THE NATO ADVANCED RESEARCH WORKSHOP
New materials for thermoelectric applications: theory and experiment
September 19th – 25th 2011, Hvar, Croatia
Scope of the ARW workshop

Abstract
The workshop will review new materials and examine mechanisms that could lead to new thermoelectric 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.

Scientific summary
Thermoelectric devices are heat engines that either convert heat into electricity or use the electricity to pump the heat from a cold to hot reservoir. The possibilities arising from the fact that electricity can be generated directly from heat, the Seebeck effect known since 1821, are beginning to be more widely appreciated. This is due to current environmental concerns to reduce waste heat loss and to find new, sustainable energy sources. The thermoelectric devices can reduce the petrol consumption in motor vehicles by 5 to 10%, reducing significantly the oil needs. They are also used for power generation in remote regions, where the thermoelectricity ensures a continuous power supply of electronic equipment. This is an important, but only one type of application of a thermoelectric effect. The other thermoelectric effects, the Peltier effect and Thompson effect, can be used for cooling without moving parts, providing microcooling for the electronics industry and refrigeration without the use of environmentally damaging CFCs and FCs. All of these can play an important role in development and efficient use of sustainable energy resources. The scientific and technological advances in this field could have important implication for modern society.

The main problem in nearly all of these applications is the rather low efficiency of the processes of energy conversion. The important factor which determines the efficiency is the dimensionless ratio, ZT, known as the figure of merit. This needs to be optimized to give a value of ZT of the order of 1 or higher for the more widespread use of thermoelectric devices. A value of ZT of the order 1 requires use of a material with a large thermopower and electrical conductivity and a low thermal conductivity. These tend to be incompatible requirements; for example, a good metal has a high electrical conductivity but also a high thermal conductivity. Materials which have a high thermopower tend also to have a low electrical conductivity. The aim of this research field, therefore, is to find or fabricate materials with the properties that enhance ZT. It is a multidisciplinary field, requiring the expertise of material physicists, chemists, metallurgists and the support of theory. There have been important recent developments in innovative synthesis techniques, the discovery of new materials, and a deeper understanding of the parameters that affect the performance of materials in thermoelectric devices. These have brought the goal of producing materials with the required characteristics for commercial application a significant step closer. The aim of this workshop is to build on the success achieved so far.
The workshop will bring together the experts in the different fields, to exchange the latest results and ideas, and to discuss the directions for future work. The programme will focus on a particular issue each day. Several strategies for increasing the figure of merit will be considered. One of them is the use of materials with strong electron correlation, which are promising due to their enhanced thermopower. Another is the use of nanostructured, layered materials and composites. There have been important developments here, in the fabrication and design of these materials, and they have considerable potential, due to the possibility of combining materials with quite different attributes to influence the various factors which contribute to the overall figure of merit. Another important class of materials are those with cages or rattlers. These tend to be rather complicated compounds as they have atoms within local rigid cages, which are relatively free to rattle, and so reduce the thermal transport by the phonons. The aim is to combine these with the favorable aspects from strong electron correlation. Yet another way of enhancing the figure of merit is by using disordered, correlated semiconductors. Semiconductors are already used in some thermoelectric devices. Disorder and increasing the electronic correlation in these materials could be a way of improving their efficiency. There will also be theoretical contributions using various of approaches, some based on simplified models, others aiming at first principles calculations for particular materials, to get a deeper understanding of the interplay of the factors that influence thermoelectric properties.

Integration of younger scientists:

Every effort will be made to involve younger scientists in the program. The organization and form of the workshop will be such as to encourage the informal exchange of ideas, and to promote discussion. The one-hour poster session will be held each afternoon, before the afternoon lecture session. The posters will be continuously on the display and the organizers will print-out all the presentations and put them on poster-boards as well. The lecturers will be available at their posters for answering additional questions. The island of Hvar is an ideal location as it provides an informal and relaxing atmosphere, free from the usual time pressures and distractions of the big city. We have had a very positive feedback from earlier occasions.

Webcasting and proceedings:

The lectures and discussions will be recorded and put on the web, together with the PowerPoint presentations. The material will edited and presented as ‘virtual proceedings’ which will be available to the public over the Internet. This material should provide an up-to-date summary of the thermoelectricity of correlated systems. The DVD with the virtual proceedings will be made available free of charge to all the participants and at the cost of the postage to everyone else.
Organization

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THE NATO ADVANCED RESEARCH WORKSHOP
New materials for thermoelectric applications: theory and experiment  
Hvar 2011, Croatia
Programme of the Workshop

Monday, September 19

14:00-18:30 Registration
20:00-21:00 Welcome party

Tuesday, September 20

8:50 - 9:00 V. Zlatic and A. Hewson
Opening of the workshop.

9:00 – 10:00 Bauer E., Technical University, Vienna, Austria.
From superconductivity towards thermoelectricity: Germanium based skutterudites.

10:00 – 11:00 Kotliar G., Rutgers University, Piscataway, NJ, USA.
First principles calculations of thermoelectric properties of materials: Quo Vadis?

11:00 - 11:30 Coffee break

11:30 - 12:30 Behnia K., Ecole Normale Superier, Paris, France.
Nernst effect in Bismuth and graphite beyond the quantum limit.

12:30 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session.

16:30 - 17:30 Snyder J., California Institute of Technology, CA, USA.
Carrier Pocket Engineering to Improve Thermoelectric Transport in Semiconducting PbTe.

17:30 - 18:30 Delaire O., Oak Ridge National Laboratory, Oak Ridge, USA.
Phonons in thermoelectrics probed with neutron scattering experiments and DFT calculations: electron-phonon and phonon-phonon couplings in FeSi and PbTe.

18:30 - 20:30 Dinner break

20:30 - 21:30 After dinner talk
Shastry S. University of California Santa Cruz, CA, USA.
Extreme Correlations: or How I learned Not to Worry and Love the Infinite U limit.
Wednesday, September 21

9:00 – 10:00 Gelbstein Y., Ben-Gurion University of the Negev, Beer-Sheva, Israel.
General Trends in Thermoelectrics.

10:00 – 11:00 Maple B., University of California, San Diego, USA.
Experiments on new correlated electron systems.

11:00 - 11:30 Coffee break

11:30 - 12:30 Rogl P. F., University Vienna, Austria.
Clathrate Type I Thermoelectrics: \( (\text{Ba, Sr})_x \text{M}_y \{\text{Ge, Si}\}_{46-x-y} \text{□}_y \).

12:30 - 13:00 Mravlje J., Ecole Polytechnique, Palaiseau, France.
Thermopower in strongly correlated \( \text{Sr}_2\text{RuO}_4 \) from first principles.

13:30 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session.

16:30 - 17:30 Mori M., Advanced Science Research Center, JAEA, Tokai, Japan.
Thermopower in correlated electron systems revisited: non-monotonic temperature dependence.

17:30 - 18:00 Pruschke T., Goettingen University, Germany.
Monte-Carlo Approach to Stationary Non-equilibrium of Mesoscopic Systems.

18:00 - 18:30 Hewson A., Imperial College, London, UK.
Fusion of energy scales on the approach to a local quantum critical point.

18:30 - 20:30 Dinner break

20:30 - 21:30 After dinner talk
Kotliar G., Rutgers University, Piscataway, NJ, USA.
Title to be announced

Thursday, September 22

9:00 - 10:00 Buehler-Paschen S., Vienna University of Technology, Vienna, Austria.
Anisotropic Kondo insulators.

10:00 - 11:00 Fauque C., Ecole Normale Superier, Paris, France. Entropy transport in (topological insulator) Bi$_2$Se$_3$.

11:00 - 11:30 Coffee break

11:30 - 12:30 Tomczak J., Rutgers University, Piscataway, NJ, USA.
Signatures of correlation effects and thermopower in FeSi.
12:30 - 13:00 Shastry S., University of California Santa Cruz, CA, USA. Universal features of Thermopower in High Tc systems and Quantum Criticality.

14:30 - 19:30 Workshop trip

Friday, September 23

9:00 - 10:00 Held K., Technical University, Vienna, Austria. Enhancement of the Na0.7CoO2 thermopower due to electronic correlations.

10:00 - 10:30 Arsenault L-F., Universite de Sherbrooke, Canada. Optimal doping and entropic origin of giant thermopower in doped Mott insulators.

10:30 - 11:00 Hess C., Leibniz Institute, Dresden, Germany. Nernst effect of iron pnictide and stripe ordering cuprate superconductors.

11:00 - 11:30 Coffee break

11:30 - 12:00 Goncalves A. P., Instituto Tecnologico e Nuclear, Sacavem, Portugal. Alternative strategies for thermoelectric materials development.

12:00 - 12:30 Pernau H-F., Fraunhofer Institut, Freiburg, Germany. Contributions to physical clarification of high ZT-Bi2Te3/Sb2Te3 nanoscale superlattices.

12:30 - 13:00 Prelovsek P., University of Ljubljana, Slovenia. Transport in disordered systems of interacting fermions.

13:00 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session

16:30 - 17:30 Costi T., Forschungszentrum Juelich, Germany. Charge Kondo effect in molecular quantum dots and Pb1−xTex and a mechanism for large thermopower.

17:30 - 18:30 Freericks J., Georgetown University, Washington DC, USA. Enhanced thermal transport in strongly correlated multilayers.

18:30 - 19:00 Pernau H-F., Fraunhofer Institut, Freiburg, Germany. Contributions to physical clarification of high ZT-Bi2Te3/Sb2Te3 nanoscale superlattices.

20:00 Workshop Dinner

Saturday, September 24

9:00 - 9:30 Fabrizio M., Scuola Normale Superiore, Trieste, Italy. Out-of-equilibrium dynamics in correlated systems: a variational approach.
9:30 - 10:00 Mierzejewski M., Institute of Physics, University of Silesia, Poland.
Nonlinear Current Response of an Isolated System of Interacting Fermions.

10:00 – 10:30 Oles A., Max-Planck-Institut fur Festkörperforschung.
Spin-Orbital Entangled States in Transition Metal Oxides.

10:30 - 11:00 Svaika A., Institute of the Academy of Sciences, Lviv, Ukraine.
Many-body dynamics and inelastic scattering in strongly correlated electron systems.

