The Abdus Salam
International Centre for Theoretical Physics

Institute for Complex Adaptive Matter

INTEL-BIOMAT funded by:

Advanced Science Institute

smr2157

Workshop on
Principles and Design of Strongly Correlated Electronic Systems
(2 - 13 August 2010)

(Miramare, Trieste - Italy)

CO-ORDINATORS:

Andrey CHUBUKOV	University of Wisconsin, Madison, U.S.A.
Piers COLEMAN	Rutgers University, Piscataway, U.S.A.
Andy SCHOFIELD	University of Birmingham, U.K.
Hide TAKAGI	University of Tokyo, Japan

LOCAL ORGANIZER:

Erio TOSATTI	ICTP-SISSA-DEMOCRITOS Trieste, Italy

BOOK OF ABSTRACTS

web-page: http://agenda.ictp.trieste.it/smr.php?2157

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PREFACE

Strongly correlated electron systems remain at the center of experimental and theoretical activities in condensed-matter physics. These are complex systems, which exhibit self-organized behavior driven by unifying principles. The search for these principles is fueled by a continuing stream of discoveries of new materials, particularly new superconductors, by new insights into the interplay of solid-state chemistry and correlated electron behavior, by new findings from high-precision experiments, and the profound connections between theoretical methods in high energy physics and those of the many-body problems. This is a field that continues to re-invent itself through a stream of new discoveries.

The aim of this Workshop is to explore, understand, and exploit the interconnections and clarify distinctions across the breadth of strongly correlated quantum systems with a particular focus on correlated electrons, superconductivity, Mott physics and quantum magnetism.

The Workshop will bring together cutting edge researchers- theoretical and experimental condensed matter physicists and chemists active in the area of emergent quantum materials: heavy fermions, frustrated spin systems, oxide metals and high temperature superconductors - both cuprates and pnictides.

This event is co-sponsored by the Institute for Complex Adaptive Matter (ICAM-I2CAM), Interdisciplinary Approaches to Functional Electronic and Biological Materials, (INTEL-BIOMAT) funded by the European Science Foundation (ESF) and RIKEN Advanced Science Institute.

The Organizers wish you a most exciting and enjoyable Workhsop.

Andrey CHUBUKOV
Piers COLEMAN
Andy SCHOFIELD
H. TAKAGI
Erio TOSATTI
Doreen M. SAULEEK

PROGRAMME

(as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

The Abdus Salam
International Centre for Theoretical Physics

Workshop on Principles and Design of Strongly Correlated Electronic Systems

Cosponsor(s): Institute for Complex Adaptive Matter (ICAM-I2CAM)Interdisciplinary Approaches to Functional Electronic and Biological Materials (INTEL-BIOMAT) funded by the European Science Foundation (ESF)RIKEN Advanced Science Institute
Organizer(s): Directors: A. Chubukov, P. Coleman, A. Schofield and H. Takagi. Local Organizer: E. Tosatti
Trieste - Italy, 02 - 13 August 2010

Venue: Leonardo da Vinci Building Main Lecture Hall

Preliminary Programme

Monday, 2 August 2010 - HEAVY FERMIONS (Room:Leonardo da Vinci Building Main Lecture Hall)

2 August 2010

08:30 - 09:20 (Room: Leonardo da Vinci Building, Lobby)
--- Registration at the Leonardo Building, Reception area ---

09:20 - 09:30 **Opening Remarks by Profs. Chubukov, Coleman, Schofield, Takagi and Tosatti**

09:25 - 10:25 --- SESSION CHAIR: Piers COLEMAN ---

09:30 - 10:30 **J.C. SEAMUS DAVIS** / *Cornell University, Ithaca, U.S.A.*
Imaging the Fano lattice to "hidden order" transition in URu2Si

10:30 - 11:00 --- Coffee Break ---

10:55 - 12:55 --- SESSION CHAIR: Andy SCHOFIELD ---

11:00 - 12:00 **Dai AOKI** / *CEA/SPSMS, Grenoble, France*
Re-entrant superconductivity and the field-induced magnetic instability in uranium compounds

12:00 - 13:00 **S. WIRTH** / *MPI, Dresden, Germany*
Magnetotransport and tunneling investigations on heavy-fermion systems

13:00 - 15:00 --- Lunch Break ---

Monday, 2 August 2010 - MATERIALS DESIGN (Room:Leonardo da Vinci Building Main Lecture Hall)

2 August 2010

14:55 - 16:55 --- SESSION CHAIR: James C. SEAMUS DAVIS ---

15:00 - 16:00 **E. BAUER** / *Los Alamos National Lab., U.S.A.*
Understanding anisotropy to develop superconductors by design

16:00 - 16:30 --- Coffee Break ---

16:30 - 17:30 **J. GRIN** / *MPI, Dresden, Germany*
Chemistry of strongly correlated systems

18:30 - 20:30 (Room: Leonardo da Vinci Building Terrace)
--- WELCOME RECEPTION ---

Tuesday, 3 August 2010 - PNICTIDES / STRONG CORRELATIONS (Room:Leonardo da Vinci Building Main Lecture Hall)

3 August 2010

08:55 - 10:55 --- SESSION CHAIR: Andrey CHUBUKOV ---

09:00 - 10:00 **S. SEBASTIAN** / *University of Cambridge, U.K.*
Quantum oscillations

10:00 - 11:00 **Z.B. TESANOVIC** / *Johns Hopkins University, Baltimore, U.S.A.*
Magnetism and superconductivity in pnictides

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Lara BENFATTO ---

11:30 - 12:30 **P. HIRSCHFELD** / *University of Florida, Gainesville, U.S.A.*
Accidental order parameter nodes in Fe-pnictides: Origins and implications

12:30 - 14:30 --- Lunch Break ---

Tuesday, 3 August 2010 - Session to be determined (Room:Leonardo da Vinci Building Main Lecture Hall)

3 August 2010

14:25 - 16:25 --- SESSION CHAIR: Dirk K. MORR ---

14:30 - 15:30 **M. CAPONE** / *University of Rome La Sapienza, Italy*
Signatures of strongly correlated superconductivity in expanded Cs3C60

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **Lu YU** / *Institute of Physics, Chinese Academy of Sciences, Beijing, China*
Non-BCS superconductivity in underdoped cuprates by spin-vortex attraction

Wednesday, 4 August 2010 - PNICTIDES (Room:Leonardo da Vinci Building Main Lecture Hall)

4 August 2010

08:55 - 10:55 --- SESSION CHAIR: Peter HIRSCHFELD ---

09:00 - 10:00 **I. EREMIN** / *Ruhr University Bochum, Germany*
Selection of the magnetic order and spin excitations in the SDW state of iron-based superconductors

10:00 - 11:00 **L. BENFATTO** / *CNR-ISC and University of Rome La Sapienza, Italy*
Superconducting properties of pnictides within a low-energy multiband approach

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Henri ALLOUL ---

11:30 - 12:30 **K. ISHIDA** / *Kyoto University, Japan*
NMR Studies on Iron-Pnictide Superconductors BaFe$_2$(As$_{1-x}$P$_x$)$_2$ and LaFeAs(O$_{1-x}$F$_x$)

12:30 - 14:30 --- Lunch Break ---

Wednesday, 4 August 2010 - POSTER SESSION

4 August 2010

14:25 - 16:55 --- SESSION CHAIR: Andy SCHOFIELD ---

14:30 - 17:00 **Poster Session**
Refreshments will be available during the Poster Session

Thursday, 5 August 2010 - MOTT and KONDO PHYSICS (Room:Leonardo da Vinci Building Main Lecture Hall)

5 August 2010

08:55 - 10:55 --- SESSION CHAIR: Kenneth BURCH ---

09:00 - 10:00 **M. VOJTA** / *Universitat zu Koeln, Germany*
Quantum critical Kondo screening in graphene

10:00 - 11:00 **H. ALLOUL** / *Universite Paris XI (Paris-Sud), Orsay, France*
Mott transition in the fullerene compounds

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Piers COLEMAN ---

11:30 - 12:30 **D. MORR** / *University of Illinois at Chicago, U.S.A.*
Defects, density of states, and differential conductance in heavy fermion systems

12:30 - 14:30 --- Lunch Break ---

Thursday, 5 August 2010 (Room:Leonardo da Vinci Building Main Lecture Hall)

5 August 2010

14:25 - 16:25 --- SESSION CHAIR: Andrey CHUBUKOV ---

14:30 - 15:30 **SHORT TALKS BY PARTICIPANTS**

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **SHORT TALKS BY PARTICIPANTS**

19:30 - 19:30 --- SOCIAL DINNER ---
to be confirmed

Friday, 6 August 2010 - To be determined (Room:Leonardo da Vinci Building Main Lecture Hall)

6 August 2010

08:55 - 10:55 --- SESSION CHAIR: Natalia PERKINS ---

09:00 - 10:00 **K. BURCH** / *University of Toronto, Canada*
Tuning materials with mechanical exfoliation

10:00 - 11:00 **Y. IWASA** / *Tohoku University, Sendai, Japan*
Electric field induced superconductivity with electric double layer transistors

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Eric BAUER ---

11:30 - 12:30 **G. BLUMBERG** / *Rutgers, The State Univ. of New Jersey, Piscataway, U.S.A.*
Title to be announced

12:30 - 14:30 --- Lunch Break ---

Monday, 9 August 2010 - QUANTUM CRITICALITY (Room:Leonardo da Vinci Building Main Lecture Hall)

9 August 2010

08:55 - 10:55 --- SESSION CHAIR: Andrey CHUBUKOV ---

09:00 - 10:00 **S. NAKATSUJI** / *Kyoto University, Japan*
Quantum criticality and spin liquid in Kondo lattices

10:00 - 11:00 **M. GARST** / *Universitaet zu Koeln, Germany*
Multiscale quantum criticality: Nematic instability in metals

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Piers COLEMAN ---

11:30 - 12:30 **S. BUEHLER-PASCHEN** / *Vienna University of Technology, Austria*
Recent developments in heavy-fermion quantum criticality

12:30 - 14:30 --- Lunch Break ---

Monday, 9 August 2010 - UNCONVENTIONAL SUPERCONDUCTORS (Room:Leonardo da Vinci Building Main Lecture Hall)

9 August 2010

14:25 - 16:25 --- SESSION CHAIR: Andrew MacKENZIE ---

14:30 - 15:30 **A. KAPITULNIK** / *Stanford University, U.S.A.*
Time reversal symmetry breaking effects in unconventional superconductors

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **H. TAKAGI** / *University of Tokyo, Japan*
New superconducting transition metal pnictides and quasi-particle interference in Fe(Se,Te) superconductor

Tuesday, 10 August - RUTHENIDES, STRONG CORRELATIONS (Room:Leonardo da Vinci Building Main Lecture Hall)

10 August 2010

08:55 - 10:55 --- SESSION CHAIR: Andy SCHOFIELD ---

09:00 - 10:00 **A.P. MacKENZIE** / *University of St. Andrews, Scotland, U.K.*
Thermodynamic studies of Sr3Ru2O7

10:00 - 11:00 **R. FLINT** / *Rutgers, The State Univ. of New Jersey, Piscataway, U.S.A.*
How spins become pairs: composite pairing and magnetism in the 115 heavy fermion superconductors

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Satoru NAKATSUJI ---

11:30 - 12:30 **M. ARONSON** / *Brookhaven National Lab., Upton, U.S.A.*
Quantum criticality in geometrically frustrated heavy fermion compounds

12:30 - 14:30 --- Lunch Break ---

Tuesday, 10 August 2010 - MULTIFERROICS, VANADATES (Room:Leonardo da Vinci Building Main Lecture Hall)

