Below $R_H$ suddenly drops and becomes negative which indicates a change of the majority charge carrier concentration. At 4K $R_H$ seems to saturate yielding $-1.2 \cdot 10^{-6}$m$^3$/C. Thus, evidently our data shows a change from a $p$-type semiconductor to an $n$-type semiconductor. Plotting $\log|n|$ vs. $1/T$, where $n$, the charge carrier concentration in a simple one band model, shows the presence of at least one impurity level. The energy gap is estimated from this Arrhenius plot yields roughly 0.1eV, which is a reasonable value taking values for $\text{Ba}_8\text{TM}_6\text{Ge}_{40}$ (TM is transition metal) as reference [2]. The distance of the impurity level to the band edge is about $\approx 1.5$meV, thus two orders of magnitude smaller than the value of the intrinsic gap. In order to get deeper insight into the charge carrier concentrations, we fitted the $T$-dependence of $R_H$ in a first attempt using the same model as in ref. [4]. As shown in figure (1b) the fit (red solid line) describes the data well.
Figure 1: (a) Semiconductor-like behaviour of the resistivity over a wide range of temperatures. (b) Temperature dependence of the Hall constant.

Cold atoms in optical lattices offer a new laboratory where quantum many-body phenomena can be realized. One key advantage of cold gases is the tunability of interactions, quantum statistics and geometry. In this talk I will focus on two recent developments:

I) Random optical potentials (e.g. speckle) have already been applied to realize the disordered Bose-Hubbard model, raising questions about the nature and extent of the Bose glass phase. I will present a new stochastic mean-field approach which describes the Bose glass in the thermodynamic limit.

II) Ultracold gases are generically inhomogeneous and strongly correlated quantum systems. Any type of long-range order will thus be crucially modified by the presence of a harmonic trap. I will discuss antiferromagnetic ordering of cold fermions in the trap, analyzed within a recently developed extended dynamical mean-field algorithm.
Particle-Hole Asymmetry in the Pseudogap Phase of the High Tc Superconductors

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In the pseudogap phase of the cuprate superconductors, a significant portion of the Fermi surface is still gapped at temperatures above the transition temperature Tc. Instead of a closed Fermi surface, the low-energy electronic excitations appear to form unconnected Fermi arcs separated by gapped regions. It is generally assumed that the spectral function is particle-hole symmetric (at low energies) in both regions - with a peak at the Fermi level on the Fermi arcs centered around the nodes and a local minimum at the Fermi level in the gapped regions away from the arcs. Using high resolution angle-resolved photoemission and new methods of analysis, we show that on a sizable portion of the Fermi surface, including the Fermi arcs, the electronic structure in the immediate vicinity of the Fermi level is not particle-hole symmetric in the pseudogap phase. This is clear evidence that superconducting pairing does not originate from the Fermi arcs. The observations are also consistent with the possibility that the Fermi arcs are in fact the inner surface of the predicted Fermi pockets.
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Rare-earth-based half-Heusler compounds as prospective materials for thermoelectric applications

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Heusler phases of the general compositions \(XYZ\) and \(XY_2Z\), where \(X\) and \(Y\) stand for \(d\)- or \(f\)-transition metals and \(Z\) denotes a \(p\)-element, continuously attract much attention because of a large variety of their interesting physical properties. With respect to the character of electrical conductance they range from good metals to wide-gap semiconductors. Magnetically they may behave like diamagnets or weakly-temperature-dependent paramagnets but they may also show Curie-Weiss paramagnetism. Frequently these materials exhibit long-range magnetic ordering that may have itinerant character but it may show a well localized nature as well. Last but not least some Heusler phases exhibit unusual properties characteristic of strong electronic correlations. Due to all these features Heusler-type compounds are being intensively studied in the context of plenitude of topics, e.g. metal-insulator transition, Kondo effect, heavy fermions, superconductivity, giant magnetoresistance, half-metals, semimetals, magnetic semiconductors, shape-memory alloys, etc.

In half-Heusler alloys \(XYZ\) the presence of vacancies often leads to the formation of a narrow gap in the density of electronic states near the Fermi level. Owing to that these compounds usually exhibit large magnitudes of the thermoelectric power, which together with their relatively low electrical resistivity and thermal conductivity make them promising materials for thermoelectric applications. In the course of our systematic investigations of \(4f\)-electron based Heusler compounds, the physical properties of two series of \(XYZ\) phases with the composition \(REPdSb\) and \(REPdBi\) (\(RE = Y, Nd, Gd, Dy, Ho, Er\)) have recently been studied by means of magnetization, magnetic susceptibility, electrical resistivity, magnetoresistivity, thermoelectric power and Hall effect measurements, performed in the temperature range 1.5—300 K and in magnetic fields up to 12 T. All these ternaries, but diamagnetic YPdSb and YPdBi, exhibit localized magnetism of \(RE^{3+}\) ions. The compounds DyPdSb, HoPdB, NdPdBi, GdPdBi, DyPdBi and HoPdBi order antiferromagnetically at low temperatures \((T_N = 2–13 K)\), whereas ErPdSb and ErPdBi remain paramagnetic down to 1.5 K. Both series show half-metallic conductivity, presumably due to the presence of narrow gaps of the order of tens meV in the electronic band structures near \(E_F\). All these ternaries show very high values of the Seebeck coefficient at room temperature \((S\) up to 200 \(\mu V/K)\), characteristic of semimetals. The carrier concentrations estimated from the Hall data are of the order of \(10^{19} - 10^{20}/cm^3\). The measured thermal conductivities are rather low being few \(W/mK\) at 300 K. As a result, the thermoelectric figure of merit reaches values of about 0.2 at room temperature, i.e. \(ZT\) is similar to those found for doped 36-electron transition metal based \(XYZ\) phases and "rattling" systems like skutterudites and clathrates, which are currently intensively investigated in a field of possible applications as novel thermoelectrics. Furthermore, the heat conductivity in the \(REPdSb\) and \(REPdBi\) compounds is dominated by the phonon contributions, and hence it should be possible to improve their thermo-electrical performance by means of controlled doping (alloying) of the host lattice or/and by increasing the level of structural disorder by appropriate heat treatment.
Breakdown of the Luttinger sum rule within the Mott-Hubbard insulator

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Keywords: strong correlations, Fermi volume, Mott insulator

The validity of Luttinger sum rule (LSR) , which determines the Fermi volume [1]

\[ N = \sum_{k, G_x(k,0) > 0} 1, \]  

was previously investigated for finite systems of correlated electrons [2] where violation was found only for \( t-J \) model, but not for Hubbard model. This can mainly be attributed to small wave vector resolution on finite systems. However, with the use of frequency moment expansion violation was found at half filling for Hubbard model on triangular lattice [3] which does not have particle-hole symmetry relevant for the violation of the LSR[4]. In this paper we show the breakdown of the LSR within the \( t-V \) model including the next-nearest neighbor hopping. Scaling analysis of finite-system results reveals evident breakdown of the sum rule in regime of large gap at \( V \gg t \), while the sum rule appears to recover together with vanishing of the Mott-Hubbard gap [5].

Figure 1: Calculated Luttinger momentum \( k_L \) vs. \( V/t \) for two values of \( t'/t \) and the line [blue] corresponding to satisfied LSR.

Strong correlations in quantum gases

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Submitted : 14-09-2008

Keywords : cold atoms, fermions in optical lattices

Atomic gases cooled to Nanokelvin temperatures are a new exciting tool to study a broad range of quantum phenomena. In particular, the outstanding degree of control which has been achieved over these quantum systems facilitates access to strongly correlated quantum many body physics. For example optical lattices have been created to mimic condensed matter systems. We perform a theoretical study of a fermionic gas with two hyperfine states confined to an optical lattice. We derive a generic state diagram as a function of interaction strength, particle number, and confining potential and discuss the connection to current experiments.
An important goal of condensed matter theory is to contribute to the development of higher thermoelectric materials, and given the advances in our capabilities to describe materials from first principles, it is likely that eventually success stories will be found. In this talk, I will describe some of my own attempts in that direction, considering first thermoelectricity of materials near a Mott transition, and near a quantum critical point. We will first discuss the concepts briefly the computational tools available. We will argue, on empirical grounds and with some theoretical justification, that we should search for optimal thermoelectricity in correlated materials, in systems that display SuperMottness, and we will substantiate this point with examples drawn from the titanites and the cobaltates.

Thermoelectricity in double-barrier structure with the resonant tunneling

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Submitted : 01-09-2008

Study of charge transport in molecules is fundamental interest with potential application in molecular electronics. STM to study the thermoelectric phenomena is molecular nanosystems [1]. Conception of resonant tunneling have been used for explanation of thermo electrical phenomenon in molecular nanosystems [2].

Electronically soft matter
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Submitted: 11-09-2008

Keywords: manganite, density wave

The phenomenon of colossal magnetoresistance in manganites is generally understood to be a result of competition between crystal phases with different electronic, magnetic, and structural order; a competition which can be strong enough to cause phase separation between metallic ferromagnet and insulating charge modulated states. Nevertheless, closer inspection of phase diagrams in many manganites reveals complex phases where the two order parameters of magnetism and charge modulation unexpectedly coexist. I will discuss how such experiments can be naturally explained within a phenomenological Ginzburg-Landau theory, where magnetic and charge modulation coexist in new thermodynamic phases, structured on the nanoscale \cite{1}. It seems possible that this is a general phenomenon, which commonly pre-empts first-order transitions. Remarkably, it is also found that the charge modulated insulating states seem to be better regarded as charge density waves instead of the expected strongly localised striped phases \cite{2, 3}. The disjunction of the phenomenology versus the expectations from microscopic models and measurements raises some conundrums about the treatment of strong electron-phonon interactions in oxides.