11:00 - 11:30 Coffee break

11:30 - 12:00 Bonca J., J. Stefan institute and University of Ljubljana, Slovenia.
Nonequilibrium dynamics of many-body systems driven by a constant electric field.

12:00 - 12:30 Zotos X., University of Crete, Heraklion, Greece.
Open issues on the transport phenomena of 1D quantum magnets.

12:30 - 15:30 Lunch & afternoon break

15:30 - 16:30 Posters and discussion session

16:30 - 17:30 Oganesyan V., City University of New York, USA.
Tutorial lecture: Magnetothermoelectric effects - experiments and theories.

17:30 - 18:00 Rogl G., University Vienna, Austria.
Severe Plastic Deformation (SPD) using High Pressure Torsion (HPT) a new route to high ZTs?

18:00 - 18:30 Pfau H., MPI for Chemical Physics of Solids, Dresden, Germany.
Thermoelectric transport across the metamagnetic transition in CeRu$_2$Si$_2$.

18:30 - 19:30 Očko M., Institute of Physics, Zagreb, Croatia.
Silicon goes thermoelectric.

Sunday, September 25

9:30 – 10:00 Andergassen S., RWTH-Aachen, Germany.
Dynamical transport in correlated quantum dots: a renormalization-group analysis.

10:00 - 10:30 Oganesyan V., City University of New York, USA.
The many-body localization.

10:30 - 11:00 Coffee break

11:00 - 11:15 Hewson A., Imperial College, London, UK.
Workshop summary.

11:15 - 11:30 Zlatić V., Institute of Physics, Zagreb, Croatia.
Closing of the workshop.
Abstracts
Signatures of non-Fermi liquid behavior in the thermopower of MnSi

Ana Akrap$^2$, Stevan Arsenijević$^4$, Cedomir Petrović$^3$, László Forró$^5$

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Submitted : 12-09-2011

Keywords : MnSi, high pressure, thermopower

Signatures of non-Fermi liquid (NFL) behavior are commonly found through the resistivity measurements, which give the power-law exponent $n$. Another transport coefficient which may bring additional information is Seebeck coefficient, $S(T)$. Focusing on a well-established, genuine NFL system MnSi, we have determined $S(T)$ for pressures up to 2.8 GPa. At ambient pressure, $S$ saturates above 400 K, showing no linear dependence in any temperature range. It drops precipitously at the ferromagnetic transition temperature $T_c$. Above the critical pressure $p_c \sim 1.4$ GPa, $T_c = 0$ and the system shows NFL behavior with the resistivity exponent $n \approx 1.5$. Simultaneously in $S(T)$ we observe a clear enhancement below 10 K with respect to the values below $p_c$. As pressure is increased to $2p_c$, the NFL contribution to $S(T)$ is gradually suppressed. We interpret our results in a scenario where the anomalous transport properties are caused by the scattering of the conduction electrons on helicoidal magnetic fluctuations.
Dynamical transport in correlated quantum dots: a renormalization-group analysis

S. Andergassen
RWTH, Aachen, Germany.
Submitted: 13-09-2011

We present results for the nonlinear transport and the time evolution into the stationary state for two minimal models for quantum dots: the interacting resonant level model describing a dot dominated by charge fluctuations, and the Kondo model for a dot with spin fluctuations. Using recently developed renormalization-group approaches in non-equilibrium, the analytical solution of the corresponding flow equations allows to identify the microscopic cutoff scales that determine the relaxation and decoherence rates. Exploring the entire parameter space we find rich non-equilibrium physics which cannot be understood by simply considering the bias voltage as an infrared cutoff. The relaxation dynamics towards the steady state features characteristic voltage-dependent oscillations as well as an interplay of exponential and power-law decay.
Optimal doping and entropic origin of giant thermopower in doped Mott insulators

Louis-François Arsenault, B. Sriram Shastry, Patrick Sémon, A.-M. S. Tremblay

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Submitted: 10-09-2011
Keywords: Thermopower, Doped Mott Insulator, Frustrated Lattice

Empirically, strong correlations can lead to giant thermoelectric power. It is however necessary to develop our theoretical tools to better understand this physics. We thus study the Seebeck coefficient of the Hubbard model on the 3-dimensional FCC lattice at various fillings and interaction strengths using dynamical mean-field theory (DMFT) for the one-band Hubbard model.

To solve the impurity problem of DMFT, we use two different methods. 1) The numerically exact continuous time quantum Monte Carlo method (CTQMC) [1], that relies on the Monte Carlo summation of all diagrams obtained from the expansion of the partition function in powers of the hybridization. 2) Iterated Perturbation Theory (IPT), an approximation method that relies on an interpolation from 2nd order perturbation theory for the Anderson impurity problem [2]. It was realized during this work that, for large couplings, the popular condition of Refs. [3] to fix the bath chemical potential gives unphysical results at low temperature. We thus developed a new condition for IPT. Indeed, at large enough coupling and in the paramagnetic state, the double occupancy ($D$) becomes a simple function of the density and is practically independent of the temperature. We thus fix this condition instead.

We show how the high frequency limit [4] and the Kelvin approach [5] of the thermopower give reliable estimates of the DC limit at weak to intermediate couplings and in the strongly interacting case without the need for analytical continuation. For the former, we look at the infinite limit of an AC thermopower to obtain $S^* = \lim_{\omega \to \infty} S_{Kubo}(\omega)$. While, for the latter, by first considering $\omega \to 0$ and, afterward, letting the system going to the thermodynamic limit we obtain $S_{Kelvin} = \left. \left( \frac{\partial \sigma}{\partial n} \right) \right|_T = \left. \left( \frac{\partial \mu}{\partial T} \right) \right|_n$, where $\sigma$ is the entropy. This expression looks very much like the Mott-Heikes result which states that at large enough temperature (or large enough incoherence) the thermopower is given by $S_{MH} = \left. \left( \frac{\partial \sigma}{\partial n} \right) \right|_E$. Fixing temperature is a much more natural process.

This also allows us to discuss to what extent, in doped Mott insulators, the enhancement of the thermopower can be understood on entropic grounds. The enhancement of thermopower is particularly important at strong coupling in this highly frustrated FCC lattice. These results will be useful in the quest for finding optimal conditions for large Seebeck coefficients.


1Supported by DOE (BSS), NSERC, CFI, MELS, RQCHP and Compute Canada (L.-F.A. and A.-M.S.T)
The antiferromagnetic (AFM) ground state of cubic TbB$_6$ is characterized by multiaxial ordering and a complex magnetic phase diagram. Magnetic susceptibility and magnetostriction show a tetragonal symmetry of AFM phase [1]. The x-ray diffraction shows the charge reflections resulting from the formation of static atomic displacement waves which can be described as a compromise between the exchange and a single-ion elastic couplings [2].

The single crystal of TbB$_6$ is studied at the first order AFM phase transition and within the ordered phase by means of magnetostriction and anisotropic magnetic susceptibility in magnetic fields up to 6 T. The tetragonal AFM phase below $T_N = 21$ K is a mixture of three equivalent AFM domains. Based on the symmetry of spontaneous deformation and the magnetostriction data we conclude that Tb magnetic moments lay in the tetragonal plane. If we apply magnetic field of about 5 T along one of the fourfold axes, the energetically most favorable domain is selected, and the whole crystal tunes into a single-domain state. This state is stable even in zero magnetic field. The observed behaviors are consistent with the tetragonal symmetry of the AFM state.

In this work we discuss the the domain selection line observed in the magnetic phase diagram. We relate this line to the measured anisotropic magnetic susceptibilities and the magnetic energy difference for the magnetic field applied along the two characteristic directions of AFM domain. For a sudden change of the field direction to another fourfold axis the nucleation and the growth of another domain emerge. We attain to explain the temperature and field dependent time evolution of this process. We use the time dependence of magnetostriction to study the domain nucleation and growth dynamics.

From superconductivity towards thermoelectricity: Germanium based skutterudites


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Submitted: 09-09-2011

Keywords: Ge-based skutterudites, electronic band-structure, electronic and thermal transport

Cage-forming compounds such as 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. In skutterudites, the majority of cage forming elements is essentially based on volatile and/or toxic pnictogens like P, As and Sb. Recently, skutterudites MPt₄Ge₁₂ (M = Ba, Sr, La, Pr, Eu, Th, U) [1,2,3] have been discovered as the first members of a new class of skutterudites, based on a framework, entirely formed by Ge-atoms. These ternary compounds are well behaving metals and the majority of them are superconductors with transition temperatures below 10 K.

The aim of the present work is to demonstrate that a partial substitution of Ge by Sb modifies the metallic state leaving behind a metal with a substantially reduced charge carrier density. This is clearly demonstrated from first principle DFT calculations revealing a shift of the Fermi energy towards a gap in the electronic density of states. Accordingly, transport properties change and appreciably large improvements of the Seebeck coefficient are observed for LaPt₄Ge₇Sb₅.

Nernst effect in Bismuth and graphite beyond the quantum limit

Zengwei Zhu, Benoît Fauqué, Kamran Behnia
LPEM-ESPCI, Paris, France
Submitted : 09-09-2011
Keywords : quantum oscillations, Nernst effect, Semimetals

A rare opportunity to explore the fate of a three-dimensional gas of highly mobile electrons confined to their lowest Landau levels is provided by elemental semi-metals such as bismuth and graphite. Coulomb interaction, neglected in the band picture, is expected to become significant in this extreme quantum limit, with poorly understood consequences. The Nernst response sharply peaks when a Landau tube is squeezed inside the thermally fuzzy Fermi surface[1]. Our study of the angular-dependent Nernst effect in bismuth resolves these peaks with a complex angular dependence in very good agreement with the theory. Beyond the quantum limit, we resolve additional unexpected Nernst peaks of unknown origin[2]. According to our study of the Nernst effect in graphite extended up to 45 T, the onset of the field-induced phase transition leads to a drastic drop in the Nernst response signaling the sudden vanishing of Landau tubes. The magnitude of this drop suggests the destruction of multiple Landau tubes possibly because of simultaneous nesting of the electron and hole pockets[3].