10 August 2010

14:25 - 16:25 --- SESSION CHAIR: Richard GREENE ---

14:30 - 15:30 **N. PERKINS** / *University of Wisconsin-Madison, U.S.A.*
Spin-orbital physics in vanadates

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **Sang-Wook CHEONG** / *Rutgers State University, Piscataway, USA*
Multiferroic vortices

Wednesday, 11 August 2010 - CUPRATES (Room:Leonardo da Vinci Building Main Lecture Hall)

11 August 2010

08:25 - 10:25 --- SESSION CHAIR: Sang-Wook CHEONG ---

09:00 - 10:00 **R. GREENE** / *University of Maryland, College Park, U.S.A.*
Correlation between spin fluctuations and pairing in electron-doped cuprates

10:00 - 11:00 **B. KEIMER** / *MPI, Stuttgart, Germany*
Neutron studies of the cuprates

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHIAR: Meigan ARONSON ---

11:30 - 12:30 **A. KAMINSKI** / *Iowa State University, Ames, U.S.A.*
Competing ground states in cuprates: disentangling Cooper-pair formation above Tc from the pseudogap state

12:30 - 14:30 --- Lunch break ---

Wednesday, 11 August 2010 - Session to be determined (Room:Leonardo da Vinci Building Main Lecture Hall)

11 August 2010

14:25 - 15:25 --- SESSION CHAIR: Tetsuo HANAGURI ---

14:30 - 15:30 **L. GREENE** / *University of Illinois at Urbana Champaign, U.S.A.*
Point contact spectroscopy of strongly-correlated electron materials: Andreev reflection multiband superconductivity and magnetism. The search for innovative avenues towards developing new families of superconducting materials

15:30 - 16:00 --- Coffee Break ---

15:55 - 17:55 --- SESSION CHAIR: Piers COLEMAN ---

16:00 - 18:00 **POSTER SESSION - Poster Gallery (behind the Main Lecture Hall)**
Refreshments will be available during the Poster Session

Thursday, 12 August 2010 - PNICTIDES (Room:Leonardo da Vinci Building Main Lecture Hall)

12 August 2010

08:55 - 10:55 --- SESSION CHAIR: Laura GREENE ---

09:00 - 10:00 **B. BUECHNER** / *Leibniz Inst. for Solid State & Materials Research, Dresden, Germany*
Nanoscale electronic order in underdoped iron pnictides

10:00 - 11:00 **P. CANFIELD** / *Iowa State University, Ames, U.S.A.*
Fe-pnictides

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHIAR: Adam KAMINSKI ---

11:30 - 12:30 **S. SHIN** / *The University of Tokyo, Japan*
Laser-ARPES study on Fe-pnictides superconductors

12:30 - 14:30 --- Lunch Break ---

Thursday, 12 August 2010 - SPIN LIQUIDS/FRUSTRATED MAGNETISM (Room:Leonardo da Vinci Building Main Lecture Hall)

12 August 2010

14:25 - 16:25 --- SESSION CHAIR: Silke BUEHLER-PASCHEN ---

14:30 - 15:30 **Y. MATSUDA** / *Kyoto University, Japan*
Bipartite elementary excitations in a two-dimensional quantum spin liquid

15:30 - 16:00 --- Coffee Break ---

16:00 - 17:00 **A. FURUSAKI** / *RIKEN Advanced Science institute, Saitama, Japan*
Unconventional ordered phases in frustrated ferromagnetic spin chains

Friday, 13 August 2010 - PNICTIDES / TOPOLOGICAL INSULATORS (Room:Leonardo da Vinci Building Main Lecture Hall)

13 August 2010

08:55 - 10:55 --- SESSION CHAIR: Paul CANFIELD ---

09:00 - 10:00 **P. PAGLIUSO** / *State University of Campinas "Gleb Wathagin", Brazil*
Low symmetry structures and strong f-s(d-s) hybridization as key ingredients to find new unconventional superconductors

10:00 - 11:00 **Z. HASAN** / *Princeton University, U.S.A.*
Discovery of topological insulators and related superconductors

11:00 - 11:30 --- Coffee Break ---

11:25 - 12:25 --- SESSION CHAIR: Andrey CHUBUKOV ---

11:30 - 12:30 **T. HANAGURI** / *RIKEN Advanced Science Institute, Saitama, Japan*
Landau-level spectroscopy of helical Dirac fermions in a topological insulator Bi2Se3

12:30 - 14:30 --- Lunch Break ---

Friday, 13 August 2010 - DISCUSSION AND CLOSING REMARKS (Room:Leonardo da Vinci Building Main Lecture Hall)

13 August 2010

14:30 - 16:00 **P. COLEMAN, A. CHUBUKOV, A. SCHOFIELD, H. TAKAGI and E. TOSATTI**
Discussion and Closing Remarks

ABSTRACTS

OF

INVITED TALKS

(in order of presentation, as per Programme updated 27 July 2010)

MONDAY, 2 AUGUST 2010

(updated as of 27 July 2010)

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Imaging the Fano lattice to 'hidden order' transition in URu_2Si_2

J.C. Séamus Davis Cornell University & Brookhaven National Lab., USA.

Within a Kondo lattice, the strong hybridization between electrons localized in real space (r-space) and those delocalized in momentum-space (k-space) generates exotic electronic states called 'heavy fermions'. In URu2Si2 these effects begin at temperatures around 55 K but they are suddenly altered by an unidentified electronic phase transition at To=17.5 K. Whether this is conventional ordering of the k-space states, or a change in the hybridization of the r-space states at each Uranium atom, is unknown. We use spectroscopic imaging scanning tunneling microscopy (SI-STM) to image the evolution of URu2Si2 electronic structure simultaneously in r-space and k-space. Above To, the 'Fano lattice' electronic structure predicted for Kondo screening of a magnetic lattice is revealed. Below To, a partial energy gap without any associated density-wave signatures emerges from this Fano lattice. Heavy-quasiparticle interference imaging within this gap reveals its cause as the rapid splitting below To of a light k-space band into two new heavy fermion bands. Thus, the URu2Si2 'hidden order' state emerges directly from the Fano lattice electronic structure and exhibits characteristics, not of a conventional density wave, but of sudden alterations in both the hybridization at each U atom and the associated heavy fermion states.

Re-entrant superconductivity and the field-induced magnetic instability in uranium ferromagnets

Dai AOKI

INAC/SPSMS, CEA-Grenoble, France

The coexistence of ferromagnetism and superconductivity has attracted much attention in the strongly correlated electron systems. In the past, it had been believed that superconductivity is antagonistic to ferromagnetism, since the Cooper pairs are easily destroyed by the strong internal field due to the ferromagnetism. The first breakthrough was the discovery of UGe_2 [1], where the superconductivity emerges in the ferromagnetic phase under pressure, and the superconducting critical temperature T_{sc} is lower than the Curie temperature T_{Curie}.

Soon after the discovery of UGe_2, the weak ferromagnet URhGe was found to be a superconductor at ambient pressure [2]. T_{sc} (=0.25K) is much lower than T_{Cruie} (=9.5K). In spite of the small T_{sc}, the upper critical field H_{c2} is very large, exceeding the Pauli paramagnetic limit. Thus the nonunitary spin-triplet paring is most likely realized as a paring symmetry. Surprisingly, the field-reentrant superconductivity was found between 8 and 13T in URhGe, when the field is applied along the hard magnetization axis, H // b-axis, where the metamagnetic transition occurs at H_R=12T [3]. Thus the field induced quantum critical point is discussed. Recently we found the enhancement of effective mass near H_R, which can explain the reentrant superconductivity by a crude model, using the McMillan-type formula [4].

A new ferromagnetic superconductivity was recently found in UCoGe [5,6]. We performed magnetoresistivity measurements with fine tuning of the field direction on high quality single crystals [7]. H_{c2} is quite anisotropic. H_{c2} for H // b-axis is strongly enhanced with decreasing temperature with an S-shape and reaches nearly 20T at 0K. These results indicate that the field-induced magnetic instability or magnetic quantum criticality reinforces superconductivity.

[1] S.S. Saxena, P. Agarwal, K. Ahilan, F.M. Grosche, R.K.W. Haselwimmer, M.J. Steiner, E. Pugh, I.R. Walker, S.R. Julian, P. Monthoux, G.G. Lonzarich, A. Huxley, I. Sheikin, D. Braithwaite and J. Flouquet, Nature 406, 587 (2000).
[2] D. Aoki, A. Huxley, E. Ressouche, D. Braithwaite, J. Flouquet, J.-P. Brison, E. Lhotel and C. Paulsen, Nature 413, 613 (2001).
[3] F. Lévy, I. Sheikin, B. Grenier and A.D. Huxley, Science 309, 1343 (2005).
[4] A. Miyake, D. Aoki and J. Flouquet, J. Phys. Soc. Jpn. 77, 094709 (2008).
[5] N.T. Huy, A. Gasparini, D.E. de Nijs, Y. Huang, J.C.P. Klaasse, T. Gortenmulder, A. de Visser, A. Hamann, T. Görlach and H.v. Löhneysen, Phys. Rev. Lett. 99, 067006 (2007).
[6] E. Hassinger, D. Aoki, G. Knebel and J. Flouquet, J. Phys. Soc. Jpn. 77, 073703 (2008).
[7] D. Aoki, T.D. Matsuda, V. Taufour, E. Hassinger, G. Knebel and J. Flouquet, J. Phys. Soc. Jpn. 78, 113709 (2009).

Magnetotransport and tunneling in heavy fermion metals

Steffen Wirth
Max Planck Institute for Chemical Physics of Solids Dresden, Germany

Heavy fermion metals have advanced to suitable model systems by means of which electronic interactions can be studied in great detail. Here we focus on the combination of magnetotransport and tunneling investigations on CeMIn$_5$ and $YbRh_2Si_2$.

In the CeMIn$_5$ class of compounds the relation between superconductivity and antiferromagnetism will be discussed. From pressure-dependent Hall effect measurements on $CeCoIn_5$ we find strong spin fluctuations associated with the departure from Landau Fermi liquid behavior [1]. We infer related, yet separate quantum and superconducting critical fields. Through Cd-doping into $CeCoIn_5$, antiferromagnetic order can be established. For the specific case of $CeCo(In_{0.925}Cd_{0.075})_5$ neutron scattering, magnetotransport and heat capacity measurements on identical samples have been combined to comprehensively map out the phase diagram [2]. Moreover, from these data we infer that both types of order, superconductivity and antiferromagnetism, not only coexist on a microscopic scale but, more importantly, mutually influence each other indicating a common origin. Magnetotransport measurements on this specific system do not give any hint towards the existence of a quantum critical point.

Magnetotransport measurements on materials with 115 structure indicate a precursor state to superconductivity [3]. In an effort to scrutinize these findings we conducted also low temperature Scanning Tunneling Microscopy/Spectroscopy. A gap detected in $CeCoIn_5$ is compatible with $d_{x^2-y^2}$ symmetry of the superconducting order parameter. In addition, its observation above the superconducting transition temperature is, again, consistent with a precursor state to superconductivity.

The heavy fermion metal $YbRh_2Si_2$ and its doped counterparts $Yb(Rh_{1-x}M_x)_2Si_2$ (M = Co, Ir) are of specific topical interest [4] due to a quantum critical point which appears to result not only from an antiferromagnetic instability but also from a Kondo break-down of the heavy quasiparticles. Corresponding Hall effect data that support such a scenario [5] will be discussed briefly. We also present very recent STM and STS at low temperature conducted on these materials. The topography confirms an excellent low temperature *in situ* cleave of the single crystals. The hybridization of conduction and 4*f* electrons results in a gap-like feature in the tunneling conductance. In addition, STS unambiguously reflects the crystal field excitations for the first time. A strongly temperature dependent peak in tunneling conductance is attributed to a resonance resulting from the Kondo lattice.