Kondo effects in multi-level quantum dots

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Submitted: 00-00-2008
Keywords: Kondo effects, quantum dots, nanobioecoattophysics

Kondo physics in semiconducting quantum dots coupled to metallic leads is commonly associated with a single ‘active’ dot level, and hence with the spin-1/2 Kondo effect. But this is not ubiquitously so: if several dot levels are relevant to charge transport, higher spin Kondo effects may arise, and have been observed experimentally. This talk will discuss a two-level, correlated quantum dot coupled to conducting leads, studied largely via RG. Particular consideration will be given both to the spin-1 and spin-1/2 Kondo regimes which occur on sweeping the dot levels through the Fermi level by tuning a gate voltage; and to the nature of the resultant quantum phase transition between the two regimes occurring in a two-lead, one-channel setup. Comparison to experiment, in the form of zero-bias conductance measurements and differential conductance maps, will also be made.
Thermal Current, Spin Current and Charge Current in Strongly Correlated Materials

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Submitted: 12-09-2008
Keywords: Seebeck effect, spin current, orbital

In the Seebeck effect, the electric voltage is generated in a conductor placed in a temperature gradient. The efficiency of the effect is given by the density and the scattering of the conduction electrons in usual metals and semiconductors. Recently, the transition metal oxides with strong electron correlation have attracted much attention as thermo-electric materials. Since the Seebeck effect is due to the entropy carried by the electric current, the spin and orbital degrees of freedom of conducting electrons in the strongly correlated materials may enhance the Seebeck effect [1]. In the first part of this presentation, the enhanced Seebeck effect is discussed in the transition metal oxides. In the second part, the spin-Seebeck effect is proposed [2], where the spin voltage, i.e., spin accumulation, is generated in a ferromagnetic metal placed in a temperature gradient. Then by utilizing the spin-detection method based on the spin-Hall effect, the spin voltage is converted to the electric voltage. The Spin-Seebeck effect is induced by a pure spin current, a flow of electron spin without electric charge current, and provides a variety of spintronics applications.

Electron spectroscopic study of correlated transition metal oxides

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Keywords : electron correlations, photoemission spectroscopy

The investigation of the role of electron correlation in various electronic properties is a paradigmatic problem in solid state physics. 3d transition metal oxides have drawn much attention in this direction during last few decades due to various exotic properties exhibited by these systems. Various recent studies show that 4d and 5d transition metal oxides (TMO) also exhibit varieties of interesting and unusual properties although the electron correlation strength is expected to be weak due to large radial extensions of the 4d and 5d orbitals. We have employed high resolution photoemission spectroscopy to study these systems. For example, ruthenates (4d TMO) in the perovskite structure exhibit a transition from Fermi liquid to Non-Fermi liquid behavior and unusual magnetic properties[1], although the electron correlation is found to be significantly weak[2, 3]. Doping of Ti at the Ru sites leads to a transition from weakly correlated metal to a band insulating phase[4] via a half metallic phase[5]. A 5d TMO, BaIrO$_3$ exhibits CDW/unusual electronic phase transition despite being an insulator. High resolution photoemission studies show that such unusual ground state appear due to localized electronic states at the Fermi level[6]. Electron correlation strength may not be strong in this system[7]. Y$_2$Ir$_2$O$_7$ is proposed to be a Mott insulator although the partially filled 5d orbitals are expected to be highly extended[8]. In this talk, I will provide a brief overview of our findings in these systems and try to bring out open questions related to these studies. The details can be found in the following references.

Unconventional superconductivity in novel d- and f-electron materials

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Submitted: 09-14-2008

Keywords: superconductivity, charge density wave, magnetic order

A wide variety of strongly correlated electron ground states and phenomena are found in novel d- and f-electron materials: e.g., valence fluctuations, hybridization gap semiconductivity, heavy fermion behavior, non-Fermi liquid behavior, anisotropic superconductivity involving pairing of electrons in states with non-zero angular momentum, high temperature superconductivity, magnetic order, coexistence of superconductivity and magnetic order, quadrupolar order, etc. The occurrence in these materials of such a broad range of ground states and phenomena apparently arises from competing interactions that can be tuned by partial or complete substitution of one element for another, as well as the application of pressure and magnetic fields, resulting in rich and complex electronic phase diagrams in the hyperspace of temperature, chemical composition, pressure and magnetic field. In this talk, we describe several recent experiments on novel d- and f-electron materials that illustrate the delicate interplay between superconductivity and various charge and spin ordered states, such as charge density waves, spin density waves, magnetic order, and quadrupolar order, and the sensitivity of these states to changes in composition, pressure and magnetic field. Materials considered include the filled skutterudites MT$_4$X$_{12}$ (M = alkali metal, alkaline earth, lanthanide, actinide; M = Fe, Ru, Os; X = P, As, Sb) [1], certain lanthanide (Ln) and actinide intermetallic compounds such as URu$_2$-xRe$_x$Si$_2$ [2] and CeTIn$_5$ (T = Co, Rh, Ir), and layered compounds such as LnTe$_3$ [3] and transition metal pnictides [4, 5]. This research was supported by the U.S. Department of Energy (DOE) under Grant Number DE-FG02-04ER46105, the National Nuclear Security Administration (NNSA) under the Stewardship Science Academic Alliance Program through the U.S. DOE under Grant Number DE-FG52-06NA26205, and the U.S. National Science Foundation under Grant Number DMR0802478.


Strongly correlated electron phenomena in filled skutterudites

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Submitted: 09-14-2008

Keywords: filled skutterudite, magnetic order, superconductivity

The filled skutterudite compounds MT$_4$X$_{12}$ (M = alkali metal, alkaline earth, lanthanide, actinide; T = Fe, Ru, Os; X = P, As, Sb) display a wide variety of strongly correlated electron phenomena and are candidates for thermoelectric applications. The strongly correlated electron phenomena include conventional BCS superconductivity, unconventional superconductivity, magnetic order, quadrupolar order, valence fluctuation behavior, heavy fermion behavior, non-Fermi liquid behavior, and hybridization gap semiconductor (Kondo insulator) behavior. When M is a lanthanide or actinide atom, the localized f-states hybridize with the ligand-states of the surrounding pnictogen atoms that form atomic cages within which the M atoms reside. The ground states are determined by a delicate interplay between the hybridization of the f- and ligand-states, crystalline electric field splitting of the f-electron energy levels, magnetic and quadrupolar interactions, and electron band structure. Examples of the strongly correlated electron phenomena found in filled skutterudite compounds are reviewed in this talk. The examples will primarily be drawn from recent experiments on single crystals of ternary La-, Ce-, and Pr-based filled skutterudite arsenides and antimonides LnT$_4$X$_{12}$ (Ln = La, Ce, Pr; T = Ru, Os; X = As, Sb) and pseudoternary Pr-based skutterudite antimonides Pr(1-x,Ru$_x$)$_4$Sb$_{12}$ and Pr$_{1-x}$Nd$_x$Os$_4$Sb$_{12}$. For example, CeOs$_4$As$_{12}$ was found to be a Kondo insulator, while CeRu$_4$As$_{12}$ was observed to display non-Fermi liquid behavior. The compounds Pr$_4$As$_{12}$ were found to exhibit ferromagnetic order below 18 K for T = Ru, BCS superconductivity below 2.4 K for T = Ru, and an unknown type of order and antiferromagnetic order below 2.3 K respectively, for T = Os. The temperature and field dependences of the specific heat and electrical resistivity indicate that PrOs$_4$As$_{12}$ is a Kondo lattice system with a small Kondo temperature T$_K$ of 1 K and an electronic specific heat coefficient of 1 mJ/ mol K$^{-2}$. The T-x phase diagrams of Pr(1-x,Ru$_x$)$_4$Sb$_{12}$ and Pr$_{1-x}$Nd$_x$Os$_4$Sb$_{12}$ reveal regions of superconductivity with different order parameter symmetry and magnetic order. This research was supported by the U.S. Department of Energy (DOE) under grant number DE-SC-04ER46105, the National Nuclear Security Administration (NNSA) under the Stewardship Science Academic Alliance Program through the U.S. DOE under grant number DE-FG02-06NA26205, and the National Science Foundation under grant number MRI-0802478.
Inhomogeneity–induced enhancement of the pairing interaction in cuprate superconductors

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Submitted : 10-09-2008
Keywords : high-temperature superconductors, STM, \( t-J \) model

Scanning tunneling spectroscopy has recently discovered a positive correlation between the magnitude of the superconducting gap and positions of dopant oxygen atoms in Bi-based cuprates[1]. We propose a simple mechanism that could be responsible for this effect. In particular, we demonstrate that the dopant-induced spatial variation of the atomic levels always enhances the superexchange interaction[2]. As a result the superconducting gap could increase in the vicinity of the dopant atoms. It has been known for some time that an enhancement of the pairing potential close to impurities leads to the correct sign of the impurity–gap correlation function[3]. However, in these papers the spatial variation of the pairing potential is of phenomenological origin. Contrary to this, we have proposed a microscopic mechanism that gives an explicit form of this dependence.