Nonequlibrium dynamics of many-body systems
driven by a constant electric field

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Submitted : 9-9-2011

Keywords : strong correlations, electron-phonon coupling, driven systems

We present a fundamental study of a Holstein polaron in one dimension and a single hole in the two dimensional t-J-Holstein model driven by a constant electric field. Taking fully into account quantum effects we follow the time-evolution of systems from their ground state as the electric field is switched on at $t = 0$, until they reach a steady state. At small electron phonon coupling (EP) the Holstein polaron experiences damped Bloch oscillations (BO) characteristic for free electron band [1]. An analytic expression of the steady state current is proposed in terms of EP coupling and electric field. In the strong coupling limit weakly damped BO, consistent with adiabatic evolution along the polaron band, persist up to extremely large electric fields. In the t-J model adiabatic regime is observed followed by the positive differential resistivity (PDR) at moderate fields where carrier mobility is determined [2]. At large field the system enters negative differential resistivity (NDR) regime where current remains finite, proportional to $1/F$. The crossover between PDR and NDR regime is accompanied by a change of the spatial structure of the propagating spin polaron, see Fig. 1. Finally we discuss the interplay between strong correlations and lattice effects in a driven t-J-Holstein model.

Figure 1: Spin disturbance behind the propagating spin polaron.


¹This work was supported by P-0044, MVZT, Slovenia and REIMEI, JAEA, Japan
Anisotropic Kondo insulators

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Submitted : 12-09-2011

Keywords : Kondo insulator, anisotropy, hybridization nodes

Kondo insulators represent a special class of heavy fermion systems where one half-filled conduction band hybridizes with an almost dispersionless 4f level, resulting in a heavy quasiparticle band with a small energy gap of a few meV at the Fermi level [1]. Due to their large (“giant”) thermopower, they are interesting candidates for thermoelectric applications [2]. The chances to realize the above described situation experimentally has been considered highest in simple, cubic compounds. Indeed, most Kondo insulators known to data are cubic [1,3]. More recently, non-cubic compounds with anisotropic properties, frequently referred to as Kondo semiconductors or semimetals, have arisen considerable interest. To describe the anisotropic properties of orthorhombic CeNiSn, for instance, it has been suggested that the hybridization vanishes along a symmetry axis of the crystal to produce nodes in the gap [4,5]. Also, more exotic models such as a topological Kondo insulator [6], have recently been discussed. These topics shall be discussed on the basis of experimental results on anisotropic Kondo insulators.


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New materials for thermoelectric applications: theory and experiment
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Charge Kondo effect in molecular quantum dots and Pb$_{1-x}$TeTlx and a mechanism for large thermopower

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Submitted: 09-09-2011

Keywords: Charge Kondo effect, molecular quantum dots, Lead Telluride

The negative-$U$ Anderson model is believed to be a relevant low energy effective model for molecular quantum dots with strong local electron-phonon interactions, for valence skipping Tl impurities in semiconducting PbTe and possibly also for many other systems, e.g. H$^{+/-}$ at interstitial sites in Si. The negative-$U$ Anderson model supports a charge Kondo effect, in which the role of spin up and spin down states in the conventional spin Kondo effect is played by the empty and doubly occupied states. Dynamic valence fluctuations between these lowest pseudospin states results in the charge Kondo effect. This has some remarkable thermoelectric properties which we elucidate here in the context of two systems, (1), molecular quantum dots, and, (2), semiconducting PbTe doped with Tl impurities.

1. For molecular quantum dots described by the negative-$U$ Anderson model we show that the charge Kondo effect provides a mechanism for enhanced thermoelectric power via a correlation induced asymmetry in the spectral function close to the Fermi level. A dramatic enhancement of the Kondo induced peak in the thermopower is found with Seebeck coefficients exceeding 50 $\mu$V/K over a wide range of gate voltages [1].

2. For PbTe doped with a small concentration $x$ of Tl impurities acting as acceptors we use the numerical renormalization group method to show that the system self-tunes to a charge Kondo state upon increasing $x$ above a critical concentration $x^* \approx 0.5\%$. The resulting charge Kondo effect naturally accounts for both the observed superconductivity at $x > 0.3\%$ [2, 3, 4] and the unusual low temperature and doping dependence of normal state properties, including the self-compensation effect in the carrier density and the non-magnetic Kondo anomaly in the resistivity, which we find to be in good qualitative agreement with experiment [5]. Our results for the Tl s-electron spectral function provide a new interpretation of point contact data [6].

We conclude that Tl impurities in PbTe constitute the first convincing physical realization of the charge Kondo effect, albeit a complex one due to the strong dependence of the chemical potential on temperature, and the presence of local disorder, phonons etc. Hence, we suggest that negative-$U$ molecular quantum dots may eventually offer cleaner realizations of the charge Kondo effect with enhanced thermopowers and figures of merit of potential use in low temperature thermoelectric applications [1].

Phonons in thermoelectrics probed with neutron scattering experiments and DFT calculations: electron-phonon and phonon-phonon couplings in FeSi and PbTe.

O. Delaire, B.C. Sales, J. Ma, A.F. May, M.A. McGuire, M.-H. Du, D.J. Singh
Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA Submitted : 09-09-2011

Keywords : FeSi, PbTe, thermoelectrics, electron-phonon, anharmonicity

Thermoelectric materials are of broad interest for sustainable-energy applications, as they can convert waste heat into electricity, and provide solid-state refrigeration. Achieving high thermoelectric conversion efficiency requires limiting the thermal conductivity, through the disruption of phonon propagation. A detailed understanding of phonon dispersions and linewidths is thus critical in microscopic theories of thermal conductivity. We investigate the phonon dispersions and linewidths in thermoelectric materials for both refrigeration (FeSi) and waste heat recovery (PbTe), with an integrated approach combining neutron and x-ray scattering measurements with first-principles computer simulations. Our experiments benefit from the unprecedented neutron flux of the Spallation Neutron Source at Oak Ridge National Laboratory, to map phonon excitations throughout reciprocal space. The synergy between experiments and computer simulations is often a source of new insights into nature. We leverage powerful electronic structure calculations, including effects of finite temperatures, to analyze our experimental results. Our detailed investigations of the phonons and electronic structure in $\text{Fe}_{1-x}\text{Co}_x\text{Si}$ show that an adiabatic electron-phonon coupling leads to pronounced anomalies in the temperature dependence of both phonons and electron states [1]. The mechanism is general and could affect a broad class of materials. In PbTe, our measurements revealed a strong anharmonicity of the transverse-optic phonons, coupled to acoustic modes, providing a critical insight into the origin of the very low thermal conductivity in this rocksalt compound [2].


Out-of-equilibrium dynamics in correlated systems: a variational approach

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There is increasing interest in correlated materials driven far away from equilibrium conditions. On one side, one hopes that probing the time evolution of these materials far from equilibrium may unveil important dynamical properties otherwise unaccessible by other techniques. On a more practical side, since correlated materials are often on the verge of a Mott metal-to-insulator transition, it could be feasible to switch on/off their conducting properties much faster than e.g. changing temperature or pressure, a great opportunity for possible applications.

In this talk, I shall present a novel technique to study correlated systems in out-of-equilibrium conditions, which is based on a proper time-dependent extension of the Gutzwiller approximation.[1, 2] In spite of its simplicity and degree of approximation, this method has the capability to deal at the same time with the dynamics of both low energy quasiparticles and high energy Hubbard bands, a distinctive feature of correlated metals close to a Mott transition. I will present some applications of the technique that could be relevant to pump-probe experiments in correlated materials.[3]

Inverse Clathrates: Formation, Crystal Chemistry and Thermoelectric Properties

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Keywords : inverse clathrate, thermoelectric properties

Besides the general class of intermetallic clathrates bearing positively charged fillers like Cs, Sr or Ba inside the cages, there also exist the so-called inverse clathrates incorporating group VI (Te) or VII (Cl, Br, I) elements. Up to now approximately 40 different compounds were reported for this class. This work provides a comprehensive compilation of investigations performed hitherto on these compounds [1]. Despite most of the compounds reported crystallize in the clathrate type-I structure, a wide range of different superstructures is observed for inverse clathrates due to atom or vacancy ordering. Similar to the polyanionic clathrates features like the SrattlingT of the guest atoms were reported for inverse clathrates, and thus they are considered as potential thermoelectric materials. Most of the compounds exhibit semiconducting behaviour with a p-type electrical conductivity. Although substitution allows modifying the thermoelectric properties, for most of them the high electrical resistivity does not allow to achieve attractive ZT-values.

Entropy transport in (topological insulator) Bi$_2$Se$_3$

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Keywords : entropy transport, quantum oscillation, topological insulator

Bi$_2$Se$_3$ and Bi$_2$Te$_3$ are well know compounds in the thermoelectricity community since they realize a high figure of merit[1]. More recently this compounds have been proposed as a host of a new class of quantum state of matter, namely topological insulator. Topological insulators are insulating materials that display massless, Dirac-like surface states in which the spin of the electron is locked perpendicular to its momentum by strong spin-orbit interaction[2]. However in practice, it is know from decade that Bi$_2$Se$_3$ is a low carrier concentration in bulk due to the result of charged Se vacancies.

Motivated by their high thermoelectric response, we start to explore the electronic grounds state of Bi$_2$Se$_3$ with a bulk carrier concentration from $n \approx 10^{19} \text{cm}^{-3}$ to $\approx 10^{17} \text{cm}^{-3}$ by entropy measurement. In this presentation we will report our measurement of $S_{xx}$ and $S_{xy}$ down to 300mK and up to 17T. We can resolved, as in the case of bismuth and graphite [3, 4], significant quantum oscillation in thermoelectricity response. By combining the Fermi surface topology deduce from our high field measurement and the low temperature and low field measurement of $\frac{S}{T}$ and $\nu$, we will propose a simple description of the electronic and entropy transport measurement in Bi$_2$Se$_3$ (in the range of concentration studied). In deed, Bi$_2$Se$_3$ (a non compensated system) appears as a complementary system of bismuth and graphite (compensated system) to understand the low temperature thermoelectricity response in the low carrier concentration limit.