[1] S. Singh et al., Phys. Rev. Lett. **98** (2007) 057001.
[2] S. Nair et al., Proc. Natl. Acad. Sci. USA **107** (2010) 9537.
[3] S. Nair et al., Phys. Rev. Lett. **100** (2008) 137003.
[4] S. Friedemann et al., Nature Phys. **5** (2009) 465.
[5] S. Friedemann et al., accepted for publication in Proc. Natl. Acad. Sci. USA.

Understanding Anisotropy to Develop Superconductors by Design

Eric D. Bauer
Los Alamos National Laboratory

In this talk, I will present an overview of our progress for identifying the relations among the evolution of correlated electron properties and T_c, as a function of tuning parameters, such as pressure or magnetic field in the heavy fermion superconductors. Our research focuses on using new theoretical tools guided by measurements on these prototypical correlated electron superconductors to identify the microscopic structural origin for changes in these physical properties that lead to a higher T_c. I will discuss our progress in identifying these key materials characteristics that will guide us toward designing the next generation of improved unconventional superconductors.

Chemistry of strongly correlated systems

Yuri Grin

Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Design of the new materials with strongly correlated electronic systems may be realized on the experimental way. Here the development of the new preparation routes for obtaining intermetallic compounds, e.g. utilizing the redox reactions, allows synthesis of the phases, which were previously inaccessible for thermodynamic or kinetic reasons. Another possibility for the design of new materials with strongly correlated electronic systems may be opened by investigations of chemical bonding in intermetallic compounds which seems to play an important role for observation of distinct physical behaviors. Especially for preparation of new intermetallic compounds the understanding of the atomic interactions may open also new opportunities. In particular the covalent interactions between the metal atoms seem to have an effect on physical behavior. Detection and visualization of covalent interactions in intermetallic compounds is an emerging object of research.

For this kind of investigations, new quantum chemical tools based on the electron localizability approach [1,2] were developed. In this approach, the correlations in the electron's motion in the real space are analyzed. Study of the chemical bonding using the electron localizability indicator (ELI-D representation) was shown to by especially suitable for metallic systems. Decomposition of ELI-D into contributions of the states belonging to certain energy ranges in the electronic density of states [2] allows visualizing and investigation of the role of electrons of the inner shells in the atomic interactions in $EuRh_2Ga_8$ [3] and $La_7Os_4C_9$ [4]. In particular for $EuRh_2Ga_8$, two types of atomic interactions were found between the europium cations and the $[Rh_2Ga_8]$ anion: ionic (non-directed) interaction via transfer of the electrons of the sixth shell to the polyanion and (directed) covalent interaction using the electrons of the penultimate (fifth) shell.

[1] M. Kohout, Int. J. Quantum Chem. **97** (2004) 651.
[2] F. R. Wagner et al. Chem. Eur. J. **13** (2007) 5724.
[3] O. Sichevich et al, Inorg. Chem. **48** (2009) 6261.
[4] E. Dashjav et al. J. Solid State Chem. **181** (2008) 3121.

TUESDAY, 3 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Quantum Oscillations

Suchitra E. SEBASTIAN

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Magnetism and Superconductivity: Pnictides versus Cuprates

Zlatko Tesanovic
Institute for Quantum Matter
Johns Hopkins University
Baltimore, Maryland, USA

Two years ago, the discovery of high-temperature superconductivity in iron-pnictides reshaped the landscape of condensed matter physics. Until that time, for more than two decades, the copper-oxide materials were the only game in town and their mysterious properties loomed large as perhaps the greatest intellectual challenge in our field. Cuprates are strongly interacting systems, near to the so-called Mott insulating limit, in which electrons are made motionless by strong correlations, and it is currently believed that much of their unusual behavior stems from such correlations.

In contrast, the newly discovered iron-based high-temperature superconductors exhibit a more moderate degree of correlations and do not appear to be near the Mott limit. Consequently, some of their properties are easier to understand. In this presentation, the basic ideas in theory of iron-pnictides will be introduced and illustrated with experimentally-relevant examples. Particular attention will be paid to the interband pairing mechanism of multiband superconductivity and the renormalization group description of the underlying physics. This will be contrasted with strongly correlated cuprates, where a thousand fancy theoretical ideas bloom, from quantum fluctuations to Berry phases, from gauge field theory to AdS/CMT duality. But we will never lose touch with reality and promise to keep a watchful eye on recent and sometimes conflicting experiments.

Accidental order parameter nodes in Fe-pnictides: Origins and implications

P. J. Hirschfeld, U. Florida–Gainesville (USA)

The new Fe-based superconductors have occasioned considerable excitement because transition temperatures are high and it is hoped that comparisons to cuprates can lead to new insights on the essential ingredients to high temperature superconductivity. According to conventional weak coupling spin fluctuation models, A_{1g} (sign-changing "s-wave") states are probably favored. Such states may be isotropic on each Fermi surface sheet or highly anisotropic, possibly with order parameter nodes. Experiments indicating a possible gapped-nodal crossover will be discussed in this framework, with an emphasis on the multiorbital physics which appears to be very important.

Understanding the Anomalous Properties of Expanded A_3C_{60} Fullerides as Strongly Correlated Superconductors

M. Capone [1,2,3], M. Fabrizio[3], C. Castellani[2], and E. Tosatti[3]
[1] *ISC/CNR Rome, Italy*
[2] *Physics Department, University of Rome "Sapienza", Rome, Italy*
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We show that the properties of expanded fullerides of the A_3C_{60} family (A being an alkali-metal atom) are described in terms of the interplay between phonon-mediated pairing and strong correlations. While correlation effects are already present in previously known fullerides (like Rb_3C_{60} and K_3C_{60}) they become essential in the newly discovered expanded materials such as A15 Cs_3C_{60} [1-2]. In these compounds one obtains, as a function of the lattice spacing, a phase diagram which strikingly resembles that of cuprates as a function of doping: A dome-like behaviour of the critical temperature, followed by a transition to an antiferromagnetic Mott insulator.

This finding suggests that, despite the phononic nature of pairing in fullerides, these materials can be members of a wider class of correlated superconductors which includes the cuprates, heavy fermion compounds and organic materials [3].
Solving a realistic three-band model for fullerides using Dynamical Mean-Field Theory, we obtain the same phase diagram found experimentally: A bell shaped superconducting region preceding the Mott transition for increasing cell volume (increasing repulsion) [4]. We propose several experimental tests of our scenario : (i) a pseudogap in the normal phase; (ii) gain of kinetic energy and of zero-frequency optical weight at the onset of superconductivity, as in the cuprates; (iii) spin susceptibility and specific heat jumps not especially large despite the incipient Mott transition; (iv) two different energy scales governing the renormalized single particle dispersion, electronic entropy and specific heat jump.

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Non-BCS superconductivity for underdoped cuprates by spin-vortex attraction

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Abstract

Within a gauge approach to the *t-J* model, we propose a new, non-BCS mechanism of superconductivity for underdoped cuprates. The gluing force of the superconducting mechanism is an attraction between spin vortices on two different Néel sublattices, centered around the empty sites (holes), which can be described in terms of fermionic holons. The spin fluctuations are described by bosonic spinons with a gap originating also from the spin vortices. Due to the no-double occupation constraint, there is a gauge interaction between holon and spinon, through which the spin vortex attraction induces the formation of spin-singlet (RVB) spin pairs with a lowering of the spinon gap. Lowering the temperature there appear two crossover temperatures. At the higher crossover, a finite density of incoherent holon pairs are formed, and it is identified with the pseudogap temperature. At the lower crossover temperature, a finite density of incoherent spinon RVB pairs are formed, and it is identified with the appearance of the Nernst signal. The true superconducting transition occurs at an even lower temperature, via a 3D XY-type transition. The superconducting mechanism is not of BCS-type, and it involves a gain in kinetic energy (for spinons) coming from the spin interactions. The main features of this non-BCS description of superconductivity agree with the experimental results in underdoped cuprates, especially the contour plot of the Nernst signal.

WEDNESDAY, 4 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Metallic Spin-Density Wave phase in iron-based superconductors:

selection of magnetic order, spin and charge excitations

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Recent discovery of superconductivity in the iron-based layered pnictides with Tc ranging between 26 and 56K generated enormous interest in the physics of these materials. The superconductivity has been discovered in oxygen containing RFeAsO (R=La, Nd, Sm) as well as in oxygen free AFe2As2 (A=Ba, Sr, Ca). Like the cuprates, the pnictides are quasi-two-dimensional systems, their parent material shows antiferromagnetic long-range order below 150K and superconductivity occurs upon doping of either electrons or holes into the FeAs layers.

In my talk I will analyze the properties of the magnetically ordered state. In particular, I will discuss the selection of the stripe magnetic order in the unfolded BZ within itinerant description. Selecting one hole and two electron pockets we find that SDW order is highly degenerate if electron pockets are circular and interactions involved are between holes and electrons only. Repulsive charge interactions between two electrons as well as ellipticity of the electron pockets break the degeneracy and select metallic $(0, \pi)$ $[(\pi,0)]$ SDW state in the unfolded BZ -- the same order as seen in the experiments. I will argue that the SDW state remains a metal even for the case of a perfect nesting because one combination of the two hole operators and one combination of two electron operators decouple from the SDW mixing. We also demonstrate that the quasi-one-dimensional nanostructure identified in the quasiparticle interference (QPI) is a consequence of the interplay of the magnetic $(\pi, 0)$ spin-density wave (SDW) order with the

underlying electronic structure. We show that the evolution of the QPI peaks largely reflects quasiparticle scattering between bands involved in the SDW formation. Because of the ellipticity of the electron pocket and the fact that only one of the electron pockets is involved in the SDW, the resulting QPI has a pronounced one-dimensional structure. We further predict that the QPI crosses over to two dimensionality on an energy scale, set by the SDW gap.

Finally, we address the salient experimental features of the magnetic excitations in the spin-density-wave phase of iron-based superconductors. We use a multiband random-phase approximation treatment of the dynamical spin susceptibility. Weakly damped spin waves are found near the ordering momentum and it is shown how they dissolve into the particle-hole continuum. We show that ellipticity of the electron bands accounts for the anisotropy of the spin waves along different crystallographic directions and the spectral gap at the momentum conjugated to the ordering one.

*-work done with A. V. Chubukov, J. Knolle, R. Moessner, and A. Akbari

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Superconducting properties of pnictides within a low-energy multiband approach

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The occurrence of superconductivity in pnictides renewed in the last year the interest in the physics of multi-band superconductors. However, what makes the case of pnictides very peculiar is the fact that pairing has mainly an interband character, as due to exchange of spin fluctuations between hole and electron pockets. These two characteristics make the theoretical description of pnictides much more involved than what is usually believed. In this talk I will review some of our recent results based on a four-band model with anisotropic interactions, where pairing is described within the Eliashberg theory. I will show that this approach allows us to account for several spectroscopic[1,2,3] and thermodynamic[2,4] properties of pnictides that are not directly captured by LDA+DMFT calculations.