Nonresonant electronic Raman and inelastic X-ray scattering and dc transport of the charge-density-wave phase of the spinless Falicov-Kimball model

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Submitted : 30-08-2008

Keywords : nonresonant inelastic scattering, dc transport, Falicov-Kimball model

Employing dynamical mean-field theory, we calculate the many-body density of states, the dc charge and thermal conductivities, and the nonresonant response functions for electronic Raman and X-ray scattering in the charge-density-wave phase of the Falicov-Kimball model. At zero temperature, the charge gap is exactly equal to $U$ and the system acts like a good insulator. Increasing $T$ rapidly fills the gap with subgap states and the transport rapidly becomes more metallic. The nonresonant response functions for electronic Raman and inelastic X-ray scattering show peaks connected with transitions over the gap and transitions that involve subgap states. In the case of inelastic X-ray scattering (when both energy and momentum are transferred), the response function manifests features of dynamical screening (vertex corrections) in the different (nonresonant) symmetry channels ($A_{1g}$ and $E_{1g}$). The optical sum rule (and suitable generalizations for inelastic light scattering) is also examined. In the case of X-ray scattering, the increment of the potential energy contribution into sum rule in the ordered phase depends explicitly on the square of the order parameter and the kinetic one either decreases or increases depending on the interactions strength and transferred momentum value.
Thermal expansion and specific heat of MnSi: evidence for quantum critical behavior

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Submitted: 29-08-2008

Keywords: itinerant magnetism, quantum critical point, Grueneisen parameter

In weak itinerant ferromagnets, such as MnSi or ZrZn2, the ordered magnetic moment in the ferromagnetic phase is much smaller than the Curie-Weiss-like moment found above the transition. These systems become paramagnetic with the application of modest (10 - 20 kbar) pressures and are, thus, quite close to a pressure-tuned phase transition at T=0, i.e. a so called quantum critical point (QCP). The ferromagnetic transition temperature can also be driven to zero by replacing some of the Mn by Fe. Recently it was shown (M. Garst et al. Phys Rev. B72, 205129 (2005)) that the Grueneisen parameter, i.e. the ratio of the thermal expansion coefficient to the specific heat, is expected to diverge near such a pressure-tuned QCP. Here we present both thermal expansion and specific heat data of pure and Fe doped MnSi at ambient pressure. We derive the Grueneisen parameters as a function of temperature, magnetic field and Fe doping and compare the results to the expected theoretical behavior.
Fluctuations of the superconducting order parameter as the origin of the Nernst effect

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Submitted : 12-09-2008

Keywords: thermoelectric transport, Nernst effect, superconducting fluctuations

An observation of a strong Nernst signal well above the critical temperature of the superconducting transition ($T_c$) made this phenomenon an area of high theoretical interest [1]. The Nernst effect is a transverse thermo-magnetic phenomenon in which the voltage difference is induced by a temperature gradient in the presence of a magnetic field. The Nernst effect measured in the high-Tc superconductors [2, 3] has been attributed to the motion of vortices [6, 5, 4] existing outside the region of superconductivity (vortex-liquid regime). Recent measurements of the Nernst signal in conventional amorphous superconducting films far above $T_c$ [7, 8] can not be explained by the vortex-like fluctuations. An alternative explanation suggests that the effect is caused by fluctuations of the superconducting order parameter [9, 10]. Surprisingly, a comprehensive theory of the Nernst effect outside the superconducting state in the conventional superconductors has not been developed so far. In this study we present such a calculation for a wide range of temperatures and magnetic fields. We demonstrate a quantitative agreement between our theoretical expressions and the experiment [8].

Low temperature transport in correlated systems and its evolution under pressure

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Submitted: 11-09-2008

The low-temperature transport coefficients of the degenerate periodic SU(N) Anderson model are calculated in the limit of infinite correlation between f electrons, within the framework of dynamical mean-field theory. We establish the Fermi-liquid (FL) laws in the clean limit, taking into account the quasiparticle damping. The latter yields a reduced value of the Lorenz number in the Wiedemann-Franz law. Our results indicate that the renormalization of the thermal conductivity and of the Seebeck coefficient can lead to a substantial enhancement of the electronic thermoelectric figure of merit at low temperature.

Using the FL laws, we discuss the low-temperature anomalies that show up in the electrical resistance of the intermetallic compounds with cerium and ytterbium ions when studied as a function of pressure. Our calculations explain the sharp maximum of the coefficient of the $T^2$ term of the electrical resistance and the rapid variation in residual resistance found in a number of Ce and Yb intermetallics at some critical pressure.
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Strongly correlated fermionic gases in optical lattices

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Submitted : 11-09-2008

In a solid material strong interactions between the electrons can lead to surprising properties. A prime example is the Mott insulator, where the suppression of conductivity is a result of interactions and not the consequence of a filled Bloch band. The proximity to the Mott insulating phase in fermionic systems is the origin for many intriguing phenomena in condensed matter physics, most notably high-temperature superconductivity. Fermionic quantum gases trapped in an optical lattice offer a very pure realisation of the Hubbard model, giving a new approach to understand the physics of strongly correlated systems.

After introducing fermionic atoms in optical lattices and outlining how they can be used to access the strongly interacting regime, I will focus on recent experiments in our group. In particular, I will report on the formation of a Mott insulor of repulsively interacting two-component Fermi gas, which we have recently observed.
Kondo effect in oscillating molecules

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Submitted: 06-09-2008

Keywords: break-junctions, Kondo effect, soft-mode

We consider electronic transport through break-junctions bridged by a single molecule in the Kondo regime. We describe the system by the two-channel Anderson model. We take that the tunneling matrix elements depend on the position of the molecule. We show, that if the modulation of the tunneling by displacement is large, the potential confining the molecule to the central position between the leads is softened and the position of the modulation is increasingly susceptible to external perturbation which break the inversion symmetry. In this regime, the molecule is attracted to one of the leads and as a consequence the conductance is small. We argue on semi-classical grounds why the softening occurs and corroborate our findings by numerical examples obtained by Wilson’s numerical renormalization group and Schönhammer-Gunnarsson’s variational method. We discuss also the occurrence of the two-channel Kondo fixed point in this model and its relevance in experiments with break-junctions.
Thermodynamic Analysis and Optimization of Energy Intensive System

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Keywords: thermodynamic, analysis, optimization, graphs, solar-heat pump

The processes taking place in complex energy intensive systems with renewable energy sources are characterized by mutual transformation of quantitatively different power resources. For this reason the thermodynamic analysis and optimization of such systems is based on combined application of both laws of thermodynamics and demands the exergy approach [1,3].

Meanwhile, the increasing complexity of optimization problems requires more effective and powerful mathematical methods. As it was shown in [1,3] the most effective mathematical methods used for exergetic analysis and optimization are methods of graph theory.

This paper describes the general approach for thermo economical optimization of energy intensive on example of a solar-heat pump systems with season heat storage (SHPS) with the total heat productivity of 0.5 MW [2] (see Fig. 1.) It is shown that the application of the suggested method allows to receive the minimum value of thermo economical expenditures of a system $Z_{opt} = Z_{1-1-3-2} = 2502$ USD/year.

The optimal variant for the SHPS with total heat production of 0.5 MW is the system with a Solar Collector $A_{SC}=1000 \text{ m}^2$, Season Storage Tank $V_{ST}=3000 \text{ m}^3$, use factor for Heat Pump $n=0.6$, use factor for Electric Boiler Heat $s = 0.4$.

On the energy scales of YbAl$_3$ from the thermopower data: the role of coherence on thermopower

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Submitted: 13/09/2008

Keywords: YbAl$_3$, coherence, Kondo temperature

We report on thermopower and resistivity data measured on an YbAl$_3$ single crystal from 2 K up to 320 K. The thermopower clearly reveals signatures of coherence in YbAl$_3$ up to $T_{coh}$ $\approx$ 35 K. We extracted the characteristic temperatures from our thermopower data, discuss and compare them with the ones extracted from the other experiments. To explain some unusual features of the temperature dependence of the thermopower, we relate the thermopower data with the other physical quantities measured on the same single crystals of YbAl$_3$. In addition, we compare our thermopower measurements to the thermopower data found in literature.
Transport Properties of the Ta$_x$N thin films

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Submitted: 15-09-2008

Keywords: Ta$_x$N thin films, resistivity, thermopower

We report on the low temperature transport properties of the Ta$_x$N thin films deposited on the SiO$_2$ amorphous substrate. The results was analyzed in the light of the Ta$_x$N thin films investigations deposited on the sapphire substrate where $x$ varied from 1.2 to 0.4 spanning thus the critical concentration of the metal-insulator transition at $x = 0.6$. During the deposition on the low cost SiO$_2$ amorphous substrate, the substrates were held at the same temperature, 450°C, at partial N$_2$ pressures ranging from 50 to 100 mTorr. Thus we obtain the Ta$_x$N thin film alloys in a narrow range of $x$: 0.72-0.83. The transport properties show considerable and non monotonous variation with $x$, which we attribute to the local minimum in the density of the electronic states at Fermi level of the rock salt intermetallic Ta$_4$N$_5$. The temperature dependence of the resistivities, which we fit to $\rho( -T/T_0 )$, is also discussed.

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Low-temperature thermopower and Nernst effect of the strongly correlated semimetal CeNiSn

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Submitted: 15-09-2008

Keywords: Correlated semiconductor, thermoelectric power, Nernst effect, CeNiSn

Heavy-electron semimetals have been claimed promising for thermomagnetic applications due to the anticipated large Nernst coefficients and the enhanced effective mass of the charge carriers. We present low-temperature thermoelectric power and Nernst effect measurements on the orthorhombic CeNiSn. Single crystals of highest available purity have been studied between 1.5K and 40K in different heat-current-field configuration. CeNiSn is classified as Kondo semimetal which exhibits a pseudo-gap opening at around 10K. At low temperatures residual states within the gap are revealed by transport and thermodynamic measurements. The Hall effect indicates the decrease of the charge carriers below the gap temperature. In this temperature range also the thermopower is found to change rapidly. Negative values are found for the configuration with the heat current along b. In field, the minimum shifts to lower T whereas the absolute values increase. Only at high fields the closing of the gap due to the field is observed. Furthermore, the influence of sample misalignment and transverse signals in the presence of a field are analyzed. The presented data are first reliable results which take into account the large Nernst coefficient at low temperatures. Results of different samples with the same configuration support exact orientation and alignment of the samples.