Enhanced thermal transport in strongly correlated multilayers

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We present the results for the charge and heat transport in inhomogeneous multilayered devices with strongly correlated electrons. We consider two devices: (1) for longitudinal transport, we consider metallic leads sandwiching a Mott insulator, and (2) for transverse transport, we consider one Mott insulator surrounded by two different Mott insulators, with thin conducting layers created at the interfaces by the polarization catastrophe. The electron dynamics of the device is described by the Falicov-Kimball model which is solved by an inhomogeneous DMFT algorithm[1]. By varying the parameters in these two systems, we can try to optimize thermoelectric properties by tuning the electronic density of states in the active regions to have a large slope. This procedure is different for the two different modes of current flow.

We calculate the transport properties by linear response theory[2, 3] and, thus, obtain the conductivity, the Seebeck coefficient, the power factor, and the figure-of-merit of the device.

We also discuss effects related to applying external fields to these devices. At first, one needs to evaluate how the electronic charge reconstruction is modified due to the electric field and to understand the many-body effects on the capacitance. Then one needs to determine the effect on the transport. We will give a preliminary discussion of our results here.

Thermoelectrics as a direct energy conversion method between heat and electricity is mainly used for electrical power generation and cooling applications. It is based on Seebeck effect, stating that materials subjected to a temperature difference ($\Delta T$), will develop a proportional internal electrical voltage ($V$). The proportion coefficient between $V$ and $\Delta T$ is known as Seebeck coefficient, $\alpha$, which strongly depends on Fermi energy and the electronic scattering parameter. One more growing application, utilizing the strong influence of electronic scattering centers on Seebeck coefficient, is for Non Destructive Evaluation (NDE) and monitoring of metallurgical states and atomic defects in metallic alloys.

The thermoelectric conversion efficiency depends not only on Seebeck coefficient but also on other parameters and increases with the dimensionless figure of merit, $ZT = \alpha^2 \sigma T / \kappa$, where, $Z$, $T$, $\sigma$ and $\kappa$ are the figure of merit, absolute temperature, electrical conductivity and thermal conductivity, respectively. A large variety of materials, such as intermetallic compounds (e.g. half-Heuslers such as TiNiSn), silicides (e.g. Mg$_2$Si and MnSi$_{\sim 1.75}$) and chalcogenides (e.g. (Bi,Sb)$_2$Te$_3$, PbTe and GeTe) have been investigated as thermoelectric materials due to high ZT values at different temperature ranges. Among these material classes, although currently showing lower ZTs, silicides and intermetallic compounds possess additional advantages due to improved mechanical properties, the ability to operate at higher temperatures ($>500^\circ C$) and the potential for large scale commercialization, since they are composed of naturally abundant and less toxic elements.

Global trends for improving the thermoelectric efficiency via maximizing the ZT values include, electronic doping optimizations; generation of Functionally Graded Materials (FGMs) with an optimal maximal ZT envelope over a wide temperature range; and nano-structuring formation for reduction of the lattice thermal conductivity. Nanostructures generation can be achieved by nano-powdering using energetic ball-milling followed by a rapid consolidation method such as Spark Plasma Sintering (SPS). Yet, due to the demand for high stability characteristics, required for long operation periods at high temperatures, one approach for avoiding nano-features coarsening and thermoelectric properties degradation, is based on utilizing thermodynamically driven nanostructures, due to physical metallurgy based effects such as spinodal decomposition and nucleation and growth reactions.

All of the mentioned above general trends in thermoelectric will be discussed during the talk. A focus on the related activities in the department of Materials Engineering at BGU will be given.
Alternative strategies for thermoelectric materials development

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Keywords : Phonon Glass and Electron Crystal\(\text{c}^\) concept, Thermoelectric materials

The presently used thermoelectric materials, as Bi\(_2\)Te\(_3\)-Sb\(_2\)Te\(_3\) and PbTe, were developed until the early 1960’s. However, they show a maximum \(ZT \approx 1\), which leads to device efficiencies that are not big enough to compete with the traditional compression systems. The development of the ‘Phonon Glass and Electron Crystal’ (PGEC) concept, in the middle 1990’s, led to the discovery of a large number of new and improved thermoelectric materials. Several strategies were used in the last years for this research. In the present contribution a review on the different strategies for new thermoelectric materials identification and development is made. This includes the study of selected semiconducting compounds, the choice and exploration of particular phase diagrams, the bulk materials grain size reduction to nano-scale dimensions, the investigation of low-dimensional systems, the research of disordered materials, etc. A special focus will be made on recent approaches used in our institutes to identify new thermoelectric materials.
Thermoelectric properties of the Kondo insulator CeRu$_4$Sn$_6$  

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Keywords : CeRu$_4$Sn$_6$, Kondo insulator, thermoelectrics

Kondo insulators represent a special class of heavy fermion systems where a half-filled conduction band hybridizes with an almost dispersionless 4f level resulting in a heavy quasi-particle band with a small energy gap of a few meV at the Fermi level [1]. The tetragonal crystal structure of the Kondo insulator CeRu$_4$Sn$_6$ places it inbetween the archetypal cubic Kondo insulators like YbB$_{12}$ or Ce$_3$Bi$_4$Pt$_3$ and the orthorhombic TKondo semimetals T CeNiSn and CeRhSb [1, 2, 3]. Investigations of possible anisotropies - or even nodes - of the Kondo insulating gap in CeRu$_4$Sn$_6$ are of central interest.

Previous measurements on single crystalline CeRu$_4$Sn$_6$ showed a large anisotropy of physical properties such as the electrical resistivity, the magnetic susceptibility and the specific heat [4]. Interestingly this anisotropy is observed not only in the tetragonal, but also in a quasi-cubic unit cell formed by the c-axis and the diagonal of the a-a-plane, c'. In this work we present thermopower data of single crystalline CeRu$_4$Sn$_6$. A large anisotropy between the c-axis and the tetragonal plane is observed. We analyse the low-temperature thermopower and compare it to the linear coefficient of the specific heat. In addition, we compare the thermoelectric figure of merit $ZT$ of our single crystals with polycrystal data.


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Enhancement of the Na$_{0.7}$CoO$_2$ thermopower due to electronic correlations

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Submitted : 31-05-2011

The merger of the local density approximation (LDA) and dynamical mean field theory (DMFT) has been a breakthrough for the calculation of materials with strong electronic correlations such as transition metal oxides and heavy fermion systems [1]. The reason for this success is that local correlations are the major ones, at least for these kinds of strongly correlated materials.

After a brief introduction to the method, I will show how electronic correlations increase the thermopower of Na$_{0.7}$CoO$_2$ by 200%. The newly revealed mechanism [2] is an asymmetric shift of (quasi) electrons and holes away from the Fermi level, concurrent with an asymmetry of the respective (group) velocities. Exploiting this effect in bandstructure and correlation engineering may lead to a substantial increase of the thermoelectric figure of merit.

Besides, I would like to briefly discuss the dichotomy between large theoretical and small experimental moments in iron pnictides [3] and, as an outlook into the future development, discuss a route to include non-local correlations beyond DMFT. This allows us, e.g., to calculate the critical exponents of the Hubbard model in two and three dimensions [4].

Nernst effect of iron pnictide and stripe ordering cuprate superconductors

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Keywords : Nernst effect, Iron-based superconductors, Cuprate superconductors

The Nernst effect has recently proven a sensitive probe for detecting unusual normal state properties of unconventional superconductors. Here we present a systematic study of the Nernst effect of the iron pnictide superconductor LaO_{1-x}F_{x}FeAs with a particular focus on its evolution upon doping \cite{1}. For the parent compound we observe a huge negative Nernst coefficient in the spin density wave (SDW) ordered state. Surprisingly, an unusual and enhanced Nernst signal is also found at underdoping (x = 0.05) despite the presence of bulk superconductivity and the absence of static magnetic order, strongly suggestive of SDW precursors at $T \lesssim 150$ K. These precursors seem to fade at higher doping levels, since a more conventional and rather featureless normal state Nernst response is observed at optimal doping (x = 0.1). We compare these findings with results for the Nernst effect of the stripe ordering cuprate superconductor La_{1.8-x}Eu_{0.2}Sr_{x}CuO_{4} \cite{2}. At $x = 0.125$ and $x = 0.15$ a kink-like anomaly is present in the vicinity of the onset of charge stripe ordering temperature, consistent with an enhanced positive quasiparticle Nernst response in the stripe ordered phase. However, a direct comparison between the Nernst coefficients of stripe ordering La_{1.8-x}Eu_{0.2}Sr_{x}CuO_{4} and superconducting La_{2-x}Sr_{x}CuO_{4} at the doping levels $x = 0.125$ and $x = 0.15$ reveals only weak differences, i.e., the enhancement of the Nernst response due to static stripe order as compared to that of the pseudogap phase is very small.


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Fusion of energy scales on the approach to a local quantum critical point

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Keywords : Quantum Critical Point, Heavy Fermions

We consider a two impurity Anderson model which has transitions to a local singlet and to a local charged ordered state as a function of an inter-impurity exchange interaction $J$ and direct interaction $U_{12}$. The low energy behavior of the model can be described in terms of renormalized parameters, which can be deduced from a numerical renormalization group (NRG) calculations. We show that on the approach to the transition points, where the quasiparticle weight factor $z \to 0$, the renormalized parameters can be expressed in terms of a single energy scale $T^*$, where $T^* \to 0$ at the transition. The values of the renormalized interaction parameters in terms of $T^*$ can be predicted from the condition of continuity of the spin and charge susceptibilities at the transitions. These predictions are confirmed by the NRG calculations. The results suggest how $\omega, T$ scaling can arise at a quantum critical point in heavy fermions.
Theoretical study of thermoelectric and thermomagnetic characteristics of Bismuth nanowires under a quantizing magnetic field

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Keywords : Bismuth nanowire, Nernst effect, Phonon drag

The phonon-drag contribution to the Nernst thermoelectric power $S_{yx}$ in bismuth nanowires is numerically investigated. Hasegawa et al. [1] have fabricated the single Bismuth nanowires with diameter 150 nm $\sim$ 500 nm and length over 1 mm, as illustrated in Fig. 1. The wire diameters are short enough to quantize the acoustic phonons but larger than the Fermi wave lengths of electrons. In the systems, therefore, the phonons travel one-dimensionally, while the electrons are found to be still three-dimensional. In the present study, we calculate the phonon-drag thermopower $S_{yx}$ of the nanowires under a quantizing magnetic field and discuss the effect of the dimensionality on the transport properties of the systems.