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NMR Studies on Iron-Pnictide Superconductors

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We present NMR results on iron-pnictide superconductors of $LaFeAs(O_{1-x}F_x)$ and $BaFe_2(As_{1-x}P_x)_2$. In $LaFeAs(O_{1-x}F_x)$, $1/T_1$ in the undoped LaFeAsO exhibits a distinct peak at $T_N \sim 142$ K below which NMR spectra become broadened due to the internal magnetic field attributed to an antiferromagnetic (AFM) ordering. In the x=0.04 sample, $1/T_1T$ of ^{75}As exhibits a Curie-Weiss temperature dependence down to 30 K, suggesting the development of AFM spin fluctuations, and decreases below superconducting(SC)-transition temperature $T_c \sim 16$ K. The AFM fluctuations are significantly suppressed with F-doping, and a pseudogap behavior is observed in $1/T_1T$ in the x=0.11 sample with a maximum $T_c \sim 23$ K in $LaFeAs(O_{1-x}F_x)$ [1]. The spin dynamics vary markedly with F-doping, which is ascribed to the change of the nesting between hole and electron Fermi-surfaces by the electron doping, and the pseudogap behavior in $1/T_1T$ is shown to originate from the characteristic energy dependence of the density of state around the Fermi energy. The significant suppression of $1/T_1T$ upon F doping while T_c remains nearly unchanged suggests that the low-energy AFM fluctuations probed by the NMR measurements do not play an important role in the superconductivity in $LaFeAs(O_{1-x}F_x)$[2].

On the contrary, $1/T_1T$ in $BaFe_2(As_{0.67}P_{0.33})_2$ with a maximum $T_c \sim 30$ K in $BaFe_2(As_{1-x}P_x)_2$ continues to increase down to T_c, indicating the development of the AFM fluctuations, and sharply decreases below T_c due to opening of the SC gap. The AFM fluctuations are suppressed and T_c also decreases with increasing P content. From the analyses of $1/T_1T$ in the normal state, it is shown that the maximum T_c sample is located in the vicinity of the quantum critical point of the AFM ordering, and that the AFM fluctuations are intimately related to the superconductivity in $BaFe_2(As_{1-x}P_x)_2$. It was found that the relationship between the AFM fluctuations and superconductivity are quite different between $LaFeAs(O_{1-x}F_x)$ and $BaFe_2(As_{1-x}P_x)_2$.

We also show that the SC gap in $BaFe_2(As_{0.67}P_{0.33})_2$ revealed by $1/T_1$ below T_c possesses the residual density of state near E_F, suggesting the presence of the nodes in the SC gap[3]. This is different from other iron-pnictide superconductors. We discuss possible SC state in $BaFe_2(As_{0.67}P_{0.33})_2$ and other iron pnictides, and the similarity between $BaFe_2(As_{0.67}P_{0.33})_2$ and heavy-fermion superconductors.

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POSTER SESSION

Leonardo da Vinci Building

Poster Gallery

(behind the Main Lecture Hall - reception area)

THURSDAY, 5 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Quantum critical Kondo screening in graphene

Matthias Vojta

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Magnetic impurities in neutral graphene provide a realization of the pseudogap Kondo model, which displays a quantum phase transition between phases with screened and unscreened impurity moment. In this talk, I discuss the physics of the pseudogap Kondo model with finite chemical potential μ. While carrier doping restores conventional Kondo screening at lowest energies, properties of the quantum critical fixed point turn out to influence the behavior over a large parameter range. Most importantly, the Kondo temperature T_K shows an extreme asymmetry between electron and hole doping. At criticality, depending on the sign of μ, T_K follows either the scaling prediction $T_K \propto |\mu|$ with a *universal* prefactor, or $T_K \propto |\mu|^x$ with $x \approx 2.6$. This asymmetry between electron and hole doping extends well outside the quantum critical regime and also implies a qualitative difference in the shape of the tunneling spectra for both signs of μ.

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Mott transition to Superconductivity in Fulleride Cs_3C_{60} compounds: an NMR study

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The variation with n of the electronic properties of cubic A_nC_{60} compounds, where A is an alkali, cannot be explained by a simple progressive band filling of the C_{60} six-fold degenerate t_{1u} molecular level. This has been ascribed to the influence of electron correlations and Jahn-Teller Distortions (JTD) of the C_{60} ball, which energetically favour evenly charged C_{60} molecules[1].

This approach is supported by the detection by NMR of a small spin-gap in Na_2C_{60} and K_4C_{60} which is ascribed to a transition from a fundamental spin singlet state of C_{60}^{2+} or C_{60}^{4+} to an excited spin triplet state [2]. Similarly, a charge disproportionation in the low T quenched cubic phase of Cs C_{60} [3], with a sizable fraction of the C_{60} balls in a doubly charged C_{60}^{2+} singlet ground state also confirms that Hund's rule is disfavoured by the JTD in such compounds.

More recently it has been discovered that the expanded A15 fulleride Cs_3C_{60} displays a Mott transition to superconductivity (SC) driven by an applied pressure [4]. This system has a phase diagram where dome shaped superconductivity appears in the vicinity of a Mott insulating phase, a common situation encountered nowadays in correlated electron systems.

We report here an NMR and magnetisation study on Cs_3C_{60} in both its A15 and face centered cubic structures [5]. NMR allowed us to evidence that both exhibit a similar first-order Mott transition to a SC which occur at distinct critical pressures p_c and temperatures T_c. Though the ground state magnetism of the Mott phases differs, their high T paramagnetic and SC properties are found similar, and the phase diagrams versus unit volume per C_{60} are superimposed. Thus, as expected for a strongly correlated system, the inter-ball distance is the relevant parameter driving the electronic behavior and quantum transitions of these systems. Our detailed NMR results allow us to demonstrate that, although the high temperature superconductivity found so far in the A_3C_{60} compounds admittedly results from an electron-phonon mechanism, the incidence of electron correlations has an importance on the electronic properties, as had been anticipated from DMFT calculations [6].

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Defects, density of states and differential conductance in heavy fermion systems

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SHORT TALKS

BY

PARTICIPANTS

FRIDAY, 6 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

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Tuning Materials with Mechanical Exfoliation

Materials with Nanometer thickness are an appealing platform for devices as well as exploring the roles of dimensionality, disorder, and free carrier density in complex materials. To this end we have produced exfoliated crystals of Bi2Sr2CaCu2O8 and Bi2Se3 on a variety of substrates. I will discuss unique advantages of this technique as well as some of the challenges it posses. Interestingly we have observed subtle differences in the Raman spectra between the exfoliated and bulk crystals enabling noninvasive determination of thickness (Bi2Se3) and Doping level (Bi-2212).

Electric field induced superconductivity with electric double layer transistors

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MONDAY, 9 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Quantum criticality and spin liquid in Kondo lattices

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Multiscale quantum criticality in nematic Fermi liquids

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Close to a nematic, i.e., Pomeranchuk instability, the Fermi surface in an isotropic metal becomes soft with respect to quadrupolar fluctuations. In spatial dimensions d=2, there are two critical bosonic modes that are characterized by different dynamics: one being ballistic with dynamical exponent z=2 and the other is Landau damped with z=3, giving rise to multiple dynamical scales. First, I discuss the analysis of the effective critical bosonic theory [1]. At temperature T=0, the z=2 mode governs the low-energy properties as it possesses the smaller effective dimension d+z. Its self-interaction leads to logarithmic singularities that can be summed with the help of the renormalization group. At finite T, the coexistence of two different dynamical scales leads to a modified quantum-to-classical crossover. It extends over a parametrically large regime with intricate interactions of quantum and classical bosonic fluctuations resulting in a universal temperature dependence of the correlation length. The multiple scales are also reflected in thermodynamics and the phase diagram. Second, the influence of the multiple energy scales on the electronic spectral function will be discussed [2]. Whereas the interaction with z=3 bosons gives rise to a singular local electron self-energy with a frequency dependence of non-Fermi liquid form, the exchange of z=2 bosons leads to an anomalous dimension for the electrons.

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Recent developments in heavy-fermion quantum criticality

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Quantum criticality in heavy fermion compounds has been a topic of great interest for more than a decade [1]. In the vicinity of a quantum critical point, heavy fermion materials display qualitative departures from the standard Landau Fermi liquid behavior of conventional metals over a wide temperature range.

The quantum critical behavior of some heavy fermion materials may be understood using a space-time generalization of classical criticality, often called "Hertz-Millis" theory [2, 3]. For other materials a new framework, evoking the critical breakdown of Kondo screening at the quantum critical point [4–8], appears to be required. The experimental hallmark of the latter is the presence of an additional energy scale T^* at the quantum critical point [9–11] which separates the phase diagram into a region of entangled quasiparticles with large Fermi volume and one with disentangled quasiparticles and small Fermi volume. In some systems these two energy scales can be separated from each other either by chemical [12, 13] or by hydrostatic pressure [14]. Such separation may lead to non-Fermi liquid behavior arising not from a single quantum critical point but from a finite zero-temperature region of the magnetic field- or pressure-tuned phase diagram [12]. Global phase diagrams [12, 15, 16] have been suggested to rationalize these different kinds of quantum critical behavior.

These recent developments will be discussed in the talk.

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Kerr Effect Measurements Through the Pseudogap of High-Tc Superconductors

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One of the most challenging puzzles that has emerged within the phenomenology of the high-temperature superconductors is to understand the occurrence and role of the normal-state "pseudogap" phase in underdoped cuprates. This phase exhibits anomalous behavior of many properties including magnetic, transport, thermodynamic, and optical properties below a temperature, T^*, large compared to the superconducting (SC) transition temperature, T_c

Two major classes of theories have been introduced in an attempt to describe the pseudogap state: One in which the pseudogap temperature T^* represents a crossover into a state with preformed pairs with a d-wave gap symmetry, and another in which T^* marks a true transition into a phase with broken symmetry which ends at a quantum critical point, typically inside the superconducting dome. While at low-doping this phase may compete with superconductivity, it might provide fluctuations that are responsible for the enhanced transition temperature near its quantum critical point.

In this talk I will review Kerr effect measurements on several high-Tc systems, including $YBa_2Cu_3O_{6+x}$, $Pb_{0.55}Bi_{1.5}Sr_{1.6}La_{0.4}CuO_{6+x}$ and $La_{1.875}Ba_{0.125}CuO_4$. We will show data that strongly suggest a scenario in which onset of Kerr effect signal near T^* marks a true phase transition. While Kerr effect is sensitive to time-reversal symmetry breaking, we will argue that the measured magnetic signal tracks another electronic phase transition, most likely a weak structural and/or charge-order transition. We will supplement the Kerr effect measurements with other data that adds further evidence for such a scenario.

New superconducting transition metal pnictides and quasi-particle interference in Fe(Se,Te) superconductor

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TUESDAY, 10 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Thermodynamic studies of Sr3Ru2O7

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How spins become pairs: Composite pairing and magnetism in the 115 family of heavy fermion superconductors

Rebecca Flint

In the BCS paradigm, Cooper pairs form from well-defined quasiparticles, but the highest temperature heavy fermion superconductors pose a different problem. Here, the heavy electrons are forming as they pair, and the composite structure of the pair is as important as the forces holding it together. This issue is paramount in the 115 family of superconductors, which includes both $CeMIn_5$(M=Co,Ir,Rh) and its actinide cousins, $PuMGa_5$(M=Co,Ir,Rh) and $NpPd_5Al_2$. I will argue that the internal structure of the heavy fermion condensate necessarily involves two bosonic entities: a d-wave pair of quasiparticles on neighboring lattice sites, condensed in tandem with a composite pair of electrons bound to a local moment, residing within a single unit cell. These two components draw upon the antiferromagnetic and Kondo screening interactions to cooperatively enhance the superconducting transition temperature. I demonstrate this tandem pairing within a symplectic-N solution of the two-channel Kondo-Heisenberg model, showing that the two mechanisms couple linearly to enhance the transition temperature. Tuning the relative strengths naturally leads to a two dome structure, as seen in $Ce(Rh,Ir)In_5$. Additionally, the charge aspects of composite pairing lead should lead to sharp superconducting shifts in both the valence and the condensate quadrupole moment.