The field-dependent thermopower is discussed in terms of a Zeeman split energy gap at the Fermi energy. A similar analysis was to the specific heat results.

The Nernst effect exceeds values of 100 μV/K at high fields of T. These large values correspond to a low charge-carrier concentration. CeNiSn allows for a study of the Nernst effect without concomitant ordering. The results will be compared to simple approaches. However, due to multiband effects those approximations are not sufficient to explain the temperature and field dependence of the Nernst effect of CeNiSn. More realistic theoretical models which take into account the gap structure as well as the multiband nature are desirable to understand the Nernst effect of strongly correlated semimetals and semiconductors. The large values of the Nernst effect of CeNiSn show that systems with strong correlations might be candidates for application for thermomagnetic cooling devices. The thermomagnetic figure of merit N²σT/κ reaches values of 0.05 However, it has to be noted that the thermal conductivity of these single crystals is large and degrades the figure of merit. Reducing the thermal conductivity by nanostructuring might yield high figures of merit.
Modelling of phase transitions in the $RVO_3$ perovskites

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Submitted: 12-08-2008

Keywords: spin-orbital superexchange, magnetic and orbital order, lattice distortion

Spin-orbital superexchange models provide a theoretical framework for describing magnetic and optical properties of Mott insulators with orbital degrees of freedom \textsuperscript{1}. The spin-orbital superexchange model for $(xy)(yz/zx)^1$ configuration at each $V^{3+}$ ion in $R\text{VO}_3$ perovskites captures $(yz/zx)$ orbital fluctuations along the $c$ axis \textsuperscript{2}. The model that describes both orbital transition at $T_{OO}$ and magnetic transition at $T_{N1}$ to the $C$-type antiferromagnetic order has to include as well \textsuperscript{3} the crystal field, intersite orbital interactions, and the orbital-lattice coupling which all vary with ionic radius $U$. The decreasing $U$ is accompanied by increasing GdFeO$_3$-like alternating rotations of the VO$_6$ octahedra by angles $\vartheta$ and $\varphi$, see inset in Fig. 1(a). This leads to the orthorhombic lattice distortion $u = (b - a)/a$, where $a$ and $b$ are the lattice parameters of the $Pbnm$ structure. The orthorhombic distortion $u$ acts as a transverse field $gu^2\tau^x_i$ ($\tau^x_i$ is the orbital operator at site $i$, $g_{\text{eff}} \equiv gu$), which acts as a transverse field on the orbitals and polarizes them, and therefore competes with orbital correlations induced by superexchange $J \approx 200 \text{K}\text{n}\text{B} \text{F}$, Fig. 1(a). While singlet orbital fluctuations are reduced at small values of $r_R$, the value of the Néel temperature $T_{N1}$ is lowered in agreement with experiment, Fig. 1(a). Simultaneously, the nonmonotonic dependence of $T_{OO}$ on $r_R$ can be explained by a rapid increase of the orbital polarization $\langle \tau^x \rangle$ (or $g_{\text{eff}}$), in agreement with the surprisingly large experimental increase of lattice distortions $u_0$ and $u_1$ from La to Y by one order of magnitude, see Fig. 1(b).

![Figure 1: (a) The orbital transition $T_{OO}$ and Néel temperature $T_{N1}$ (solid lines) for varying ionic size $r_R$ in $R\text{VO}_3$ perovskites, as obtained from the theory \textsuperscript{3} and from experiment (circles); dashed lines for $g_{\text{eff}} = 0$. The inset shows the $\text{GdO}_3$-type distortion, with the rotation angles $\vartheta$ and $\varphi$. (b) Experimental distortion (in percent) at $T_0 = 0$ ($u_0$, circles) and above $T_{N1}$ ($u_1$, triangles), compared with the orbital polarization $\langle \tau^x \rangle_{T=0}$ and with $g_{\text{eff}}$. Squares show the upper bound for $g^2/K$ predicted by the theory (at $u_0 = 0$).](image)

Calculated electronic structure properties of URu$_2$Si$_2$ and Ce-115 materials

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Submitted : 14022008

The Ce-115 materials are archetypal heavy-fermion superconductors that display a fascinatingly rich interplay of magnetism and superconductivity. We employ density-functional theory (DFT) based calculations to approach the correlated $f$-electronic structure of these materials. In particular, we compute the nuclear quadrupole resonance (NQR) frequencies at the $f$-sites in pure and Cd-, Sn-doped Ce-115 and compare with recent experiments. The degree of Ce $4f$-localization is treated through the application of various models (local density approximation, generalized gradient approximation, $\xi_+ U$, and $f$-core approach). We find that there is a correlation between the NQR and Ce $4f$-behavior. In another collaboration we use ARPES to study the Fermi surface of the Kudo lattice material CeCoIn$_5$ halfway the lattice coherence temperature ($T^* \approx 45$K) and compare with DFT calculations. We find that at $T=26$ K the Fermi surface of CeCoIn$_5$ is not enlarged, implying that signatures of coherence in the transport data can develop without a concomitant enlargement of the Fermi surface. We furthermore investigate Ru$_2$Si$_2$ which hidden order (HO) phase has been a mystery for many years and provide a microscopic explanation for the HO. We identify the Fermi surface “hot spots” where degeneracy induces a Fermi surface instability and quantify how symmetry breaking lifts the degeneracy, causing a surprisingly large Fermi surface gapping. We show that our electronic structure model is fully consistent with all known experimental properties of Ru$_2$Si$_2$. 
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Strongly correlated cage compounds: New thermoelectrics

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Submitted: 31-02-2008

Keywords: cage compounds, strong correlations, thermoelectrics

The dramatic increase in the world’s demand for energy together with the fact that
the major portion of the primary input is lost to the environment is alarming and calls for
new environment friendly technologies. Thermoelectric materials can convert part of this
low-grade waste heat to electricity. Equally important, they can be used in the inverses
mode, where they use electrical energy to move heat. This effect is used in solid state
Peltier coolers which work without any harmful liquid refrigerants, without movable parts,
and completely silently.

Here, our investigations of a class of materials referred to as cage compounds are pre-
mitted. Well known representatives of this class are skutterudites, clathrates, or clathrate-
like compounds. They all possess an internal crystal structure of voids or “cages”, filled
with loosely bound atoms. The much discussed phonon engineering concept for these ma-
terials is that the “rattling” of these guest atoms in the cages suppresses the lattice thermal
conductivity \(\kappa_L\) but leaves the electrical conductivity \(\sigma\) essentially unchanged. Some rare
earth cage compounds have, in addition, the potential to introduce giant thermopower (\(S\))
values via strong correlation effects which would thus doubly optimize the thermoelectric
figure-of-merit \(ZT = \sigma/\kappa S^2 T\), where \(T\) is the absolute temperature.

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Visualizing pair formation on the atomic scale in high-Tc superconductors

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Submitted: 11-09-2008
Keywords: superconductivity, STM

Unlike traditional superconductors, the density of states (DOS) of the high-Tc superconductor Bi-2212 shows large nanoscale variations that have been detected using scanning tunneling microscopy (STM) [1],[2]. Such variations are seen in the low temperature superconducting gap [1] and in features associated with the coupling of pairs to boson modes [2]. In order to understand these variations in the spectra, we perform atomic resolution STM measurements of Bi-2212 as a function of temperature [3]. Using newly developed experimental techniques, we measure the evolution of the DOS from low temperature (T«Tc) to temperatures where all gaps in the spectrum have disappeared (T>T*). Such measurements show that the pairing gap nucleates in nanoscale regions at temperatures between Tc and T*. By normalizing the low temperature DOS (T«Tc) to the DOS at high temperature, we are able to fit the superconducting DOS to the d-wave BCS form. We find that the experimental spectrum deviations from a simple d-wave fit indicating a strong coupling between electrons and bosonic modes. We will discuss the temperature evolution of these as well as other features in the DOS, and correlate such measurements with the inhomogeneity seen in the gap magnitude at low temperature.


1Work in collaboration with Ken Gomes, Aakash Pushp, Colin Parker, Shimpei Ono, Genda Gu, Yoichi Ando and Ali Yazdani.
The physics of doped Quantum Dimer Models

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Submitted: 27-02-2008

Keywords: Strongly Correlated Electrons, Frustrated Magnets, Unconventional Superconductors

Magnetic frustration commonly leads, in two-dimensional (2D) quantum spin systems, to the (dynamical) formation of spin singlets (or dimers). Generically, systems of quantum fluctuating dimers may order into Valence Bond Crystals (VBC) or remain in some unconventional quantum dimer liquid similar to Anderson’s original RVB state (see e.g. Fig. 1(A)). The two-dimensional Quantum Dimer Model [1] (QDM) plays an increasing role in the understanding of frustrated quantum antiferromagnets and quantum-disordered spin systems and offers completely new routes of investigations.

Yet, little is known theoretically on itinerant frustrated systems and the investigation of doped quantum dimer models (see Fig. 1(B)) is a promising route towards a better understanding of e.g. doped frustrated antiferromagnets or the pseudogap phase of the high-$T_c$ cuprates. I will review recent progress on the bosonic doped QDM [5] and the “non-Frobenius” doped QDM [6] retaining the original fermi statistics of the electrons. These models show rich phase diagrams including, in the latter case, a d-wave hole-pair unconventional superconductor at small enough doping and a bosonic superfluid at large doping. The hole kinetic energy is shown to favor binding of topological defects to the bare fermionic holons turning them into bosons, in agreement with arguments based on RVB wave-functions [7]. Under an applied Aharonov-Bohm flux, the superfluid exhibits quantization in terms of half-flux quanta, consistent with $Q = 2e$ elementary charge quanta [5].