We utilize a theory of a single Bismuth crystal that includes the contribution of both holes and electrons [2]. The theory revealed that the phonon drag is dominant in the prominent magneto-oscillations in the $S_{yx}$ of a bulk bismuth [3]. Thus, the phonon-drag effect is expected to play a dominant role also in nanowires.

Figure 1: (Left) An optical microscope image of a Bismuth nanowire encased in a quartz template, which is fabricated by Hasegawa et al. [1]. (Right) SEM images at the edges of the nanowires show that they have diameters of 150 $\sim$ 850 nm.

Superconductivity and magnetism in lanthanide platinum germanium compounds

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Keywords: strongly correlated electrons, unconventional superconductivity, filled skutterudite

Filled skutterudite compounds have several well known characteristics that are advantageous for an enhanced thermoelectric figure of merit Z [1]. To aid in the search for increased efficiency in filled skutterudite thermoelectric materials, it is important to improve our understanding of their strongly correlated electron phenomena. We have therefore performed a study of the Pr$_{1-x}$Ce$_x$Pt$_4$Ge$_{12}$ system. PrPt$_4$Ge$_{12}$ is an unconventional superconductor exhibiting evidence for time-reversal symmetry breaking [2], while CePt$_4$Ge$_{12}$ is a nonmagnetic Fermi liquid in which Ce assumes an intermediate valence [3]. Preliminary measurements of magnetization, resistivity, and specific heat down to $\sim$2 K show that superconductivity is suppressed linearly with increasing Ce concentration up to $x = 0.4$, above which, no superconductivity was observed. Powder diffraction measurements show that the lattice parameter increases slightly with increasing $x$, consistent with previous work [3]. Power law analysis of the resistivity measurements show that the system remains a Fermi liquid throughout the entire series. The magnetization decreases with increasing Ce concentration.


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Thermal conductivity measurements

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Keywords: thermal conductivity, meltspinning, 3ω-method

The thermal conductivity $\kappa$, the Seebeck coefficient $S$ and the resistivity $\rho$ enter the expression for the dimensionless figure-of-merit $ZT$,

$$ZT = \frac{S^2 \cdot T}{\kappa \cdot \rho}$$

which characterizes a material’s efficiency concerning thermoelectric power generation or cooling. Thus, by lowering the thermal conductivity, $ZT$ can be enhanced. By introducing rattling modes or increasing the contribution of grain boundaries, the phonon thermal conductivity can be lowered.

Here we present thermal conductivity measurements on meltspun Ba$_8$Ga$_{16-x}$Ge$_{30+x}$ clathrates [1] as well as on nanostructured polycrystalline (SrTiO$_3$)$_{1-x}$(SrCO$_3$)$_x$ samples, synthesized by the evaporation induced self-assembly approach used in Ref. 2. The melt spinning technique [3, 4] can produce Ba$_8$Ga$_{16-x}$Ge$_{30+x}$ in a metastable state, where $x$ can be varied continuously from negative to positive values, resulting in both p- and n-type materials. The temperature dependent thermal conductivity of the p-type ($x = -0.1$) compound shows no maximum at low temperatures, which might be explained by strong phonon charge carrier coupling. Steady-state heat-flow experiments on meltspun Ba$_8$Ga$_{16-x}$Ge$_{30+x}$ flakes had to be carried out by means of a parallel thermal conductance technique to mechanically stabilise the 20 $\mu$m thin samples.

In comparison to single crystalline SrTiO$_3$, the thermal conductivity of nanostructured polycrystalline (SrTiO$_3$)$_{1-x}$(SrCO$_3$)$_x$ is found to be reduced by a factor of 10. The substitution with SrCO$_3$ was done to lower the thermal diffusivity. A systematic dependence of the diffusivity on the SrCO$_3$ content could not be observed.

A new thermal conductivity setup based on the 3ω-method [5] is also presented. Such a setup is particularly well suited for thin film samples. In comparison to the standard steady-state heat-flow technique, thermal radiation and heat loss in the temperature measuring probes hardly affect the measurement. Thus, thin samples with low thermal conductivity can be measured.


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Superperturbation theory approach to thermoelectric transport in strongly correlated quantum dots

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Submitted : 14-09-2011

The description of transport in correlated matter beyond the linear response regime is usually based on the semiclassical Boltzmann equation in the relaxation time approximation. Such an approach relies on the existence of well-defined quasiparticles which is not always warranted. Perturbative methods on the other hand are straightforwardly extended onto the Schwinger-Keldysh contour but often suffer from internal inconsistencies like non-conservation of the charge current away from particle-hole symmetry. We devise a superperturbation approach on the Schwinger-Keldysh contour to treat the transport through a quantum dot. This method is free of such issues as the non-conservation of the current and allows to study various transport properties at and away from particle-hole symmetry. Perturbative in nature, this approach is generalizable to more complex situations.
First principles calculations of thermoelectric properties of materials: Quo Vadis?

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Keywords: thermoelectrics

There is increase interest in using computational and theoretical methodologies to accelerate thermoelectric materials discovery. In this talk will describe some aspects of the methodology available to evaluate the thermoelectric response based on modern electronic structure tools. Using DMFT, we will discuss the validity of simpler estimates of the thermoelectric response such as the infinite frequency limit and the Kelvin formulae. We will stress qualitative considerations that can guide the search for improved thermoelectric response in correlated electron materials. This talk will complement the much more rigorous results LDA+DMFT to be presented by Jan Tomczak.
Experiments on new correlated electron systems

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Submitted : 13-09-2011

Keywords : strongly correlated electrons, non-Fermi liquid behavior, quantum criticality

Multinary $d$- and $f$-electron compounds have proven to be a rich reservoir of strongly correlated electron ground states and phenomena: e.g., valence fluctuations, heavy fermion behavior, non-Fermi liquid behavior, quantum criticality, unconventional superconductivity, high temperature superconductivity, exotic forms of magnetic order, quadrupolar order, etc. These ground states and phenomena arise from a delicate interplay between competing interactions that can be tuned by variation of chemical composition ($x$), pressure ($P$) and magnetic field ($H$), resulting in complex electronic $T(x, P, H)$ phase diagrams. In this talk, we describe recent research performed in our laboratory on correlated electron phenomena in two classes of materials: (1) the noncentrosymmetric compounds with the formula $M_2T_{12}Pn_7$, where $M$ = a rare earth or an actinide element, $T$ = Mn, Fe, Co, Ni, and $Pn$ = P, As, and (2) the filled skutterudite compounds $MPt_4Ge_{12}$, where $M$ = an alkaline earth, a rare earth, or an actinide element [1, 2]. An extensive investigation of single crystals of $M_2Fe_{12}P_7$, where $M$ = Sm, Yb, Th, and U, grown in a Sn flux, was carried out by means of electrical resistivity, specific heat, and magnetization measurements as a function of temperature ($T$) and magnetic field ($H$). The $T$−$H$ phase diagram for single crystals of Yb$_2$Fe$_{12}$P$_7$ reveals a crossover from a magnetically ordered non-Fermi-liquid (NFL) phase at low $H$ to another NFL phase at higher $H$ [3].

The crossover occurs near the value of $H$ where the magnetic ordering temperature ($T_M$) is no longer observable, but not where $T_M$ extrapolates smoothly to $T = 0$ K at a possible quantum critical point (QCP), indicating the occurrence of a quantum phase transition between the two NFL phases. The lack of a clear relationship between the extrapolated QCP and NFL behavior suggests an unconventional route to the NFL ground states.

We have also explored the behavior of other members of this “2-12-7” family of compounds including U$_2$Fe$_{12}$P$_7$, which displays antiferromagnetic behavior below 14 K and possible metamagnetism [4], and Sm$_2$Fe$_{12}$P$_7$, which appears to be a new heavy fermion, itinerant ferromagnet with a Curie temperature of $\sim$6 K [5]. Superconductivity and correlated electron behavior in the pseudoternary Pr-based filled skutterudite system Pr$_{1-x}$Ce$_x$Pt$_4Ge$_{12}$ were studied by means of electrical resistivity, specific heat, and magnetization measurements down to 2 K. The compound PrPt$_4Ge$_{12} exhibits unconventional superconductivity below $T_c = 7.9$ K [2] with evidence for point-like nodes in the gap function [6] and time reversal symmetry breaking [7], while CePt$_4Ge$_{12} is a nonmagnetic Fermi liquid in which Ce has an intermediate valence [8]. The experiments show that $T_c$ is suppressed linearly with increasing Ce concentration up to $x = 0.4$ and Fermi liquid behavior persists throughout the entire series ($0 \leq x \leq 1$).

1Synthesis of samples and characterization measurements for superconductivity were supported by the US Air Force Office of Scientific Research under MURI Grant No. FA 9550-09-1-0603. Low temperature measurements were funded by the US National Science Foundation under Grant No. DMR 0802478. Single crystal growth and electronic and magnetic properties measurements were sponsored by the US Department of Energy under Grant No. FG02-04-ER46103. Acquisition of crystal growth equipment was funded by the US Department of Energy under Grant No. FG02-04-ER46178.


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Doping dependence of the Nernst effect in Eu(Fe$_{1-x}$Co$_x$)$_2$As$_2$
- departure from Dirac fermions physics

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Keywords : Iron pnictides, Nernst effect, Dirac fermions

We report a systematic study of the transport properties in the series of Eu(Fe$_{1-x}$Co$_x$)$_2$As$_2$ single crystals with $x = 0, 0.15, 0.20$ and 0.30. Spin-density-wave (SDW) order is observed in the undoped and the least doped samples with $x = 0$ and 0.15 at $T_{SDW} = 191$ and 131 K, respectively. For $x = 0.15$ and 0.20 Eu(Fe$_{1-x}$Co$_x$)$_2$As$_2$ becomes a superconductor with $T_{c \text{onset}} = 20.5$ and 8.5 K, respectively. We find properties of the SDW state in the parent EuFe$_2$As$_2$ compound well described by the Dirac fermions model. On the other hand, the small cobalt doping significantly changes the transport coefficients below $T_{SDW}$ in Eu(Fe$_{0.85}$Co$_{0.15}$)$_2$As$_2$. Further increasing of $x$ causes an evolution of the system toward a regular metallic state. The antiferromagnetic ordering of the Eu$^{2+}$ ions at $T_N \approx 18$ K has only minor influence on the measured quantities.