Funding for this work provided by NSF DMR-0907179

Geometric Frustration and Quantum Criticality in Heavy Electron Compounds

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We have studied a number of the R2T2X `221' compounds, where R=rare earth, T=transition metal, and X=main group element, where the R atoms sit on a geometrically frustrated Shastry-Sutherland lattice (SSL). Magnetically ordered or spin liquid phases, separated by a quantum critical point (QCP), can be realized in the system, depending on the relative strengths of the near neighbor J' and next neighbor J exchange interactions that couple the R moments. Ce_2Ge_2Mg and Yb_2Pt_2Pb order antiferromagnetically at 9.7 K and 2.05 K, respectively, while Ce_2Pt_2Pb appears to form very close to the QCP. Susceptibility measurements find that the magnetic susceptibilities of all three compounds display Curie-Weiss temperature dependencies, giving the full Hund's rule moment expected for Yb^{3+} or Ce^{3+}. Specific heat measurements confirm that the ground state is a magnetic doublet, well isolated from higher lying states in the crystal field manifold.

The magnetic ground state is constructed from pairs of neighboring moments, or dimers. Magnetic fields Zeeman split the excited dimer triplet state, and above a critical field HC1 it becomes the ground state. A further increase of the field increases the population of dimer triplets, driving a sequence of magnetic ally modulated states that are evidenced by steps in the magnetization. We observe these steps in Ce_2Ge_2Mg and in Yb_2Pt_2Pb, although they are much sharper and persist to higher temperatures in the former case, implying that fluctuations associated with both the finite temperature transition in Ce_2Ge_2Mg and the nearby QCP in Yb_2Pt_2Pb reduce the stability of these interaction driven modulated states. We have used specific heat and magnetocaloric effect measurements to map out a complicated phase diagram in Yb_2Pt_2Pb and Ce_2Ge_2Mg, where the field dependence of the in-plane order $T_N \sim (H-Hc1)^{\phi}$, where $\phi \sim 2/3$, which places this transition in the Bose-Einstein class, as in other quantum magnets. Clear evidence for quantum criticality is found in Ce_2Pt_2Pb, where $C/T \sim T^{1.4}$, $\rho \sim A - aT$, and $\chi \sim T^{-0.8}$.

This research was supported by the NSF under grant NSF-DMR-0405961.

Spin-orbital physics in vanadates

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MULTIFERROIC VORTICES IN HEXAGONAL $YMnO_3$

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Hexagonal $REMnO_3$ (RE= rare earths) with RE=Ho-Lu, Y, and Sc, is an improper ferroelectric where the size mismatch between RE and Mn induces a trimerization-type structural phase transition, and this structural transition leads to ferroelectricity. For the last two decades, ferroelectric $REMnO_3$ has been extensively studied as a candidate material for ferroelectric memories and also for its multiferroicity – the coexisting nature of ferroelectricity and magnetism. Despite this research the true ferroelectric domain structure and its relationship with structural domains have never been revealed. Using transmission electron microscopy and conductive atomic force microscopy, we have investigated the relationship among trimerization antiphase domains, ferroelectric domains and antiferromagnetic domains in $REMnO_3$. We found that ferroelectric domain walls and structural antiphase boundaries are mutually interlocked. In addition, we discovered a vortex structure with six domains emerging from one point - all distinctly characterized by polarization orientation, structural antiphase, and antiferromagnetic relationships. This vortex can be considered as a topological defect in a multiferroic. We also found that ferroelectric domains and walls have distinct electronic transport properties. These fascinating results reveal the rich physics of the hexagonal system with a truly-semiconducting band gap where structural trimerization, ferroelectricity, magnetism, and charge conduction are intricately coupled.

WEDNESDAY, 11 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Correlation between spin fluctuations and pairing in electron-doped cuprates

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The origin of the electron pairing in high-T_c cuprate superconductors is still unresolved in spite of over 20 years of research on these materials. Most research has focused on hole-doped cuprates, which have a "pseudogap" phase of unknown origin in the under doped region of the phase diagram. In contrast, electron-doped cuprates have a "pseudogap" whose origin is known to come from antiferromagnetic spin density wave (SDW) fluctuations [1]. Here we report a detailed analysis of very low temperature transport measurements (30mK < T< 2K) on electron-doped $La_{2-x}Ce_xCuO_4$ ($0.10 < x < 0.21$) films in the normal state (H >Hc2). Most significantly, we find a direct correlation between the strength of the linear-in-temperature resistivity and the superconducting transition temperature (T_c). This strongly suggests that pairing and normal state scattering are both caused by the same coupling, most likely to SDW fluctuations since no other excitations are known to exist at low temperatures in the n-doped cuprates. A correlation between T-linear resistivity and Tc has also been found in hole-doped cuprates [2], however, in this case the scattering responsible for the T linear term is unknown and the measurements have not been done at low enough temperatures to access the ground state. Since the superconductivity originates in the CuO_2 planes for both electron- and hole-doped cuprates, our work suggests that the spin fluctuations must play the dominant role in the pairing for all (both hole- and electron-doped) cuprate high-T_c superconductors!

[1] P. Armitage, P. Fournier, and R. L. Greene, arXiv: 0906.2931, accepted RMP
[2] For a summary and other references see; L. Taillefer, arXiv:1003.2972

Collaborators on this work are: K. Jin, N. P. Butch, G. Droulers, K. Kirshenbaum, X. H. Zhang, P. Bach, and J. Paglione.

Funding for this work provided in part by the NSF under DMR- 0653535

Neutron studies of the cuprates

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Competing ground states in cuprates: disentangling Cooper-pair formation above Tc from the pseudogap state

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Pseudogap state in cuprates is one of most interesting topics in modern condensed matter physics. This state is characterized by anisotropic energy gap that leads to seemingly disconnected segments of the Fermi surface, so called "Fermi arcs". The relationship between the pseudogap and superconductivity is one of the central issues in physics of cuprates. One of the leading theories explaining it is so called "pre-formed" pair scenario, where pseudogap is thought to be a state of paired electrons that lack the long range coherence. Another class of theories attributes the pseudogap to an ordered state that would naturally compete with superconductivity. By studying the spectral weights associated with pseudogap and superconductivity using Angle Resolved Photoemission Spectroscopy (ARPES) we found that there is a direct correlation between the loss of the low energy spectral weight due to the opening of the pseudogap and a decrease of the spectral weight associated with superconductivity as a function of momentum and doping. High accuracy data lead us to conclude that the pseudogap competes with the superconductivity by depleting the spectral weight available for pairing in the region of momentum space, where the superconducting gap is largest. We also conducted detailed studies of the temperature dependence of the spectral weight at the chemical. We found evidence for a spectroscopic signature of pair formation and demonstrated that in a region of the phase diagram commonly referred to as the ``pseudogap", two distinct states coexist: one that persists to an intermediate temperature Tpair and a second that extends up to T*. The first state is characterized by a doping independent scaling behavior and is due to pairing above Tc, but significantly below T*. The second state is the "proper" pseudogap - characterized by a "checker board" pattern in STM images, the absence of pair formation, and is likely linked to Mott physics of pristine CuO2 planes.

Point contact spectroscopy of strongly-correlated electron materials: Andreev reflection multiband superconductivity and magnetism
The search for innovative avenues towards developing new families of superconducting materials

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POSTER SESSION

Leonardo da Vinci Building

Poster Gallery

(behind the Main Lecture Hall - reception area)

THURSDAY, 12 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Nanoscale Electronic Order in Underdoped Iron Pnictides

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Studying nuclear magnetic resonance and electronic transport properties we have investigated short range order phenomena in $RFeAsO_{1-x}F_x$ (R = La;Sm) pnictide superconductors. The charge distribution in the FeAs layers is probed using As nuclear quadrupole resonance [1]. Whereas undoped and optimally doped or overdoped compounds feature a single charge environment, two charge environments are detected in the underdoped region. Spin-lattice relaxation measurements show their coexistence at the nanoscale. Together with the quantitative variations of the spectra with doping, they point to a local electronic order in the iron layers, where low- and high-doping- like regions coexist on the nanometer scale. In the same doping range a pronounced increase of the relaxation rate is found signalling a slowing down of Fe spin fluctuations with decreasing temperatures [2]. This clearly shows the proximity of static magnetic order, which is, however, absent according to our high sensitive SR studies [3]. The appearance of the slow magnetic fluctuations as signalled by the NMR data correlates with clear-cut anomalies of the electronic transport properties resistivity [4] and Nernst coefficient [5]. On the basis of these data the possibility of nematic-like order of charges- orbitals – and/or spins in underdoped pnictides is discussed.

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Phase diagrams and physical properties of $Ba(Fe_{1-x}TM_x)_2As_2$ (TM = Co, Ni, Cu, Ru, Rh, Pd)

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A brief overview and summary of the effects of transition metal (Co, Ni, Cu, Ru, Pd, and Rh) doping and pressure on physical properties of $BaFe_2As_2$ will be presented. A detailed comparison of the phase diagrams for different dopants will be made. The range of experimental parameters that allow for the stabilization of superconductivity will be outlined [1-4]. The evolution of physical properties with doping, in particular, two possible Lifshitz transitions, bracketing the superconducting dome, as inferred from thermoelectric power and Hall measurements (as well as ARPES) will be examined [5,6]. Effects of doping will be compared with pressure [7,8]. In addition, a "universal" behavior of specific heat jump at T_c and peculiarities of thermal expansion in $Ba(Fe_{1-x}Co_x)_2As_2$ for a wide range of Co-concentrations will be discussed [9,10].

In collaboration with S. L. Bud'ko, N. Ni, E. D. Mun, A. Thaler, A. Kracher, E. Colombier and H. Hodovanets. Work at the Ames Laboratory was supported by the U.S. Department of Energy Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

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Laser-ARPES study on Fe-pnictides superconductors

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We developed laser angle-resolved photoemission spectroscopy (ARPES) with high bulk sensitivity, high resolution of 150 μeV and low temperature of 1.8 K. Laser-ARPES is employed to investigate the electronic structure of $BaFe_2As_2$ and several Fe superconductors across the magneto-structural transition and superconducting transition.

For $BaFe_2As_2$, we found a drastic transformation in Fermi surface (FS) topology with the rearrangement of its orbital component across the transition at T_N = 140 K[1]. Polarization-dependent ARPES enables us to separately observe the electronic structure from single domains in the low-temperature twinned structure. It is suggested that single Fe 3d orbital component dominates the highly 3-dimensional FSs in antiferromagnetic (AF) state. We conclude that $BaFe_2As_2$ shows AF state coexisting with orbital-polarized metallic state.

We will also discuss on the superconducting gap and its anisotropy of each Fermi surface on $(Ba_{1-x}K_x)Fe_2As_2$, $BaFe_2(As,P)_2$[2], and KFe_2As_2 measured by polarization-dependent laser-ARPES. We found that orbital fluctuation mechanism is also important as well as the spin fluctuation mechanism in the superconductivity.