Figure 1: (A) Schematic phase diagrams of the (undoped) QDM on triangular and square [2] lattices. Only the triangular lattice exhibits a liquid (RVB) phase [3]. A novel mixed phase on the square lattice has been reported in [4]. (B) Schematic plots of the dimer flip (a) and holon hopping (b) in the doped QDM on the square lattice.

Spectral functions and high-energy kink in cuprates

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Keywords : spectral functions, cuprates, ARPES

Anomalous properties of quasiparticles in cuprates, a system with strongly correlated electrons, are most directly probed by angle-resolved photoemission spectroscopy (ARPES). Recently, large attention has been devoted to the high-energy kink followed by a waterfall quite universally observed by ARPES in hole-doped cuprates. We show (1) that spectral functions within the extended t-J model appropriate for cuprates and evaluated using the finite-temperature diagonalization of small clusters, exhibit such a high-energy kink in single-particle dispersion. The kink and waterfall-like features persist up to large doping and to temperatures beyond J. Hence the origin can be generally attributed to strong correlations and incoherent hole propagation at large binding energies. In contrast, our analysis predicts that electron-doped cuprates do not exhibit such phenomenon in photoemission.

Competing interactions and magnetic order in correlated electron systems

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Submitted: 12-08-2008
Keywords: Strongly correlated electrons, Mott-Hubbard transition, magnetism

We study the interplay between antiferromagnetism and the paramagnetic metal-insulator-transition (PMI) on a Bethe lattice with nearest and next-nearest neighbor hopping $t_1$ and $t_2$, respectively. $t_2/t_1 \rightarrow 1$ the PMI outgrows the antiferromagnetic phase and shows a scenario which resembles the phase diagram of the system V$_2$O$_3$. However, in contrast to earlier expectations we do not find a hint for an antiferromagnetic metal at half filling.

Off half filling frustration stabilizes the otherwise phase-separated antiferromagnet for filling $n < 1$. Around $n \approx 0.5$ we in addition are able to stabilize a ferromagnetic phase at moderate interaction. Note that on the Bethe lattice such a phase does not exist for $t_2 = 0$, even in the limit $U \rightarrow \infty$ due to missing closed loops necessary for Nagaoka’s theorem.
Density-functional study of the formation of a magnetic impurity in quantum point contacts

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Submitted: 06-09-2008

Keywords: quantum point contact, 0.7 anomaly

A quantum point contact (QPC), a narrow region separating two wider electron reservoirs, is the standard building block of sub-micron devices, such as quantum dots - small boxes of electrons, and qubits - the proposed basic elements of quantum computers. As a function of its width, the conductance through a QPC changes in integer steps of \( G_0 = \frac{2e^2}{h} \), signalling the quantization of its transverse modes. Such measurements also reveal an additional shoulder at a value around \( 0.7 \times G_0 \) which has become known as the 0.7 anomaly. Recently it has been suggested that this phenomenon can be explained if one invokes the existence of a magnetic impurity in the QPC at low densities. Here we report on our extensive density-functional calculations [1] that reveal the formation of an electronic state with a spin-1/2 magnetic moment in the channel as the density increases above pinch-off, under very general conditions.

The present paper gives an overview on a systematic study of the formation, crystal chemistry and physical properties of intermetallic clathrates in various ternary and higher order systems. In these systems alkaline earth elements act as cage filler atoms, whereas the M-atoms act as stabilizers of the clathrate compounds with frameworks made of Ge and/or Si. The ratio of M-atoms to the vacancy content of the framework defines the doping level and consequently the thermoelectric characteristics of the material. The thermoelectric potential of this class of materials will be discussed.
Thermoelectric properties of metal / excitonic insulator junctions

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Submitted: 15-09-2008
Keywords: Falicov-Kimball model, excitonic insulator, Andreev reflection

The excitonic insulator (EI) is a paradigm of a strongly correlated semiconductor whose ground state is dramatically renormalized by electron-hole interaction [1]. Here we propose that its unusual physical properties may be uncovered by making a junction with a metal, as well as that the EI /metal junction is a promising thermoelectric device. We first theoretically consider the class of mixed-valent EIs with high dielectric constants, such as SmB$_6$ and Sm$_2$Se$_3$, whose ground states may be regarded as a condensate of $d$ electron and $f$ hole pairs. If an overlayer of rare-earth atoms differing from the EI bulk is placed at the junction interface, then high values of the figure of merit $ZT$ can be reached at low temperature [2]. This is due to the strong dependence of the transmission coefficient on the energy. In the case of the EI with dispersive bands [3] we are able to address the coherence properties of the ground state. We predict that the thermal and electrical transport across the junction shall exhibit high resistance behavior and low entropy production, distinct from a junction of a metal and a normal semiconductor [4]. At small electrical bias and low temperature, exciton flow dominates over the free charges, substantially increasing the electrical and thermal interface resistance. The rate of entropy production is low due to the coherent and dissipationless character of exciton flow, which is analogous to the supercurrent flowing through a metal /superconductor junction.


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Studying correlation effects in metallic band-insulator / Mott-insulator heterostructures by means of slave bosons

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Submitted: 30-08-2008

Keywords: multilayer structures, electronic reconstruction, slave bosons

Recent experiments have shown that a metallic state can be stabilized at the interface between a Mott insulator (LaTiO$_3$) and a band insulator (SrTiO$_3$) [1]. In such systems, electronic charge is redistributed in order to compensate for the mismatch of the work functions. The resulting mutual doping of the two insulators induces free carriers which have, however, highly renormalized properties.

In order to discuss certain correlation effects relevant for such multilayer structures, we study a model of a band-insulator/Mott-insulator heterostructure by use of the slave-boson mean-field theory introduced by Kotliar and Ruckenstein [2]. We focus on the (renormalized) normal state properties of the quasiparticles and their dependence on model parameters [3]. Furthermore, we compare our results with alternative approaches, like the dynamical mean-field approximation [4] and discuss strengths and limitations of our treatment.

Role of multiple subband renormalization in the electronic transport of correlated oxide superlattices

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Submitted: 25-08-2008

Keywords: perovskite superlattices, optical conductivity, Seebeck coefficient

Metallic behavior of band-insulator/Mott-insulator interfaces was observed in artificial perovskite superlattices such as in nanoscale SrTiO$_3$/LaTiO$_3$ multilayers [1]. For the theoretical description of the parallel transport at low temperatures we identify two major ingredients relevant for such systems: a) the quantum confinement of the conduction electrons leads to a complex, quasi-two dimensional subband structure with both hole- and electron-like Fermi surfaces. b) strong electron-electron interaction answers for a substantial renormalization of the quasi-particle dispersion. Both aspects are well captured in the finite-$U$ slave-boson mean-field description of an extended Hubbard model for the band-insulator/Mott-insulator heterostructure [2].

In our study we focus on the optical conductivity and on the Seebeck coefficient [3]. The results for the optical conductivity can be compared with recent experiments [4] to estimate key parameters. On the other hand, the Seebeck coefficient is sensitive to details of the dominant scattering mechanism. As an example, we study the s-wave impurity scattering in the Born and the unitary limit. Since the subband contributions are weighted differently in the two limits, the Seebeck coefficient is either dominated by the weakly or the strongly renormalized subbands leading to different characteristic behavior.

Recent Results from Oak Ridge National Laboratory on the Layered Iron Arsenide Superconductors with Tc = 55 K

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Submitted: 29-05-2008

The recent discovery by Kamihara et al. [1] of a layered compound, LaFeAsO$_{0.89}$F$_{0.11}$ with T=26K ignited an intense research effort in condensed matter physics laboratories around the world. Within a month, scientists at the Institute of Physics in Beijing had pushed Tc above 50 K by substituting smaller rare earths (Ce, Pr, Nd, Sm or Gd) for La. The first samples in the US were synthesized and characterized within our group at Oak Ridge [2]. The arsenide superconductors are but a small subset of a much larger class of oxypnictide compounds with the same structure originally discovered by d’Jitschko’s group in 1994. In this presentation I will discuss our current results and understanding of the properties and physics of the arsenide superconductors, as well as the possible use of these compounds for thermoelectric applications.

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An Overview of Recent Progress in Thermoelectric Materials Research

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Submitted: 29-08-2008

In the past year there have been two significant breakthroughs in thermoelectric materials research on bulk materials. The best thermoelectric figure of merit near room temperature has been increased by more than 50% to groups have demonstrated room temperature values for near 1.5. As was first found in carefully prepared thin films, the increase in near nanocomposites is almost entirely due to a decrease in the lattice thermal conductivity. Second, a novel method to modify the electronic structure and increase near was demonstrated recently by Heremans, Snyder and co-workers. The modification depends on creating a sharp density of states near the Fermi energy using non-magnetic valence-skipping dopants such as Tl. After presenting a brief history of thermoelectric materials research and a discussion of the basic physics of thermoelectric devices, the new developments will be briefly discussed. Research was sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy.
Geometrical frustrated magnetism in spin-chain oxides crystallizing in
K$_4$CdCl$_6$-type rhombohedral structure

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Submitted : 15-09-2008

We have been investigating a novel class of oxide systems of the type (Ca,Sr)$_3$XYO$_6$, (X,Y= transition metal ions) crystallizing in K$_4$CdCl$_6$-type rhombohedral structure, in which the spin-chains are arranged in a triangular fashion in the basal plane. In many cases, the intrachain interaction is ferromagnetic. As a result of interchain antiferromagnetic interaction, a variety of novel magnetic features attributable to geometrically frustrated magnetism are observed in this family of oxides. A overview of our important results will be given. Specific attention will be paid to Sr$_3$NiRhO$_6$, in which intrachain interaction appears to be antiferromagnetic in contrast to the behavior in family, whereas Sr$_3$NiPtO$_6$ behaves like a spin-liquid – a phenomenon so common among S=1 systems.
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Superconductivity in the Intercalated Graphite Compounds
C$_6$Yb and C$_6$Ca