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Total Raman scattering features in the CDW chess-board phase of the Falicov-Kimball model

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Submitted : 30-08-2011

Keywords : Raman scattering, Falicov-Kimball model, dynamical mean-field theory

Exact solution for the total electronic Raman scattering response function is derived for case of the insulating phase with charge-density-wave (CDW) order. We examine the spinless Falicov-Kimball model on an infinite-dimensional hypercubic lattice. The Falicov-Kimball model is one of the simplest strongly correlated many-body models, which displays rich physics and has an exact solution within dynamical mean-field theory (DMFT), as well as its charge vertex is known.

When the temperature is less than $T_c$, the density of states (DOS) displays strong dependence on temperature. That DOS features are reflected in the Raman spectra which also show significant features in $T$. Our main result is that there are a large number of strong resonances, which are connected with the peculiarities of the ordered-phase DOS.

We study three common experimental symmetries, which define the polarization of incident and scattered light. The complicated shape of the Raman spectrum and its strong reconstruction with the change of the incident photon energy is caused by the presence of the subbands with strong temperature dependence. The results for the resonance effects give information about the many-body charge dynamics of the CDW-ordered phase. We examine both weakly and strongly correlated cases.
Nonlinear Current Response of an Isolated System of Interacting Fermions

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Submitted : 01-09-2011

Keywords : charge transport, nonlinear response, one-dimensional systems

Nonlinear real-time response of interacting particles is studied on the example of a one-dimensional tight-binding model of spinless fermions driven by electric field. Using equations of motion and numerical methods we show that for nonintegrable (metallic or insulating) systems at high temperatures the major effect of nonlinearity can be accounted by internal heating \[1, 2\]. On the other hand, integrable metals show on constant driving a different universality with a damped oscillating current whereby the frequency is related but not equal to the Bloch oscillations \[1\]. Finally, for integrable insulators we obtain strongly nonlinear dc response (see Figure 1) with vanishingly small dc conductivity in the linear-response regime \[2\]. The latter finding is consistent with equilibrium results for dc limit of the optical conductivity determined in the presence of a weak and decreasing perturbation.

Figure 1: dc response of integrable and nonintegrable insulators at high temperatures: \( F \) is the electric field, \( \beta_{\text{eff}} \) is an effective inverse temperature and \( I \) is dc current induced by \( F \).

Thermopower in correlated electron systems revisited: non-monotonic temperature dependence

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Keywords : thermopower, Hubbard model, dynamical mean-field theory

We examine the role of the strong Coulomb interaction on thermopower, whose temperature dependence will be particularly discussed in detail. For this purpose, the single band Hubbard model is adopted as a minimum model and the strong Coulomb interaction is treated in the dynamical mean field theory. We find that the strong Coulomb interaction brings about the coherent-to-incoherent crossover as temperature increases, and then gives rise to a non-monotonic temperature-dependence [1]. Such a overall behavior is well described by the entropy consideration at high temperatures, i.e, the Mott-Heikes formula. In the light of our theoretical results, we discuss the thermoelectric response in some transition metal oxides [2]. Magnetic field dependence and multi-orbital effects will be discussed as well.

Thermopower in strongly correlated Sr$_2$RuO$_4$ from first principles

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Submitted : 09-09-2011

Keywords : thermopower, electronic correlations, ruthenates

Sr$_2$RuO$_4$ is a correlated metal with the specific heat enhancement about 4 times over the LDA value. NMR and ARPES measurements reveal the crossover to incoherent regime at about 100K. Remarkably, quantum oscillations reveal larger mass enhancement of the carriers in the widest band. We analyze Sr$_2$RuO$_4$ within LDA+DMFT, which reproduces and explains these experimental observations. The low coherence scale and the anomalous mass renormalizations are related to the Hund’s rule coupling and to the proximity to the van Hove singularity [1]. Encouraged by good agreement with experiment, we calculated also the transport quantities. The dependence of Seebeck coefficient on temperature is reproduced well. The semi-saturation which occurs above 150K is related to the crossover to the incoherent regime. Our results demonstrate LDA+DMFT method is promising for investigation of thermopower in correlated electron systems.

Silicon goes thermoelectric
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Submitted : 12-09-2011
Keywords : heavily doped silicon, thermoelectrics, MIT

We discuss on the possibility that boron and phosphorous heavily doped silicon can/could be applied as a working material in thermoelectric (TE) devices. The cheapness and the availability of the ingredients combined with the relative simplicity of production all go in favour to their application. Also, some recently published works indicate enhancement of TE figure of merit, $Z$, by lowering grain size of polycrystalline samples and dimensionality. We are also presenting some of our very recent investigations on the Si:B system near MIT. The results are interesting just in terms of TE properties.

Content:

a) the problem of silicon as thermoelectric,
b) the newest results,
c) heavily boron doped silicon - high concentrations (our investigations),
d) heavily phosphorous doped silicon - high concentrations (our investigations),
e) heavily boron doped silicon - near MIT (our investigations),
f) ferroelectrics.
Many-body localization

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Submitted : 11-09-2011
Keywords : localization, transport, dynamics

I will review some recent theoretical and numerical results that suggest the existence of a novel localization transition in ensembles of interacting particles at a finite temperature. This purely dynamical transition lacks thermodynamic signatures akin to the Anderson transition and can be realized provided coupling to environment is sufficiently weak. Signatures of this phenomenon range from vanishing diffusion constants, divergence of lifetimes of local excitations and concomitant suppression of entanglement in excited multiparticle states, and, fundamentally, the breakdown of statistical mechanics.
Spin-Orbital Entangled States in Transition Metal Oxides

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Submitted : 05-09-2011
Keywords : spin-orbital superexchange, entanglement, quantum phase transition

Superexchange models provide a theoretical framework for describing magnetic and optical properties of Mott insulators. Spin-orbital entanglement (SOE) determines finite temperature properties of systems with active orbital degrees of freedom, for instance the phase diagram of the RVO$_3$ perovskites ($R$=La,⋯,Lu) [1]. To describe SOE one needs to use exact diagonalization of finite clusters, or combine it with the self-consistent Bethe-Peierls-Weiss (BPW) cluster method. The latter is employed to investigate the ground state of a bilayer in the ($d^9$) Kugel-Khomskii model [2], depending on Hund’s exchange $\eta \equiv J_H/U$ ($U$ is the intraorbital Coulomb element) and the $e_g$ orbital splitting $E_{z^2}/J$ ($J \equiv 4t^2/U$ is the superexchange constant). When spin and orbital degrees of freedom are disentangled in mean-field theory (MFT), the $G$-type antiferromagnetic ($G$-AF), $A$-type antiferromagnetic ($A$-AF) and ferromagnetic (FM) order compete, see Fig. 1(a). The BPW approach gives a quite different phase diagram, see Fig. 1(b), including: (i) interlayer valence-bond phase with holes in $3z^2−r^2$ orbitals (VB$_z$), (ii) alternating plaquette valence-bond (PVB), and (iii) two phases with SOE in the regime of strongly frustrated interactions, ESO and EPVB.

In the $d^1$ spin-orbital model on a triangular lattice the Lanczos diagonalization suggests that the Goodenough-Kanamori rules are violated [3] — here the geometrical frustration prevents long-range order and leads to the spin-orbital liquid state that involves SOE on the bonds. However, ordered states may be stabilized on frustrated lattices by strong orbital-lattice coupling in presence of interorbital hopping, as for instance in KO$_2$ or RbO$_2$ [4].

![Phase diagrams of the $d^9$ bilayer model.](image)

Figure 1: Phase diagrams of the $d^9$ bilayer model [2]: (a) MFT, and (b) BPW approach with a cubic cluster of 8 sites. Green area in (a) indicates phases with alternating orbitals; yellow area in (b) marks singlet phases while orange area indicates phases with SOE.


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Contributions to physical clarification of high ZT-Bi$_2$Te$_3$/Sb$_2$Te$_3$ nanoscale superlattices.$^1$

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Keywords : thermoelectrics, figure-of-merit, superlattice

Since the 1990’s it is well known, that nanostructuring of thermoelectric(TE) Materials should reduce the lattice part of the thermal conductivity and therefore increase the ZT-value. With this knowledge in 2001 Venkatasubramanian et al. [1] achieved the breakthrough of the ZT=1 wall. By using nanofabricated superlattice structures of p-type Bi$_2$Te$_3$/Sb$_2$Te$_3$ they obtained a ZT of 2.4 (see Figure 1) and ZT=1.5 for n-type Bi$_2$Te$_3$/Bi$_2$Te$_2$.83Se$_{0.7}$.

In normal case MBE processes are used to deposit nanoscale multilayered films and superlattice structures [2]. For the mass production of thin film TE-devices an established high throughput technique like sputtering or electroplating for the film preparation would be more preferable. For example multilayered magnetic films, used in up-to-date hard drives, are sputtered in inline processes with throughput rates up to m$^2$/min [3].

As Fraunhofer IPM had already an expertise in nanoalloying of thermoelectric thin films, a project was started to fabricate nanoscaled superlattice structures using nanoalloying of sputtered films. The combination of sputtering and nanoalloying seems to be a promising way for future TE-device manufacturing.

This talk will give an overview of Fraunhofer IPM’s efforts for the online ZT-determination for bulk as well as thin film TE-materials and the results we obtained using these techniques within our superlattice project.