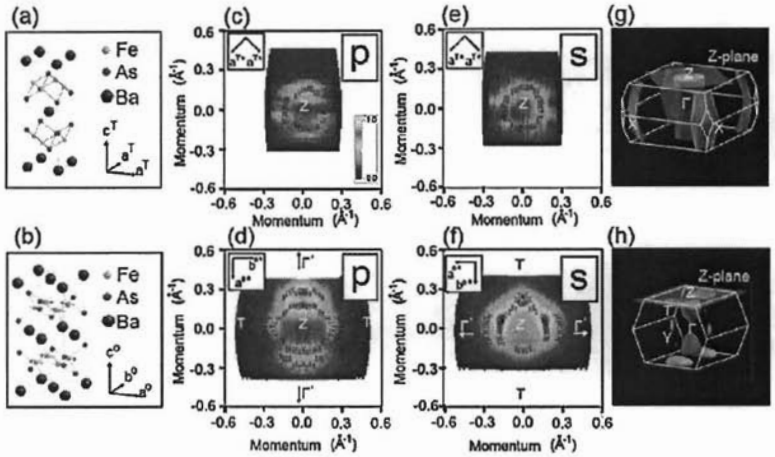

Figure 1: (a) Crystal structure of $BaFe_2As_2$ in the tetragonal structure. (b) Crystal and magnetic structure in the stripe-type AF ordered orthorhombic structure. (c),(d) FS of $BaFe_2As_2$ measured by p polarization at 180 K (above TN) and 30 K (below TN), respectively. (e),(f) FS of $BaFe_2As_2$ measured by s polarization at 180 K (above TN) and 30 K (below TN), respectively. (g),(h) Whole FS in the first BZ obtained by LDA calculation considering PM tetragonal and stripe-type AF orthorhombic structure, respectively, using the experimentally obtained structural parameters.

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Bipartite Elementary Excitations in Two-Dimensional Quantum Spin Liquid

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Spin systems confined to low dimensions exhibit a rich variety of quantum phenomena. Particularly intriguing are quantum spin liquids (QSLs), antiferromagnets with quantum fluctuation driven disordered ground states, which have been attracting tremendous attention for decades. In dimension greater than one, it is widely believed that QSL ground states are likely to emerge in the presence of geometrical frustrations. In 2D, typical examples of systems where such geometrical frustrations are present are the triangular and kagomé lattices. Largely triggered by the proposal of the resonating-valence-bond theory on a 2D triangular lattice and its possible application to high-T_c cuprates, realizing/detecting QSLs in 2D systems has been a long-sought goal. Two recently discovered organic insulators, κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ and $EtMe_3Sb[Pd(dmit)_2]_2$, both featuring 2D spin-1/2 Heisenberg triangular lattices, are believed to be promising candidate materials which are likely to host QSLs.

Here, to unveil how the elementary excitations above a QSL ground state behave, we study the low-temperature heat-transport properties of κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ [1] and $EtMe_3Sb[Pd(dmit)_2]_2$ [2]. In the temperature dependence of thermal conductivity, a sizable linear term is clearly resolved in the zero-temperature limit in $EtMe_3Sb[Pd(dmit)_2]_2$, indicating the presence of gapless excitation. Meanwhile its magnetic-field dependence suggests a concomitant appearance of spin-gap-like excitations at low temperatures. These findings expose a highly unusual dichotomy which characterizes the low-energy physics of this quantum liquid.

In collaboration with M. Yamashita, T. Shibauchi, Y. Senshu, M. Nagata, S. Fujimoto (Kyoto Univ.), T. Sasaki(Tohoku University), H.M. Yamamoto and R. Kato (RIKEN)

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Unconventional phases in frustrated ferromagnetic spin chains

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The search for exotic orders in (low-dimensional) quantum spin systems with geometric frustration has been a very active field of both theoretical and experimental studies. I will discuss some unconventional spin orders, such as vector chiral order, spin nematic and other multipolar spin orders, which appear in the one-dimensional spin-1/2 Heisenberg model with competing nearest-neighbor J_1 and antiferromagnetic next-nearest-neighbor J_2 exchange couplings in the presence of either magnetic field or easy-plane anisotropy, eigher one of which breaks the SU(2) spin symmetry down to U(1). The J_1-J_2 model, or the zigzag spin chain, is a minimal model of frustrated quantum magnets and is a host of various types of exotic spin orders. With a ferromagnetic nearest-neighbor coupling J_1, the model is considered to describe magnetic properties of quasi-one-dimensional edge-sharing cuprates such as $Rb_2Cu_2Mo_3O_{12}$ and $LiCuVO_4$.

In the recent publications listed below we obtained the ground-state phase diagram of the J_1-J_2 spin chain which contains various types of unconventional phases including a vector chiral ordered phase, a spin nematic phase, etc. For example, the vector chiral ordered phase is a quantum analogue of classical helical spin ordered phase, and the spin nematic phase can be regarded as a superfluid of two-magnon bound states. The spin nematic and higher-order multipolar phases appear near saturation field. In the presence of easy-plane exchange anisotropy (but without magnetic field), we find a series of quantum phase transtions between a dimer phase and an antiferromagnetically ordered (Neel) phase near the degeneracy point $J_1/J_2 = -4$. If time allows, I will briefly discuss the case of antiferromagnetic J_1 as well.

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FRIDAY, 13 AUGUST 2010

(updated as of 27 July 2010)

web-page: http://agenda.ictp.trieste.it/smr.php?2157

Low symmetry structures and strong f-s(d-s) hybridization as key ingredients to find new unconventional superconductors

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Abstract Submitted to the "Workshop on Principles and Design of Strongly Correlated Electronic Systems", Abdus Salam ICTP, Trieste, Italy, 2010

Discovery of 3D Topological Insulators and related Superconductors using Spin-sensitive novel spectroscopic methods

D. Hsieh[1], Y. Xia[1], Y.S. Hor[1], L.A. Wray[1], D. Qian[1], S.-Y. Xu[1], A. Fedorov[2], J.H. Dil, J. Osterwalder, H. Lin[3], A. Bansil[3], C.L. Kane[4], R.J. Cava[1], M.Z. Hasan[1]
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The topological insulator is a fundamentally new phase of quantum matter, which exhibits exotic quantum-Hall-like behavior even in the absence of an applied magnetic field and unlike the quantum Hall liquids can be turned into superconductors [1]. In this talk, I will briefly review the first experimental discovery and realization of the topological insulator in Bi-Sb [2,3], and then report our discovery a new generation of topological insulators with order-of-magnitude larger bulk band gaps and a single spin-helical surface Dirac cone [4,5,6] and experimentally demonstrate *all* defining properties of topological insulators such as (1) Topological Spin-Textures [3,5,6], (2) Spin-momentum helical locking [3,6], (3) Non-trivial Berry's phases [3,6], (4) Absence of backscattering or no U-turn [5,7], (5) Protection by time-reversal symmetry [1,5], (6) Room temperature topological order [6], (7) Superconductivity and Magnetism in doped topological insulators [8,9] and (8) a new platform for topological quantum phenomena [10].

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Landau-level spectroscopy of helical Dirac fermions in a topological insulator Bi_2Se_3

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Topological insulators are emerging materials which have energy gap in the bulk but possess robust gapless edge (2-dimensional case) or surface (3-demensional case) states [1,2]. In 3-dimensional case, the surface state is characterized by Dirac fermions which would give rise to unique quantum phenomena in a magnetic field [3]. Although the Dirac surface state has been confirmed by angle-resolved photoemission spectroscopy (ARPES) experiments, magnetic-field effects on a topological insulator are poorly understood because ARPES is not magnetic-field compatible and contributions from bulk bands dominate magneto-transport properties.

Here we use scanning tunneling spectroscopy to study the Dirac surface state of a topological insulator Bi_2Se_3 under magnetic fields [4]. Bi_2Se_3 crystals are naturally doped with electrons and the Dirac point is located ~0.3 eV below the Fermi level. Under magnetic field perpendicular to the cleaved surface, a series of Landau levels (LLs) has been observed in the tunneling spectrum. Remarkably, there is a field-independent LL at the Dirac point, which is a hallmark of Dirac fermions. We developed a scaling analysis scheme of LLs based on the Bohr-Sommerfeld quantization condition which allowed us to determine the energy-momentum dispersion of the surface state. Near the Fermi energy, complicated fine structures mixed with LLs appear in the spectra, which may be responsible for the anomalous magneto-fingerprint effect [5]. We anticipate that these observations provide spectroscopic basis for understanding the nature of topological insulators under magnetic fields.

This work has been done in collaboration with K. Igarashi, M. Kawamura, H. Takagi and T. Sasagawa.

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ABSTRACTS

OF

POSTERS

(in alphabetical order of author name as of 27 July 2010)

Title:
Effect of interband interactions of phonon and charge fluctuation on the superconductivity of MgB2

Authors: ***O CAbah***[1,2], G C Asomba[1] and C M I Okoye[1]

Affiliation: 1. Department of Physics and Astronomy, University of Nigeria, Nsukka.
2. Department of Quantum nanoscience, Delft University of technology, Netherlands.

Abstract:

We have recently investigate the effect of an unconventional pairing mechanism in MgB2 using a two-band model within the framework of Bogoliubov–Valatin formalism. The approach incorporates the intraband s-wave interaction in the s- and p-bands, as well as interband s-wave interaction between them. The analysis assumes that the pairing interaction matrix comprises of attractive electron–phonon, charge fluctuation and repulsive electron–electron (Coulomb) interactions to account for superconductivity in MgB2. The model is used to estimate the transition temperature and isotope effect exponent as well as to elucidate the importance of interband contributions in the superconductivity of the system.

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Study of the optoelectronic properties of semiconductors and nanostructures based on silicon carbide (SiC)

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Abstract

Silicon carbide nanostructures have very unique properties which bode well for applications in microelectronics and optoelectronics and have thus attracted much interest from the materials and device communities. In the microelectronics industry, silicon carbide is regarded as a promising substitute for silicon, especially in high power, high temperature, and high frequency devices. Recent advances in the preparation of ultra-high quality SiC single-crystals have in fact paved the way for wider uses of silicon carbide in microelectronic devices.

Among the different kinds of SiC nanostructures, SiC nanocrystals which have potential applications as nanoscale light emitters were the first to receive attention and have been studied extensively in the last ten years. Optically, bulk SiC shows weak emission at room temperature on account of its indirect band gap. However, the emission intensity can be significantly enhanced when the crystallite size diminishes to several or tens of nanometers. This is thought to be caused by depressed non-radiative recombination in the confined clusters.

In accordance with the quantum confinement (QC) effect, photoluminescence (PL) of the crystallites with diameters below the Bohr radius of bulk excitons is shifted to blue with decreasing sizes. Consequently, wavelength-tunable emissions can be achieved by preparing crystallites with different sizes. The large band gap of SiC (2.23 eV for 3C-SiC) renders the nanocrystals a good candidate as blue and ultraviolet (UV) light emitters in displays. This is in contrast to silicon crystallites from which strong and stable emissions in these spectral ranges are difficult to achieve. Moreover, the high chemical and thermal stabilities of silicon carbide make the luminescence from these nanocrystals very stable enabling the use of the materials in harsh environments and demanding applications. Combined with their excellent biocompatibility, especially blood compatibility, low density, and high rigidity, SiC nanocrystals are potentially useful in biology and medicine as well, for example, in bio-labeling.

Keywords: Nanostructures; Nanocrystals; Quantum confinement effect ; Recombination ; Photoluminescence

Electrical properties of AlN metal-insulator-semiconductor structures

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Abstract

Capacitance-voltage measurements of high-quality PECVD prepared aluminum nitride (AlN) thin films have been performed. These films have shown polycrystalline (002) preferential orientation, and were deposited on p-type Si (100) substrates with Pt forming the metal in a metal-insulator-semiconductor (MIS) structure. As the structure, crystallinity, texture and insulating properties depended on film thickness and were substantially influenced by the increase of the thickness; we undertook the measurement of the capacitance of the grown films and investigated their insulating properties with increasing thickness (200-1000nm). Defects trapped in the MIS structure could be a key player in dominating the overall behaviour of the C-V measurement curves, and good understanding of the process dominating the transport mechanism is essential for establishing optimal conditions for the deposition of AlN using different methods.