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Submitted : 15-09-2008

Low dimensionality is generally considered as a necessary ingredient for high superconducting transition temperatures. Surprisingly, perhaps, systems based on graphite have received little attention in this context. Introducing metal atoms between the carbon layers can tune the interlayer spacing and charging of the graphite host through a variety of electronic ground states. One such ground state is superconductivity, which is not present in pure graphite. Our discovery of superconductivity in the intercalation compounds C$_6$Yb and C$_6$Ca, with transition temperatures of 6.5 and 11.5 K, respectively has reissued the debate on such systems. These critical temperatures are unprecedented in graphitic systems and have not been explained by simple mechanisms for the superconductivity. This discovery has already stimulated several proposals ranging from exotic superconducting mechanism to new structural phases. We will present an overview with particular emphasis on recent results from high-pressure experiments.
Real-Time Diagrammatic Monte Carlo for Nonequilibrium Quantum Transport

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Submitted: 01-09-2008

Keywords: Quantum Transport, Nanoconductors, Real-Time Quantum Dynamics

We propose a novel approach to nonequilibrium real-time dynamics. It is applicable to quantum impurities models coupled to biased non-interacting leads, such as those relevant to quantum transport in nanoscale molecular devices. The method is based on a diagrammatic Monte Carlo sampling of the real-time perturbation theory along the Keldysh contour. We benchmark the method on a non-interacting resonant level model and, as a first non-trivial application, we study zero temperature non-equilibrium transport through a vibrating molecule.

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Emergent $\omega/T$ Scaling of Magnetic Response from Freezing of Spin Dynamics in Doped Antiferromagnets 1

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Submitted: 0309-2008
Keywords: scaling, high-$T_c$ superconductivity, doped antiferromagnets

Since the early neutron scattering experiments on low doped La-based high temperature superconductors [1] the simple scaling form of dynamic magnetic response $\chi''(q, \omega, T)$ in the variable $\omega/T$ has been observed in other high-$T_c$ cuprate superconductors at low (hole)doping. In [2] it was shown that such behavior naturally follows from basically two assumptions, well established experimentally for doping levels for which there is no static magnetic order, i.e., a) the low- $\omega$ response is overdamped, and b) the thermodynamic spin-spin correlation length “freezes” at low temperature, i.e. remains finite and temperature independent. These two assumptions together with the sum rule obeyed by $\chi''(q, \omega, T)$ result in a linear-in-$T$ dependence of the effective damping over most of the temperature range above some $T_{QC}$ with a crossover to a finite value below $T_{QC}$. Moreover, this quantum critical behavior of damping manifests itself in the scaling of the peak position of the $q$-integrated response $\chi''(\omega, T)$ with temperature. Such behavior has been observed quite recently in underdoped YBa$_2$Cu$_3$O$_{6.45}$ compound as well [3] providing yet another test for the above assumptions. Surprisingly, however, the scaling behavior has been recently reported to apply to $\chi''(q, \omega, T)$ as well [4]. It is shown, that the above approach still remains valid, and enables one to extract the bare damping of magnetic fluctuations at low $\omega$ from experimental data. The limitations of the above approach and possible application to electron doped compounds, e.g., PLCCO [4] are also discussed.


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Thermoelectricity in correlated matter

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Submitted : 17-09-2008

Thermoelectricity is a foundational topic in statistical mechanics, dealing with reversible heat generation from a current flow. Kelvin established reciprocity using thermodynamic arguments in the nineteenth century. This is mysterious since transport is not within the domain of thermodynamics, and indeed Onsager later gave the correct framework during his seminal work on reciprocity. With regard to the Kelvin, I point out the origin of the mysterious "flaw in the ointment". Interestingly enough, Kelvin’s argument produces a fairly useful, if inexact estimator of thermopower in certain situations. After this amusing historical footnote, I turn to the transition metal oxide Correlated materials, which are classical Mott Hubbard systems. A new formalism, using dynamical heat response, enables a quantitative understanding of the sodium cobaltate materials. It also provides some new predictions for as yet unknown materials, with extremely large thermopower. I summarize a novel hydrodynamic approach that gives a clear physical picture of the new operators introduced by us, and shows that the dimensionless figure of merit ZT couples the energy and charge modes.
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Particle-Hole Asymmetry in the Pseudogap Phase of the
High Tc Superconductors

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Submitted: 16-09-2008

Spin dependence of quasiparticle mass has been observed recently in CeCoIn5 and other systems. It emerges from strong electronic correlations in a magnetically polarized state and was predicted by us earlier. Additionally, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase has also been discovered in CeCoIn5 and therefore, the question arises as to what extent these two basic phenomena are interconnected as appears in theory. Here we show [1] that the appearance of the spin-split masses essentially extends the regime of temperature and applied magnetic field, in which FFLO state is stable, and thus, it is claimed to be very important for the phase detectability. Furthermore, in the situation when the value of the spin quantum number \( \sigma = \pm 1 \) differentiates masses of the particles, the fundamental question arises as to what extent the two mutually bound particles are indistinguishable quantum mechanically? By considering the Cooper-pair state we show explicitly that the antisymmetry of the spin-pair wave function in the ground state may be broken when the magnetic field is applied.

Graphene Quantum Dots

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Graphene is the first real two-dimensional solid consisting of a hexagonal lattice of carbon atoms and revealing high carrier mobility and quantum Hall effect even at room temperature. First graphene quantum devices have been recently demonstrated, such as graphene nanoribbons, quantum interference devices, and graphene single electron transistors. The development of spin-based quantum information processing relies so far mostly on GaAs quantum dots. In such devices hyperfine coupling and spin-orbit interactions are the main mechanisms limiting spin coherence times. Spin qubits in graphene hold the promise that these decoherence mechanisms are significantly reduced. Here, we report measurements showing that excited single-particle states can be detected in graphene quantum dots via co-tunneling in the Coulomb blockaded regime as well as via related features for high voltage bias. The device consisting of a single-layer graphene island with a diameter of around 140 nm is connected via two narrow graphene constrictions and is tunable by a lateral graphene gate. From transport measurements we extract a charging energy in the range of around 8.5 meV and a single-level spacing on the order of 1.6 meV. Furthermore we demonstrate the functionality of a charge-read-out using a nearby graphene constriction. Both steps, the detection of excited states and the charge-read-out are crucial for the investigation of graphene quantum devices in general as well as for future implementations of spin qubits in graphene. In particular it allows to relate the size of the quantum dot to the relevant energy scales such as charging energy and quantum confinement energy. Estimates based on the linear energy-momentum relation of graphene give carrier numbers below 10 for our devices.
Enhanced Thermoelectricity in the Correlated Semiconductor FeSb$_2$

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Submitted: 31-08-2008

Keywords: strong correlations, thermopower, Nernst effect

Recently, FeSb$_2$ was classified as a new $d$-electron based correlated semiconductor [1], similar to the unique FeSi. The discoveries of a colossal thermopower amount to $S = 45$ mV/K and a huge thermoelectric power factor of $PF = S^2/\rho = 2300 \mu W/K^2 cm$ [2] near 10 K stimulate us to study the physics of the thermoelectricity enhancement and its possibility as practical thermoelectric material for low temperature cooling. In this work, we measure the thermoelectric properties of a new FeSb$_2$ single crystal prepared by chemical vapor transport technique, and make a comparison with the Ru-based homologue RuSb$_2$. Thermodynamic properties show strong indications of correlation effects in the former, while they are absent in the latter. Enhanced thermopower with a peak in excess of 10 mV/K was observed below $\sim 30$ K, in agreement with the previous report [2]. Together with a relatively small electrical resistivity, this leads to a large thermoelectric power factor, 650 $\mu W/K^2 cm$. On the other hand, RuSb$_2$ shows less enhanced thermopower with small power factor. Nernst coefficient is also enhanced in FeSb$_2$ in the same temperature range, however, showing a very different temperature dependence from thermopower. We argue that the enhanced thermoelectricity in FeSb$_2$ is due to the electron-electron correlation effects which are absent in RuSb$_2$. Analysis based on classical models will also be presented, which shows that the dominating term in the enhanced thermopower in FeSb$_2$ is indeed electronic in origin.

Thermoelectrics of Kondo Semiconductors and Intermetallic Clathrates

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Submitted : 14-09-2008

We report a systematic study of thermoelectric properties in two systems; Kondo semiconductors and intermetallic clathrates. Kondo semiconductors based on rare-earth elements have an extremely narrow pseudogap at the Fermi level as a result of anisotropic hybridization of 4f electronic states with conduction bands. The development of a V-shaped density of states with decreasing temperature allows enhancement of thermopower while maintaining the electrical conduction metallic. Among the isostructural compounds CeTX with the ε-TiNiSi-type orthorhombic structure, the transport property changes from semiconducting CeRhAs, semimetallic CeRhSb and CeNiSn, to metallic CePtSn and CeBiPt \cite{1}. In this sequence, both the Kondo temperature and the gap width decrease, whereas the phonon thermal conductivity at high temperatures increases. Opening of the pseudogap in CeRhAs and CeRhSb enlarges the thermopower, and leads to the thermoelectric figure of merit $1.0 \times 10^{-3} \text{K}^{-1}$ at 115K and $1.7 \times 10^{-3} \text{K}^{-1}$ at 12 K, respectively. These results are compared with those of Ce-filled skutterudite CeOs$_4$Sb$_{12}$ and Yb-based Kondo semiconductor MB$_3$.