$^1$This work was supported by the German Science Foundation (DFG) SPP 1386 and the German Federal Ministry of Education and Research(BmBF)
Thermoelectric transport across the metamagnetic transition in CeRu$_2$Si$_2$

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Submitted: 09-09-2011

Keywords: Metamagnetism, Heavy fermions, Thermopower

The nature of the metamagnetic transition (MMT) in the canonical heavy fermion compound CeRu$_2$Si$_2$ is still to be determined, after thirty years of investigation. The MMT presents only crossover-like features where thermodynamic properties peak but never diverge close to the transition field of 7.8T. They are consistent with a continuous Fermi liquid ground state at low temperatures linking the low and high field sides of the MMT [1]. Meanwhile the residual electrical transport across the MMT shows only weak anomalies, which were argued to be consistent with a non-symmetry breaking topological transition driven by strong Zeeman splitting [2].

We present a new high-resolution study of in-plane thermoelectric power and thermal conductivity in CeRu$_2$Si$_2$ at temperatures below 1K and in magnetic fields up to 12T, extending the range of previous work considerably [3]. Thermopower and thermal conductivity are unique probes that are sensitive to both thermodynamic and transport properties that provide qualitatively new information about the metamagnetic crossover.

Transport in disordered systems of interacting fermions

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Submitted: 11-09-2011

Keywords: correlated systems, disordered systems, transport properties

Interplay of disorder and correlations is at present one of challenging theoretical issues. While single-particle states of noninteracting fermions in one dimension are always localized, the influence of interactions are still controversial. First we study the effect of a single static impurity on the many-body states and on the spin and thermal transport in the 1D anisotropic Heisenberg chain at $T > 0$. Whereas the pure Heisenberg model reveals Poisson level statistics and dissipationless transport due to integrability, we show using the numerical approach that a single impurity induces Wigner-Dyson level statistics and at high enough temperature incoherent transport within the chain. Next, dynamical conductivity in a disordered 1D model of interacting fermions is studied numerically at high temperatures and in the weak-interaction regime in order to find a signature of many-body localization and vanishing d.c. transport coefficients. On the contrary, we find in the regime of moderately strong local disorder that the d.c. conductivity $\sigma_0$ scales linearly with the interaction strength questioning the possibility of a many-body metal-insulator transition at $T > 0$. Finally, evidence is shown that in a Mott insulator the disorder can even enhance d.c. transport.

Monte-Carlo Approach to Stationary Non-equilibrium of Mesoscopic Systems

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Keywords: Stationary non-equilibrium, Quantum Monte-Carlo

Calculating properties of correlated systems out of equilibrium is a challenging task, even if on targets only stationary situations. In particular, transport through nano-objects like molecules or quantum dots is of strong interest, and a theory to calculate transport properties or merely local quantities in a reliable way for reasonably strong correlations very desirable.

Based on a suggestion by Han and Heary [1] we show that one can use advanced quantum Monte-Carlo techniques to calculate quantities with high accuracy [2]. Although the actual goal is to extract current or conductance respectively thermoelectric effects, a first step is to calculate local properties, like the double occupancy, as function of external bias.

We present results for this quantity, which shows interesting non-monotonic behavior. This feature has been observed earlier [3], but was restricted to $T = 0$ and comparatively weak correlations.

Severe Plastic Deformation (SPD) using High Pressure Torsion (HPT) a new route to high ZTs?

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Submitted : 08-09-2011
Keywords : SPD, HPT, Skutterudites

For thermoelectric devices bulk materials with a high figure of merit ZT and high efficiencies are indispensable. Skutterudites are among the favourable materials reaching after ball milling and hot pressing ZTs of 1.2 (p-type) and 1.4 (n-type) at 800 K. For many materials lowering of the thermal conductivity via phonon scattering mechanisms has proven a key issue to increase ZT. High pressure torsion (HPT) is known as an outstanding technique to produce ultrafine grained materials under severe plastic deformation (SPD). Both p- and n-type skutterudites have been deformed by HPT with 2 - 4 GPa at room temperature and temperatures up to 500°C resulting in an oriented lamellar shaped nanograined structure with a crystallite size of about 50 nm as well as amorphous aggregates and an enhanced dislocation density. In comparison with ball milled and hot pressed skutterudites the HPT treated samples show a reduction of the thermal conductivity of about 40%. This and the slightly higher Seebeck coefficient in spite of a markedly enhanced electrical resistivity are the reason why HPT proved to enhance ZT values up to a factor 2. Vickers hardness of HPT treated p-type skutterudites was investigated showing clearly a dependence on the crystallite size.
Clathrate Type I Thermoelectrics: \( \{\text{Ba, Sr}\}_8M_x\{\text{Ge, Si}\}_{46-x-y}\square_y \)

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Submitted : 09-09-2011
Keywords : Clathrates, Thermoelectrics, Phase stability

Thermoelectric properties among the manifold of "intermetallic" clathrates have hitherto shown most interesting features in two series of clathrate type I compounds: \( \text{EA}_8M_{16}X_{30} \) and \( \text{EA}_8M_xX_{46-x-y}\square_y \) (EA=earth alkaline metal; X is Si or Ge; \( \square \) is a structural vacancy in a lattice site). The present talk will focus on a systematic study of clathrate formation, phase relations, clathrate structures, bonding and structure-property relation in novel multi-component clathrate type I materials \( \text{EA}_8\{M, M'\}x\{\text{Si, Ge}\}_{46-x-y}\square_y \) where M, M’ are predominantly 3d, 4d, 5d elements from the end of the d-series. Significant differences in formation and consequently in thermodynamic stability exist between barium-based and strontium-based clathrate type I compounds defining the existence of a clathrate phase. These differences are partially due to the different thermodynamic stabilities of the phases surrounding the clathrate phase, but in part are due to the intrinsic lower thermodynamic stability of the strontium based clathrate compounds and/or solid solutions. Density functional theory calculations of the ground state energies of the corresponding Ba- and Sr-containing clathrate I solid solutions confirm the differences in stability. The implications of these stabilities on physical properties will be outlined particularly with respect to thermoelectric applications.
Peculiarities of magnetic properties of nanostuctured $\text{Ba}_6\text{Mn}_{24}\text{O}_{48}$

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Submitted : 01-08-2011

Keywords : strongly correlated system, magnetic properties, spin - glass system

Static and dynamic magnetic properties of nanostructured compound $\text{Ba}_6\text{Mn}_{24}\text{O}_{48}$ was investigated in temperature range 4.2-100 K in magnetic fields up to 6 kOe. Two types of samples were investigated: a powder and a compacted powder. The magnetic moment temperature dependences for both samples demonstrate an anomaly around 50 K caused by phase transition in the magnetically ordered state. Temperature dependences of magnetic moment measured in field cooling FC and zero field cooling ZFC regimes in magnetic fields from 24 to 3000 Oe are strongly different for two type of samples. Magnetization at 4.2 K in a field 200 Oe differs by almost two-fold. Existence of splitting point between FC and ZFC regimes indicates that in this compound exists a phase separation at low temperature. The temperature of the splitting for both samples, $T^*$ is weakly dependent on the external magnetic field. This indicates that the compound is in a state of spin glass. Conducted study of the temperature dependence of the dynamic magnetization of pressed powder $\text{Ba}_6\text{Mn}_{24}\text{O}_{48}$ in the frequency range 10 - 10 000 Hz allowed to determine the frequency dependence of the freezing temperature $T_f$. Based on these data determined the rate of frequency shift of the freezing temperature $T_f$. This rate is approximately equal to 0.013, resulting value is consistent with similar estimates for the spin - glass systems.
As part of the energy crisis and the search for alternative to fossil fuels, the interest in thermoelectric devices for waste heat conversion has grown. For green applications the most well known thermoelectric materials based on IV and group V chalcogenides, have several drawbacks, the main ones being price and toxicity. A group of materials that has recently gained much attention due to their low price and high availability are the metal silicides such as FeSi, MnSi\textsubscript{1.74}, and Mg\textsubscript{2}Si. The metal silicides have shown high ZT values for both \textit{n}-type Mg\textsubscript{2}Si (ZT \sim 1.1) and \textit{p}-type higher manganese silicides (ZT \sim 0.7). In the current research highly efficient thermoelectric higher manganese silicide based materials were developed. The synthesis methods included furnace melting, mechanical alloying and arc melting, all followed by powder metallurgy using spark plasma sintering (SPS). The resulted samples, prepared by all of these three techniques contained some residual MnSi and some residual Si. A comparison between the thermoelectric and the structural properties of the various materials will be described.
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Universal features of Thermopower in High $T_c$ systems and Quantum Criticality

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Submitted : 12-09-2011
Keywords : thermoelectrics

I will discuss the qualitative insights in the computation intensive field of thermoelectric constants, especially in correlated electronic systems. My efforts in the last few years have yielded two new simple and yet powerful formulas for the thermopower, the high frequency formula $S^*$ and the Kelvin formula. These are not exact in general, but capture the essential physics in different regimes. Using these powerful formulas, the role of features in the DOS, and of electronic frustration in triangular lattices becomes transparent, as compared to the "the computer (and perhaps God) understand the details" viewpoint of the computational efforts using the indisputably exact but opaque Kubo formula. I will summarize these formulas, some new applications, and prospects for the future.
Extreme Correlations:  
or How I learned Not to Worry and Love the Infinite U limit  

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Submitted : 12-09-2011

My frustrating and apparently eternal engagement, in the problem of infinite U systems may yet have a happy ending- as I will try to convince you in this talk.

In particular, the physics of the tJ model, and in particular the one electron propagator is discussed in a new scheme that I have recently proposed [1].

The state that emerges is termed as the Extremely Correlated Fermi Liquid, and the constituent equations describing its Physics are explicitly written down as a “double barrel” hierarchy involving a Fermi liquid type self energy, a dynamical spectral weight and two vertex functions. An initial solution is discussed, arising from considerations usual to high dimensions. Remarkable agreement is observed in the spectrum with ARPES data from optimally doped BISSCO families, with both synchrotron and laser source light sources as outlined in Ref. [2].

[1] B. S. Shastry, Extremely Correlated Fermi Liquids,  

Many-body dynamics and inelastic scattering in strongly correlated electron systems

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Submitted : 09-09-2011
Keywords : many-body dynamical response, inelastic light and x-ray scattering, Falicov-Kimball model

Some problems of the development of microscopic theory of many-body dynamics in strongly correlated electron systems within the dynamical mean field theory are considered. In particular, results for the many-body susceptibilities and resonant cross-sections of inelastic (Raman) scattering for the Falicov-Kimball model are presented.