Fernando Assis Garcia – IFGW - Unicamp

Title

Correlated and dispersive rattling modes in skutterudite compounds.

Abstract

Skutterudite compounds are cage systems inside which a guest rare earth ion may be allocated. By many accounts, macroscopic physical properties (specific heat, thermal conductivity, thermoelectric power, etc.) may be well understood by adding, to the electronic contribution, a bosonic term describing an Einstein oscillator. This term is an isolated and non-dispersive harmonic vibration that is included to describe the excursion of the guest rare earth ions within the skutterudite cage, the so-called rattling modes. In this work, we present experimental evidence, from Gd^{3+} and Eu^{2+} ESR measurements, that such picture does not hold when one deals with a microscopic probe of the guest ion dynamics, and that both a correlated and dispersive rattling mode is necessary to explain our results.

Financial Support: FAPESP and CNPQ

The severe failure of a variational method used to describe the correlated molecular electron transport

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The field of molecular electronics is plagued by large discrepancies (often by several orders of magnitide) between the electric current through single molecules measured experimentally and computed theoretically. Because most theoretical approaches are based on the combination of the Keldysh nonequilibrium Green's functions and the density functional theory (NEGF+DFT), which heavily rely upon the single-particle description, one is tempting to assume that (presumably strong) electron correlations make the theoretical estimations unreliable.

Among the several attempts to incorporate electron correlation effects within transport theory, a method proposed by Delaney and Greer (DG) [1] a couple of years ago and subsequently used in a few studies of that group [1–5] seemed particularly appealing, as it claimed to correctly reproduce measured currents and yielded a few other plausible results.

Basically, the DG approach is a variational method based on two ingredients. One ingredient is the (constrained) minimization of the total energy of a *finite* cluster, which comprises the molecule of interest and parts of electrodes, in the presence of an external (source-drain) bias (zero-temperature case). DG claimed that this condition follows from the principle of maximum entropy [6, 7]. The second ingredient is the imposition of the open boundary conditions in terms of the Wigner function (WF). In authors' view, utilizing the WF is particularly advantageous, because, unlike the single-particle Fermi distribution, it can also be employed for correlated electrons.

However, these authors did not demonstrate that their approach is physically sound. Therefore, in two recent papers we scrutinized the DG approach and unabmiguously demonstrated that (i) its results are completely unphysical [8], and (ii) it cannot be remedied [9]. To demonstrate the lamentable failure of the DG method we considered the simplest models: a point-like quantum dot both with and without onsite Coulomb interaction [8]. As a rare example demonstrating the lamentable failure of a theory on which we are aware, in Fig. 1 we present results for the case of a noninteracting point contact.

In our most recent work devoted on this topic [10], we completed the evidence on the failure of the DG method, and demonstrated that this method also lamentably fails not only in the case of *discrete* models, but also in the case of the simplest *continuous* model employed to discuss electric transport in the early days of quantum mechanics [11]. In the same work [10] we unreveled the physical reasons why the DG method fails. Briefly, it amounts to compute the electric response by considering

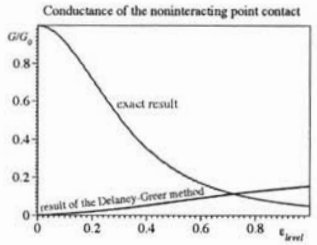

FIG. 1: Results on the normalized conductance G/G_0 ($G_0 = 2e^2/h = 77.5\,\mu$S) obtained exactly and by using the DG method for a noninteracting point contact as a function of the offset energy ε_{level}. (After Ref. 8.)

the time limit $t \to \infty$ *before* taking (or, more precisely speaking, mimicking) the infinite volume limit (in one dimension, $L \to \infty$); from transport theory it is well known that these two limits cannot be interchanged and the correct order is just the opposite.

The authors acknowledge with thanks the financial support for this work provided by the Deutsche Forschungsgemeinschaft (DFG).

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Metamagnetism and the anomalous phase of $Sr_3Ru_2O_7$

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The phase diagram of $Sr_3Ru_2O_7$ contains a metamagnetic transition that bifurcates to enclose an anomalous phase with intriguing properties - a large resistivity with anisotropy that breaks the crystal-lattice symmetry [1]. We propose that this is a magnetic analogue of the spatially inhomogeneous superconducting Fulde-Ferrell-Larkin-Ovchinnikov state. Based on a microscopic theory of Stoner magnetism we derive a Ginzburg-Landau expansion where the magnetisation transverse to the applied field can become spatially inhomogeneous. We show that this reproduces the observed phase diagram of $Sr_3Ru_2O_7$ [2]. We consider the thermodynamic signatures of such transitions and the effect of the complex bandstructure of $Sr_3Ru_2O_7$ on simple models of the transition.

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Generalising spin ice: the magnetic ground state of pyrochlore $Gd_2Ti_2O_7$

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Recently there has been much interest in the magnetic monopole excitation of spin ice. This is a consequence of the 'ice rules' which give rise to a large low energy degeneracy. Both spin ice and gadolinium titanate have a pyrochlore lattice of corner sharing tetrahedra. In spin ice the strong crystal field interactions mean that the spins have an Ising character: they are constrained to point along the local tetrahedral axes. The degenerate ground state configurations consist of all tetrahedra containing two spins pointing inwards and the remaining two outwards (and, therefore, each tetrahedron has a ferromagnetic component). In contrast, in gadolinium titanate the antiferromagnetic nearest neighbour Heisenberg interaction is dominant, which is extremely frustrated on the pyrochlore lattice. This gives rise to a similar but much larger degeneracy than is seen in spin ice.

We investigate the residual degeneracy in gadolinium titanate. Firstly we enforce the Mössbauer experimental restriction that the spins are confined to planes perpendicular to the local crystal directions in order to reduce the degeneracy to a manageable level. This XY-like anisotropy can be seen to be a result of minimising the dipolar interactions. Our assumptions generate a more complex analogue of the ice rules for gadolinium titanate.

Theoretically the frustrated antiferromagnetic interaction leads to the absence of classical long range magnetic order in the ground state. $Gd_2Ti_2O_7$ shows precisely this behaviour by magnetically ordering well below the Curie-Weiss temperature as a result of other much weaker interactions becoming relevant. In the current literature there are apparently conflicting interpretations of neutron scattering and Mössbauer data. In particular the only magnetically ordered ground states previously proposed to fit the neutron scattering data required a quarter of the gadolinium spins to have no magnetic moment. The Mössbauer experiments however, clearly indicate that in the ground state all the spins have magnetic moments of the same classically expected magnitude. We therefore attempt to resolve some of this confusion.

At low temperature we require that our rules discussed above are also consistent with the neutron scattering experiments, which show a magnetic scattering vector $\mathbf{k} = (\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$. This turns out to lead to two distinct magnetic states which are unrelated to previous proposals. The energetics are complicated. The residual degeneracy appears to be lifted by a compromise between longer range Heisenberg and direct dipolar interactions of a similar energy scale. Our proposed states, however, do not appear to fit the neutron scattering Bragg peak intensities at all well. We therefore believe that it is possible to find still lower energy $\mathbf{k} = (\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$ states, of equal magnitude spins, by relaxing the restriction that the spins must lie exactly within the planes indicated by the Mössbauer data.

Lifshitz transitions and crystallization of fully-polarised dipolar Fermions in an anisotropic 2D lattice

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We consider a two dimensional model of non-interacting chains of spinless fermions weakly coupled via a small inter-chain hopping and a repulsive inter-chain interaction. The phase diagram of this model has a surprising feature: an abrupt change in the Fermi surface as the interaction is increased. We study in detail this meta-nematic transition, and show that the well-known $2\frac{1}{2}-$order Lifshitz transition is the critical endpoint of this first order quantum phase transition. Furthermore, in the vicinity of the endpoint, the order parameter has a non-perturbative BCS-like form. We also study a competing crystallization transition in this model, and derive the full phase diagram. This physics can be demonstrated experimentally in dipolar ultra-cold atomic or molecular gases. In the presence of a harmonic trap, it manifests itself as a sharp jump in the density profile.

Common Features of Magnetic Properties and Thermal Entanglement on a Triangulated Kagomé Lattice

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The common features of concurrence, as a measure of pairwise thermal entanglement, and magnetic properties of spin-1/2 Ising-Heisenberg model on a triangulated Kagomé lattice are studied within the framework of variational mean-field like treatment based on Gibbs-Bogoliubov inequality. Because of the separable character of Ising-type exchange interaction between the Heisenberg trimers, the calculation of quantum entanglement in effective field can be performed for each of them individually. The concurrence is studied in terms of a three qubit XXX Heisenberg model in effective magnetic field and is found being non-zero in absence of external magnetic field. The critical temperature for the phase transition and threshold temperature for concurrence coincide in the case of antiferromagnetic coupling between qubits. The magnetic and entanglement properties exhibit common (plateaux, peak) behavior observable via coupling constant and external magnetic field. The fact that saturated and frustrated phases are entangled and non-entangled respectively is obtained.

Novel microwave–induced resonances on the current-voltage characteristics of YBCO/Nb Josephson junctions

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Recently it has been shown that to achieve a strong THz radiation from Josephson junctions (JJs) we need to develop an approach allowing us to tune the current-voltage characteristics (CVC) of JJs until resonance conditions are met [1]. Here [2] we show that the control of CVC can be achieved if a strong microwave signal (MW) is applied to a JJ.

Experiments. We prepared thin film ramp-edge JJs between 170 nm untwinned $YBa_2Cu_3O_{7-x}$ and 150 nm Nb using a 30 nm Au barrier. We observe a remarkable tuning of the CVCs of such JJs by the MW and some unusual resonances (see Fig.1a) when applying strong MW. Unlike the Shapiro-steps, such unusual resonances have their voltage position on the CVC dependent on the MW power rather than the MW frequency, while their amplitude is largely unaffected by an increase in the MW power. Such resonances are very robust against a change in the MW frequency f in the range $0.001<f/f_J<0.1$, f_J is the Josephson plasma frequency of JJ typically of about 100 GHz. Such behaviour indicates an intriguing Josephson dynamics associated with the switching from a parametric excitation regime induced by the magnetic field of the MW via oscillations of the Josephson critical current to an ac-current excitation regime triggered by the electric field of the MW. Such tuning of the CVC via MW could be used to optimize the output of THz emitters.

Theory. To model the CVC of the JJs we assume that the magnetic field H of the MW, induces an *ac* current in the JJ of amplitude $I_{ac} = kH$. The coupling constant k is determined by the circuit parameters and depends on f, I_{dc} and H. So, the current flowing through the junction is $I(t) = I_{dc} + I_{ac}(t)$. To compute the CVC of the JJ $V(I_{dc})$ we first solve numerically the following equation for the JJ phase difference ψ ([2]) :

$$\ddot{\psi} + \dot{\psi}/\sqrt{\beta_c} + J(\tau)\sin\psi = i(\tau). \qquad (1)$$

Here β_c is the McCumber parameter, $i(\tau) = I(\tau)/I_c$, I_c the Josephson critical current, $\tau = 2\pi f_J t = \omega_J t$ is the normalized time, and the dots above the variable represent the time derivative. $J(\tau)$ can be interpreted as a dimensionless critical current modulated by H. Then we calculate $V = \Phi_0\omega_J \langle d\psi / d\tau \rangle$ (here $\langle \ldots \rangle$ means time average, Φ_0 is the flux quanta) for every dc bias current I_{dc}, so that finally the CVC is obtained. A remarkable agreement with the measurements is reached (see Fig.1b).