The other is intermetallic clathrates A$_8$Ga$_{16}$X$_{30}$ (A=Sr, Ba; X=Si, Ge, Sn) where guest A atoms are loosely bound to the cage formed by Ga and X atoms. The structural and vibrational properties were studied through thermodynamic and transport measurements \cite{2,3} as well as microscopic techniques such as Raman scattering \cite{4} EXFS \cite{5}, inelastic neutron scattering \cite{6} and others. Type-I clathrate Ba$_8$Ga$_{16}$Sn$_{30}$ shows glasslike thermal conductivity that is actually lower than that of amorphous silica glass, while still behaving electrically as a heavily doped semiconducting crystal. The refinements of single-crystal x-ray diffraction data indicate that the Ba atom in the tetrakaidecahedron occupies the off-center 24k sites which are 0.43 Å away from the center. This displacement results from the mismatch between the guest ion size and the host cage size. The Ba vibration among off-center positions has a characteristic energy of 20 K whose energy is lowest among type-I clathrates. The low thermal conductivity is therefore ascribed to the strong scattering of acoustic phonons by the low-energy off-center rattling.

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**Multiband Effects in Fe-pnictide Superconductors**

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Submitted: 16-09-2008

*Keywords*: iron, pnictides, superconductivity

The key aspect of the newly discovered Fe-pnictide superconductors is their quasi two-dimensional multiband nature. Numerous experiments testify to the presence of a coherent, multiply connected, moderately correlated Fermi surface, and place these systems away from the Mott limit and a high local spin state of Fe dictated by the Hund’s rule [1]. By relating the problem to a negative $U$ Hubbard model and its superconducting ground state, we show that the defining instability of such a Fermi surface is the valley density-wave (VDW) a combined spin/charge density-wave at the wavevector connecting the electron and hole valleys [2]. As the valley parameters change by doping or pressure, the fictitious superconductor experiences Zeeman splitting, eventually going into a non-uniform Fulde-Ferrell-Larkin-Ovchinikov (FFLO) state, an itinerant and often incommensurate VDW of the real world, characterized by the metallic conductivity from the ungapped remnants of the Fermi surface. When Zeeman splitting exceeds the Chandrasekhar-Clogston limit, the FFLO state disappears, and the VDW is destabilized. Near this point, the VDW fluctuations are an essential ingredient of high-$T_c$ superconductivity in Fe-pnictides [2].

Magnetism and Unconventional Superconductivity in Strongly Correlated CeRhIn$_5$ and CeCoIn$_5$\textsuperscript{1}

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Submitted : 04-17-2008

Keywords : unconventional superconductivity, quantum critical, CeRhIn$_5$, CeCoIn$_5$

Magnetism and evidence for a superconducting gap with d-wave symmetry occur simultaneously in both CeRhIn$_5$ and CeCoIn$_5$. In superconducting CeCoIn$_5$, coexisting magnetism is induced either by a magnetic field or by replacing a small number of In atoms by Cd. On the other hand, superconductivity is induced to coexist with antiferromagnetism by applying pressure to CeRhIn$_5$, and at sufficiently high pressures, where there is only superconductivity, a magnetic field induces coexisting magnetism again. The tunability of these very pure materials is remarkable and has allowed progress in revealing the interplay among magnetism, quantum criticality and superconductivity. In spite of this progress, many questions remain unanswered, and these become apparent from a brief review of evidence for an unconventional superconducting gap and of relationships between magnetism and superconductivity in these materials. Perhaps, the most interesting open question is the nature of bosonic excitations involved in Cooper pairing. Growing evidence points to a magnetic origin and an enhanced susceptibility to a pairing instability near the quantum-critical regimes in these systems, but additional experiments, coupled with theoretical modeling, will be necessary to provide definitive answers.

\textsuperscript{1}In collaboration with Tuson Park, R. Movshovich, V. A. Sidorov, Z. Fisk, L. Pham, N. J. Curro, R. R. Urbano, W. K. Park, L. H. Greene, A. Bianchi, M. Nicklas, O. Stockert and M. Kenzelmann
Two Dimensional Triangular Lattice Mott-Hubbard Insulators in Real Life: Sn/Si(111), Sn/Ge(111) and other surfaces

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Genuinely two-dimensional (2D) Mott-Hubbard (MH) insulators are hard to come by in nature, although they should be interesting to work with. Semiconductor surface states form narrow half filled bands which have long been considered a natural place to look for strong electron correlations and 2D metal-insulator transitions including periodically distorted charge (and spin) density waves [1]. Surfaces isoelectronic to (1/3) coverage, (sqrt3 x sqrt3) periodic Sn/Si(111), Sn/Ge(111), Si/SiC(0001) are endowed precisely with such a narrow half filled band, and appear to provide an ideal playground [2, 3]. Among these, SiC(0001) has been known to possess an undistorted MH insulator ground state, whereas Sn/Ge(111) is a (3x3) periodically distorted metal, and Sn/Si(111) an undistorted (sqrt3 x sqrt3) metal[2,3]. While this diversity is in agreement with conventional local density functional (LDA) calculations, (where MH insulators do not exist or appear disguised as magnetic band insulators as in SiC(0001)) it is still surprising, in view of their extremely narrow half filled surface bands. The apparent diversity of behavior was recently removed by the experimental discovery that even Sn/Ge(111) and Sn/Si(111), contrary to LDA predictions, revert to undistorted MH insulators below 20 K and 60 K respectively [4, 5].

I will describe improved density functional LDA+U calculations which, while still mean field in character, enforce better the requirement of integer site occupancy. In Sn/Ge(111) at T=0, one finds that a distorted (3 x 3) metal and a (sqrt3 x sqrt3) undistorted insulator are both possible, the insulator prevailing for realistic U values. For Sn/Si(111), realistic values of U turn the ground state from a metal to a narrow gap insulator. These results naturally explain the emergence of MH ground states in agreement with experiment [6].

In these MH insulating surfaces it is predicted that each Sn adatom supports a spin 1/2. Spins on nearby adatoms interact antiferromagnetically through an exchange coupling J, in the range of 50 K for Sn/Ge(111), and 100 K for Sn/Si(111). Thus the Mott-Hubbard insulating ground state of these surfaces is a realization of the 2D triangular Heisenberg antiferromagnet. Below kT J the spins cannot fluctuate independently of one another, and in this regime spin entropy will be effectively frozen. This observation may explain the observed transition of Sn/Ge(111) and Sn/Si(111) from an undistorted low temperature MH state to a metallic band-like state at higher temperature [3, 4, 5]. The possible resonating valence bond (RVB) state of these insulating surfaces suggests that their doping through alkali adsorption or other means might lead to novel 2D d-wave (quasi) superconducting states.

Optics clues to pairing glues in the cuprates


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Keywords: superconductivity, optical spectroscopy, cuprates

Ever since the discovery of high temperature superconductivity the issue whether or not the pairing is either mediated by a bosonic glue or by a radically different mechanism, and the nature of a glue if it exists, have been highly debated[1, 2]. If the 'glue picture' is applicable, infrared optical spectroscopy can be used to measure the spectrum describing the bosonic glue and its coupling to electrons, $\alpha^2 F(\omega)$. From optical spectra of Bi-2201, Bi-2212, Bi2223, and Hg-1201 at various doping levels we observe that the two main components of $\alpha^2 F(\omega)$ are (i) a peak at 50 meV and a broad temperature and doping dependent background. The 50 meV peak is most likely due to vibrational modes around, in view of the fact that this feature is practically independent of doping, temperature and stoichiometry. The background, which extends up to approximately 0.3 eV is found to increase drastically with decreasing temperature in the range 0 - 20 meV , corresponding to a strong increase of the coupling constant in the limit $T \to 0$. In the case that we take the entire spectrum found at room temperature to be pair forming we find an upper limit on $T_c$ that is 2 times larger and has the same doping trend as the actually observed $T_c$'s.

The two observations, (i) that $\alpha^2 F(\omega)$ is temperature dependent and (ii) that the coupling constant is huge ($\sim 4$), together indicate that the strong coupling formalism probably needs to be revised or extended. The use of a temperature independent $\alpha^2 F(\omega)$ or $\lambda$ in the analysis of resistivity measurements is for example certainly not justified.

Double gap superconductivity in Mo$_3$Sb$_7$  

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Keywords: double-gap superconductivity, specific heat, muon spin relaxation

We performed specific heat and transverse field (TF) mSR experiments on Mo$_3$Sb$_7$ in order to clarify the nature of superconductivity in this compound which has a $T_c = 2.2$ K. Both the electronic specific heat and TF muon depolarization rate exhibit characteristic temperature dependencies, which can be only be described by a double-gap model assuming the relative weights of the molar electronic heat coefficients or magnetic penetration depths of these gaps of 70/30. We have determined some fundamental parameters for the studied superconductor, like the specific heat jump at $T_c$, $\Delta C_p(T_c)/\gamma_nT_c$, the electron-phonon coupling constant, $\lambda_{e-ph}$, the upper $H_{c2}$ and thermodynamic critical $H_{c0}$ fields, the penetration depth $\lambda$, coherence length $\xi$, superconducting carrier density $n_s$, effective superelectron mass $m^*$ and the Ginzburg-Landau parameter $\kappa$. The estimated values of parameters like $\Delta C_p(T_c)/\gamma_nT_c$, $N(E_F)$, and $\lambda_{e-ph}$ suggest that Mo$_3$Sb$_7$ belongs to intermediate-coupling regime. The electronic band structure calculations indicate that there exists a large difference in the density of states and Fermi velocities in different parts of the Fermi surface, that facilitates the opening of two superconducting gaps.