In the first part of the talk we present results for the total Raman scattering near a metal-insulator and charge-density-wave transitions. The problem is solved exactly for the spinless Falicov-Kimball model with dynamical mean-field theory. We include the nonresonant, mixed, and resonant contributions in three common experimental polarizations, and analyze the response functions for representative values of the energy of the incident photons. Resonant effects can yield a double resonance enhancement of nonresonant peaks, a joint resonance of peaks when the incident photon energy is on the order of interband transitions, and the appearance of an isosbestic point in all symmetry channels. The complicated scattering response can be understood from the significant temperature dependence of the many-body density of states and includes a huge enhancement for photon frequencies near the energies of the interband transitions, including the charge-density-wave gap energy.

In the second part of the talk we consider the interaction of x-rays with strongly correlated electron system. An exact solutions for the core-hole propagator, which determines the x-ray photoemission spectrum (XPS), and two-particle core-hole—band electron response function, which determines the x-ray absorption spectrum (XAS), are derived for the spinless Falicov-Kimball model. The density of states of the x-ray edge problem and XAS are considered for the different temperatures and interaction strengths. It is obtained that both XPS and XAS contain two groups of peaks one of which corresponds to the absorption edge. Besides, the resonant inelastic x-ray scattering (RIXS) response functions are analyzed for different values of the transferred momentum and incident photon energies (below and above the edge).
Carrier Pocket Engineering to Improve Thermoelectric Transport in Semiconducting PbTe

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Submitted : 09-09-2011
Keywords : thermoelectrics

High Seebeck coefficient in semiconductors generally results from a high density of states (DOS) effective mass. Many unconventional electronic structures that increase DOS are being studied or proposed for high efficiency thermoelectric materials. For example, resonant DOS enhancement demonstrated in Tl doped PbTe increases the Seebeck coefficient and the material has high thermoelectric figure of merit, $zT$, at high temperature. However high band mass of the carriers results in low mobility, which leads to lower $zT$. Instead, high DOS effective mass due to high valley degeneracy leads to high $zT$. For example, utilizing the high degeneracy second valence band in PbTe leads to nearly twice the $zT$ ($zT \sim 1.4$) than that of the first valence band. By engineering the two valence bands to converge further increases the degeneracy and $zT$. 
Signatures of correlation effects and thermopower in FeSi

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Submitted: 10-09-2011

Keywords: strong correlations, thermoelectrics, semiconductors

Iron based narrow gap semiconductors such as FeSi, FeSb$_2$, or FeGa$_3$ have received a lot of attention because they exhibit striking similarities to heavy fermion Kondo insulators. Iron silicide, FeSi, which we consider as a prototypical compound in this class, is an ordinary semiconductor at low temperatures. At high temperatures, however, it behaves as a bad metal with a Curie-Weiss like susceptibility. Signatures of this crossover are observed in particular in the thermoelectric properties: The Seebeck coefficient reaches notable values of about 700$\mu$V/K at low temperature. Above 100K, however, it is largely suppressed, while displaying multiple sign changes, i.e. a complex balance between electron and hole dominated transport.

Many proposals have been advanced to explain the unusual behavior in various observables. Among these figure Hubbard-like correlations, spin-state transitions, a thermally induced mixed valence, spin-fluctuations, as well as anomalous electron–phonon couplings. However, lacking quantitative methodologies applied to this problem, a consensus remains elusive to date.

Here, we employ realistic many-body calculations\textsuperscript{1} to elucidate the impact of electronic correlation effects on FeSi. Our methodology accounts for all substantial anomalies observed in FeSi: the metalization, the lack of conservation of spectral weight in optical spectroscopy, and the Curie susceptibility. In particular we find a very good agreement for the anomalous thermoelectric power. We find the suppression of the Seebeck coefficient to be driven by correlation induced incoherence. The change in the dominant type of carriers is correlated with the non-monotonous evolution of the chemical potential, causing a large temperature dependence of the particle/hole asymmetry. Validated by this congruence with experiment, we further present a physical picture of the microscopic nature of the crossover to the metallic state.

\textsuperscript{1}based on the combination of density-functional theory and dynamical mean field theory
Quantum Criticality and Magnetism in $Ln_2Fe_{12}P_7$ Compounds

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Submitted: 09-10-2011

Keywords: strongly correlated electrons, non-Fermi liquid behavior, quantum criticality, thermoelectric power

Recent investigations of a class of noncentrosymmetric, pnictogen-based systems with chemical formula $Ln_2Fe_{12}P_7$ ($Ln =$ Lanthanide or Actinide) have yielded a wealth of strongly correlated electron physics [1, 2, 3]. We have carried out magnetization, specific heat, and electrical resistivity measurements for compounds with $Ln =$ Yb, Sm, U, and Th. Each system exhibits an enhanced electronic contribution to specific heat and $Ln =$ Yb, Sm, and Th have a magnetically ordered ground state in zero applied magnetic field [1, 2, 3]. The $Ln =$ Sm compound exhibits multiple magnetic transitions and a meta-magnetic transition, which might suggest this system’s close proximity to a quantum critical point (QCP) [3]. The $Ln =$ Yb system exhibits a crossover from a magnetically ordered non-Fermi-liquid (NFL) phase to a second NFL phase under applied magnetic field $H$ [1]. The crossover occurs near the value of $H$ where the transition temperature $T_M$ of the ordered phase was no longer observable, but not where a possible QCP would be found if $T_M$ is extrapolated to zero temperature. The resulting $T - H$ phase diagram deviates strongly from the form typically taken by classical QCP phase diagrams, adding Yb$_2$Fe$_{12}$P$_7$ to a growing list of materials exhibiting unconventional NFL behavior.

Materials with strongly correlated electrons often exhibit enhanced thermoelectric power $S$, especially if their Fermi energy lies near a sharp peak in the electronic density of states [4]. Since such systems are potentially useful in thermoelectric applications, we measured the thermoelectric power $S$ of the $Ln =$ Yb compound. We observed that it exhibits an enhanced $S$, comparable to many other strongly correlated electron systems, but that its power factor $S^2/\rho$ (where $\rho$ is electrical resistivity) is an order of magnitude smaller than that of the power-factor record holder YbAl$_3$ [5].


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The Ternary Systems Ba-Au-Ge and Ba-Au-Si: Phase Equilibria, Crystal Structures and Physical Properties

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Formation and homogeneity ranges of the ternary clathrates of type-I, \( Ba_8T_xGe_{46-x-y}\square_y \) and \( Ba_8T_xSi_{46-x} \) (\( T = Au \) and \( \square \) is a vacancy; space group \( Pm-3n \)) at 800°C and phase relations concerning this region have been investigated. For both ternary systems, Ba-Au-Ge and Ba-Au-Si, partial isothermal sections have been derived at 800°C for the region of 0 to 33 at.% Ba. For characterization of the clathrates and other ternary compounds existing at 800°C, X-ray powder diffraction, electron probe microanalysis (EPMA) and X-ray single crystal diffraction were used. Thermoelectric properties (thermopower, electrical resistivity and thermal conductivity) have been measured for clathrate compositions \( Ba_8Au_5.1Si_{10.9} \) and \( Ba_8Au_6Ge_{40} \) between 4.2 and 900 K from which a thermoelectric figure of merit has been evaluated. These studies evidenced the closeness of the systems to a metal to isolator transition. The phase equilibria at 800°C are characterized by several new ternary phases in the investigated region up to 33 at.% barium. The homogeneity ranges have been established for \( Ba(Au_{1-x}Si_x)_2 \) and \( Ba(Au_{1-x}Ge_x)_2 \) (\( AlB_2 \)-type) and also for \( BaAu_2+xSi_{2-x} \) and \( BaAu_1+xGe_{3-x} \) (\( BaNiSn_3 \)-type, \( Ce(Ni,Sb)_4 \)-type). The crystal structures of the other novel phases in the gold-rich part have also been determined from single crystal X-ray data: \( BaAu_3Si \) and \( BaAu_3Ge \) (own type, \( tP a = 0.6459(2) \), \( c = 0.5487(2) \) nm), \( BaAu_5+xSi_{2-x} \) (\( x = 0 \), own structure type, space group \( Pnma \), \( a = 0.8981(2) \), \( b = 0.7106(2) \) and \( c = 1.0363(2) \) nm) and \( BaAu_5+xGe_{2-x} \), the latter revealing with increasing gold content a closely related derivative structure type (\( x = 0.3 \)).
Heavily phosphorus doped polycrystalline silicon with possible applications in the field of thermoelectrics

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Until recently, the field of thermoelectrics marked silicon as an utterly poorly performing material. However, in the recent few years, due to development of the experimental methods that influenced the decrease of the grain size in the polycrystalline material and lowering of dimensionality, silicon gained increased attention. In this study, we analyzed heavily phosphorus doped polycrystalline silicon samples prepared in the following way: the amorphous samples were obtained using parallel flows of silane and phosphine in LPCVD furnace at 530 °C and thereafter subjected to rapid thermal annealing in different time intervals at 950 °C. According to SIMS, the concentration of phosphorus is $2 \cdot 10^{20} \text{cm}^{-3}$ for each sample. Samples were analyzed using Raman spectroscopy, SEM, four point probe, low temperature resistivity and Seebeck coefficient measurements. Samples are in the metallic regime from the lowest temperatures measured. Seebeck coefficient shows linear temperature dependence above 150 K where the resistivity shows the $T^{3/2}$ dependence in the same temperature range.

The quality of samples obtained in this way was evaluated by comparing them to some crystalline samples in the same dopant concentration range. We also discuss application possibilities of these samples as thermoelectrics and in microelectronics.
Open issues on the transport phenomena of 1D quantum magnets

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I will discuss recent theoretical developments on the dynamics of one dimensional quantum magnets [1]. In particular, I will focus on open issues and controversial results related to the finite temperature transport of integrable models [2]. These singular systems are commonly used in the description of quasi-one dimensional materials. They are recently attracting interest in connection to experiments, following the discovery of unusual thermal conductivity in quasi-1D magnetic materials [3].


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