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Thermoelectric properties of non-fermi liquid systems

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Submitted : 00-00-2008

Keywords : non-Fermi liquid, thermoelectric power, two-channel Kondo effect

The non-Fermi liquid (NFL) ground state in strongly correlated electron systems, which
are subjects of intensive theoretical and experimental studies may have different physical
origins. On one hand, a number of NFL systems have been suggested to locate near to a
quantum critical point at \( T = 0 \) K. The NFL properties of these systems in general are
caused by fluctuations of an order parameter in the vicinity of second-order phase transition.
On the other hand, NFL behaviour observed in diluted f-electron systems has been
attributed to connect with some kind of disorder. In the latter systems, multichannel Kondo
effect or distribution of the Kondo temperatures are possible sources of NFL behaviour. To
distinguish one from another mechanisms responsible for NFL phenomenon, one usually
takes into consideration the temperature dependence of several physical quantities like spe-
cific heat, electrical resistivity and magnetic susceptibility. Here, based on the data of the
solid solutions \( U_{1-x}Y_xAl_2 \), we demonstrate that the deviation from the prediction of the
Fermi liquid theory shows up in the thermoelectric power \( S(T) \) properties for \( x = 0.9 \) and
0.95. Moreover, the observed characteristic \( S(T) \sim AT^{1/2} \) dependence in these alloys im-
plies the two-channel Kondo effect to be the most probable mechanism. Complementary
measurements of magnetoresistance in fields up to 9 T provide a consistent support for the
suggestion.

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On the applicability of bosonization and the Anderson-Yuval methods at the strong-coupling limit of quantum impurity problems

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Keywords: impurity models, strong coupling

The applicability of bosonization and the Anderson-Yuval (AY) approach at strong coupling is investigated by considering two generic impurity models: the multichannel interacting resonant-level and anisotropic Kondo models. The two methods differ in the renormalization of the conduction-electron density of states (DoS) near the impurity site. Reduction of the DoS, absent in bosonization but accounted for in the AY approach, is shown to be vital in some models yet redundant in others. The criterion being the stability of the strong-coupling fixed point. Renormalization of the DoS is essential for an unstable fixed point, but redundant when a decoupled entity with local dynamics is formed. This rule can be used to greatly enhance the accuracy of both methods at strong coupling.
Dynamical mean-field theory study of electron-electron correlation effects in multilayered structures.

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Submitted: 31-08-2008

Keywords: strongly correlated electrons, inhomogeneous DMFT, Mott insulators

We present self-consistent inhomogeneous DMFT calculations of the electronic structure of a multilayered device. It is composed of two semi-infinite leads of a ballistic metal that sandwich an interacting barrier. The barrier is described by the Hubbard model and the system is particle-hole symmetric with no electronic charge reconstruction. The problem is solved self-consistently by assuming that the self-energy is local in real space. We find that for a finite barrier no matter how strong the interaction, the system becomes a perfect metallic conductor at low enough temperature. We argue that at zero temperature and frequency the Luttinger theorem holds and that the system has a well defined Fermi surface. This is due to the restoration of translational invariance of the system and to peculiar properties of Fermi liquids in multilayers. This perfect conducting state is extremely fragile to finite temperature, finite driving electric fields, finite driving frequencies, or disorder, so it will often be difficult to see experimentally. We comment on the similarities and differences with quantum dot impurity systems in the Kondo regime. We end with a discussion of when this phenomena can be expected to be seen experimentally.
Multiple energy scales of strongly correlated electrons as revealed by the thermoelectric transport data

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Submitted : 15-09-2008

Keywords : energy scales of correlated thermoelectrics

The heavy fermions and valence fluctuators with Ce, Eu, and Yb ions can exhibit completely different behaviors, depending on temperature, pressure or magnetic field. Typically, we distinguish the local moment (LM) regime, characterized by the Kondo scale $T_K$, and the Fermi liquid (FL) regime, characterized by an energy scale $T_0$.

The LM–FL crossover is characterized by the reduction of entropy, an enhancement of the low-energy effective mass, the change of the susceptibility from Curie-Weiss to Pauli like, and the change of the transport coefficients from logarithmic to simple power laws. The question is, can we understand the crossovers induced by temperature, pressure, doping, or the field, explain the anomalies observed in the FL and LM phase, and relate $T_0$ and $T_K$ to each other?

We address these problems by representing the 4f systems by the periodic Anderson model with infinite $f-f$ correlation. Close to the ground state, the properties are obtained by the Fermi liquid theory, with the FL scale $T_0$ taken from the dynamical mean field approximation (DMFT) or from the experiment. The high-temperature properties are calculated by the diagrammatic expansion which provides the Kondo scale $T_K$ and explains most of the experimental features observed for $T \geq T_K$. However, in a stoichiometric compound, the crossover proceeds differently than in a dilute alloy and cannot be described by a single impurity model.

To infer the overall behavior of intermetallic compounds with 4f ions we solve the periodic Anderson model in the slave-boson approximation and derive an approximate relationship between $T_0$ and $T_K$. We show that the value of the ratio $T_0/T_K$ and the nature of the crossover (“fast” or “slow” with respect to the single impurity case) depends very much on the shape of the conduction electrons density of states around the chemical potential.

An understanding of the crossover allows us to interpolate between the LM and the FL solutions. Using these results we explain the anomalies found in the experimental data on thermoelectric transport. We show that the thermopower is particularly well suited for estimating the characteristic energy scales of strongly correlated systems.
Superconductivity and Magnetism in Fe-based Pnictides under Pressure\(^1\)

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Submitted : 14-09-2008

Keywords : superconductivity, high pressure

There has been a flurry of research activity following the recent discovery of a new class of high temperature superconductors which contain FeAs-based planes. We have performed high pressure electrical resistivity measurements on several of the new FeAs-based superconductors. The \(T_c\) of LaFeAsO\(_{0.89}F_{0.11}\) initially increases rapidly with pressure and then passes through a maximum and is suppressed towards zero temperature near 200 kbar. The \(T_c\) of CeFeAsO\(_{0.88}F_{0.12}\) decreases monotonically with pressure and is reduced below 1 K above 190 kbar. In undoped CeFeAsO we find no evidence for pressure induced superconductivity at pressures as high as 550 kbar. In single crystals of LaFePO, we find that \(T_c\) increases rapidly from 7.5 K at ambient pressure to nearly 14 K (onset) under only 100 kbar pressure, demonstrating that significant \(T_c\) values may also be found in the phosphorus-based oxypnictides.

![Figure 1](image)

Figure 1: (a) Superconducting critical temperature, \(T_c\), versus pressure for CeFeAsO\(_{0.88}F_{0.12}\). (b) Pressure suppresses the spin density wave (main panel) and enhances the antiferromagnetic ordering temperature (inset) of undoped CeFeAsO.

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Pressure dependence of electronic ground states in \(f\)-electron materials

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Submitted : 14-09-2008

Keywords : high pressure, superconductivity, charge and spin density waves

We present the results of several high pressure experiments on the \(f\)-electron materials URu\(_2\)Si\(_2\), the rare-earth tritellurides CeTe\(_3\) and TbTe\(_3\), and the recently discovered Fe-based superconductors LaFePO, LaFeAsO\(_{1-x}\)F\(_x\) and CeFeAsO\(_{1-x}\)F\(_x\).

![Figure 1](image)

Figure 1: (a) Pressure dependence of the transition temperatures of the phases observed in TbTe\(_3\). At 22.8 kbar, charge density wave, antiferromagnetic and superconducting order all appear upon progressively cooling the sample. (b) Spin density wave ordering temperature \(T_{SDW}\) and antiferromagnetic ordering temperature \(T_{AFM}\) versus pressure for CeFeAsO.

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LPCVD (low pressure chemical vapor deposition) was used for preparation of thin heavily boron δ-doped polysilicon samples. Investigated samples were deposited in the horizontal reactor at 750 °C for 1 hr and thereafter thermally annealed in the diffusion furnace at 1200 °C (also for 1 hr). Obtained samples had very low sheet resistances. Comprehensive Raman spectroscopy gave insight into the structure and boron concentration of polysilicon samples. Resistivity measurements revealed metallic behavior from the room temperature down to 2 K with $T^{1/2}$ dependence in an unusually wide temperature range (from 2 to 80 K). In the whole temperature range measured thermopower data show metallic behavior as well and are linear above 120 K. However, the thermopower values are rather high, even higher than the theory predicts for ordinary metals. In spite of the high thermopower and low resistance obtained, thermoelectric characteristics of the investigated Si:B are still not good enough for the applications in thermoelectric devices.

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Kondo model with magnetic anisotropy terms

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Submitted : 20-08-2008
Keywords : Kondo effect, magnetic anisotropy, tunneling spectroscopy

Recent scanning tunneling spectroscopy experiments have revealed that magnetic anisotropy strongly affects the behaviour of magnetic impurity atoms adsorbed on surfaces of noble metals. Motivated by these experiments, we have performed a systematic study of the static and dynamic properties of the single-channel Kondo model with $D S_z^2 + E(S_z^2 - S_y^2)$ longitudinal and transverse magnetic anisotropy terms for different impurity spins $S$ and for different signs and values of the anisotropy $D$. In addition to confirming some previously known results, we find a number of unexpected features. In the $S = 1$ case, we find two-stage Kondo screening with exponentially reduced second Kondo temperature if $|D| < T_K^{(1)}$, for both positive and negative $D$ (if $E \neq 0$). Effective spin-1/2 Kondo screening is also found for $S = 2$ if $|D| < T_K^{(1)}$, and for $S = 3/2$ if $|D| > T_K^{(1)}$, but with no exponential reduction of the second Kondo temperature. We also studied the non-Fermi-liquid behaviour in the negative-$D$ model in the $E \ll |D|$ case. To make contact with experiments, we also discuss the splitting of the Kondo resonance with the applied magnetic field in the presence of the anisotropy and the shifts of the magnetic excitation peaks in the tunneling spectra (spin-flip spectroscopy).
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