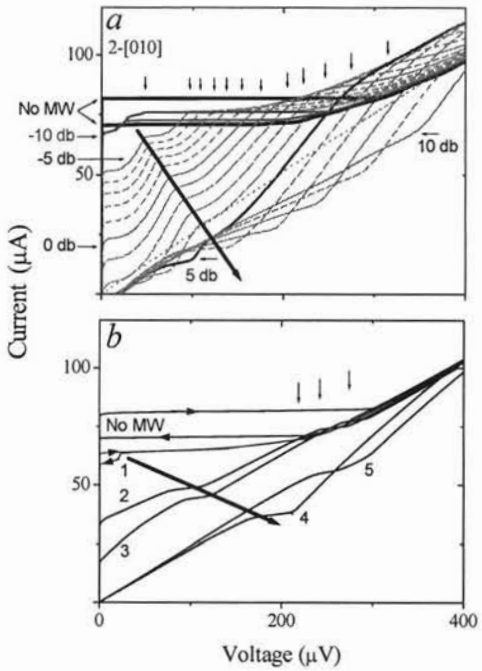

Fig. 1. *The CVC for a junction at different applied MW power. With increasing MW power of frequency 0.5 GHz the peak position of the first resonant shifts in the direction indicated by the big arrows. Vertical arrows show the peak voltage position of the second resonance.* ***(a)*** *Experimental curves. MW power increases by 1db from -5 to 10 db.* ***(b)*** *Calculated CVC: (1) -10 db and k=0.02, (2) 0 db and k=0.02, (3) 4 db and k=0.02, (4) 7 db and k=0.1, (5) 10 db and k = 0.1, dashed line 20 db and k = 0.1 increases monotonically.*

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Competition between magnetism and superconductivity in the iron arsenides

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The new iron arsenide superconductors present a very rich phase diagram, displaying superconducting, antiferromagnetic and structural order. Here, we present a microscopic model to study the competition between electronic and magnetic degrees of freedom. Expanding the microscopic free energy of the system with competing order around the multicritical point, we show that while the phonon-mediated s^{++} state is generally incompatible with the itinerant antiferromagnetic state, the unconventional s^{+-} state is able to coexist with magnetism. The sensitivity of the phase diagram to the symmetry of the Cooper pair wave-function is related to the fact that the static magnetic moment plays the role of an intrinsic inter-band Josephson coupling in the free energy expansion. Our results rely solely on the assumptions that the system is close to particle-hole symmetry and that the same electrons that form the ordered moment contribute to the superconducting condensate. On the other hand, in the case of a localized antiferromagnetic phase, we show that coexistence with the superconducting state can be easily attained. We also demonstrate that, in this case, the localized magnetic moment is little affected by the onset of superconductivity, which is at odds with experimental observations on iron arsenide compounds.

Unconventional quantum magnetism in Fermi systems with magnetic dipolar interactions

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We study the magnetic structure of the ground state of an itinerant Fermi system of spin-1/2 particles with magnetic dipole-dipole interactions. We show that, quite generally, the spin state of particles depend on its momentum, i.e., spin and orbital degrees of freedom are entangled and taken separately are not ``good'' quantum numbers. Specifically, we consider a uniform system with non-zero magnetization at zero temperature. Assuming the magnetization is along z-axis, the quantum spin states are $\mathbf{k}$-dependent linear combinations of eigenstates of the σ^z Pauli matrix. This leads to novel spin structures in *momentum space* and to the fact that the Fermi surfaces for ``up'' and ``down'' spins are not well defined. The system still has a cylindrical axis of symmetry along the magnetization axis. We also show that the self energy has a universal structure which we determine based on the symmetries of the dipolar interaction and we explicitly calculated it in the Hartree-Fock approximation. We show that the bare magnetic moment of particles is renormalized due to particle-particle interactions and we give order of magnitude estimates of this renormalization effect. We estimate that the above mentioned dipolar effects are small but we discuss possible scenarios where this physics may be realized in future experiments.

Ref: Phys. Rev. B 81, 214443 (2010)

Relationship between crystal structure, electronic structure and ground state properties in the system $Ce_{3+x}Rh_4Sn_{13-x}$

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Over the past years the compounds crystallizing in the space group $Pm\bar{3}n$ with the formula $Ce_3T_4Sn_{13}$ (T is a transition metal) have attracted considerable attention due to strongly correlated electron phenomena they exhibit. $Ce_3Ir_4Sn_{13}$ is claimed to be a heavy-fermion system ($\gamma \approx 670$ mJ mol-Ce^{-1} K^{-2}) with an antiferromagnetic phase transition at $T_N = 0.6$ K [1]. In contrast, $Ce_3Co_4Sn_{13}$ exhibits only a short-range antiferromagnetic order at 0.8 K, which can be suppressed by magnetic fields, giving way to single-impurity behaviour above 25 kOe with a Kondo temperature $T_K \approx 1.2$ K [2]. Interestingly, very recent studies of the new compound $Ce_3Rh_4Pb_{13}$ do not give any indication of a Kondo effect or magnetic order above 0.35 K [3].

In view of this diversity of low-temperature physical properties in one class of isostructural and isoelectronic compounds, it is of great interest to investigate in detail another member of this family, $Ce_3Rh_4Sn_{13}$. Although this system has been studied during the last few years, the results obtained by different research groups were contradictory [4] . Further, inconsistent reports concerning both crystal structure and superconducting properties of the reference compound $La_3Rh_4Sn_{13}$ [5-6] as well as the existence of two compounds $Ce_3Ru_4Sn_{13}$ and $CeRuSn_3$, both crystallizing in the space group $Pm\bar{3}n$ [7], prompted us to reinvestigate carefully structural properties of the parent compound $Ce_3Rh_4Sn_{13}$ and to inspect the homogeneity range of Ce and Sn in this system. The influence of the substitution of Sn by Ce on the crystal structure, electronic structure and ground state properties of $Ce_{3+x}Rh_4Sn_{13+x}$. is analysed in detail based on the results of magnetization, resistivity and specific heat measurements, X-ray diffraction and spectroscopic data (X-ray photoemission, X-ray absorption) accompanied by first principles electronic structure calculations.

Ce core level XPS spectra and Ce L_{III} XAS data reveal a stable $4f^1$ configuration of the Ce ions. The detailed analysis of the Ce 3d XPS spectra based on the Gunnarsson-Schönhammer model calculations [8] indicates a rather weak hybridization between the Ce 4*f* and the conduction band states ($\Delta \approx 35$ meV) for all investigated compounds. The crystal structure of $Ce_3Rh_4Sn_{13}$ has been determined from single crystal diffraction experiments. Superstructure has been found. Thermodynamic measurements for $Ce_3Rh_4Sn_{13}$ point to two successive magnetic phase transitions at $T_{N1} \approx 1.9$ K and $T_{N2} \approx 1.1$ K. The Kondo temperature estimated based on the scaling of isothermal magnetoresistivity curves [9] equals 1.9 K. In contrast, the resistivity of $Ce_{3+x}Rh_4Sn_{13+x}$ ($0.2 \leq x \leq 0.6$) does not give any sign of the Kondo effect and indicates a low charge carrier concentration. The specific heat shows only one broad anomaly at temperatures below 1 K, which points to a magnetic ordering (presumably of a short-range type). This is in line with first principles electronic structure calculations which show a magnetic ground state for $Ce_3Rh_4Sn_{13}$ and indicate that the compounds $Ce_{3+x}Rh_4Sn_{13+x}$ ($0.2 \leq x \leq 0.6$) have only a very weak tendency towards a magnetic ordering.

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Affiliation: Iowa State University and Ames Laboratory

Title: London penetration depth measurements of $Ba(Fe_{1-x}M_x)_2As_2$ (M=Co, Ni, Pd, Pt, Co+Cu)

Abstract:
The change in the in-plane London penetration depth with temperature, $\Delta\lambda_{ab}(T)$, has been measured across the entire superconducting region of the doping phase diagram for single crystals of the newly discovered $Ba(Fe_{1-x}Co_x)_2As_2$ series as well as other transition metal substitutions such as Ni, Pd, Pt, and Co+Cu using the tunnel diode resonator (TDR) method [1,2]. In addition, the difficult to measure zero temperature value of the London penetration depth, $\lambda_{ab}(0)$, has been determined as a function of Co doping level by a novel technique which utilized TDR frequency measurements on samples that are coated with an aluminum film [3]. This allowed for the determination of the absolute value of the penetration depth from $\lambda_{ab}(T)=\Delta\lambda_{ab}(T)+\lambda_{ab}(0)$. A clear increase in $\lambda_{ab}(0)$ for far underdoped concentrations has been attributed to the competition between the superconducting and itinerant antiferromagnetic phases for the same conduction electrons. The resulting evolution of the superfluid density, $\rho_s(T)=[\lambda_{ab}(0)/\lambda_{ab}(T)]^2$, as a function of the doping level will also be reported.

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Turning a Nickelate Fermi Surface into a Cuprate-like one Through Heterostructuring

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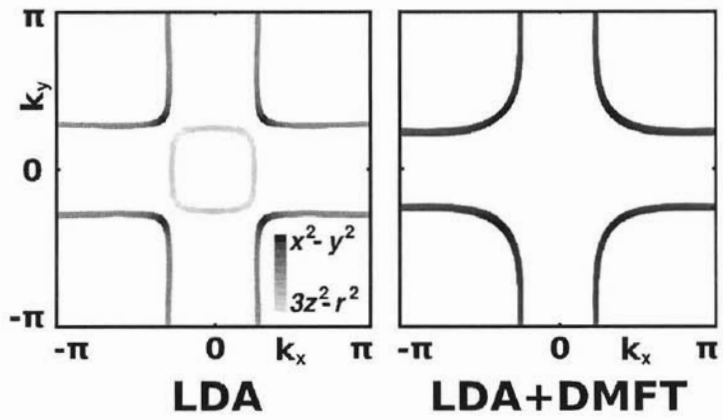
The possibility of finding bulk nickelates with an electronic structure analogous to that of high temperature cuprate superconductors was considered a while ago [1]. For the systems available at that time the results were not encouraging so the idea was discarded. However, nowadays, due to new experimental techniques, heterostructures can be engineered offering new possibilities for actual material design. Using the local density approximation and its combination with dynamical mean field theory (LDA+DMFT), we show (see figure) that electronic correlations induce a transition to a single sheet cuprate-like Fermi surface for $LaNiO_3/LaAlO_3$ heterostructures, even though both e_g orbitals contribute to it [2]. As we find also strong antiferromagnetic fluctuations, the low-energy electronic and spin excitations resemble those of high-temperature cuprate superconductors.



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Magnetic properties and Superconductivity in 5 band model for Iron Pnictides

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The most probable scenario for high T_c superconductivity in iron-based superconductors is that the magnetic fluctuation related to the stripe-type antiferromagnetic (AF) phase in the undoped materials induces an extended s-wave ($s_{\pm}$-wave) superconductivity. Indeed, calculations by the random phase approximation (RPA) for an effective 5-band Hubbard model suggest that such an AF fluctuation is induced by Fermi surface (FS) nesting, and leads to $s_{\pm}$-wave superconductivity upon the carries doping.[1] This has been verified on the basis of the fluctuation-exchange approximation (FLEX) with the self-energy correction.[2] However, straightforward addition of the FLEX self-energy also revealed a problem with double counting of the interaction effects in the multiband systems, accompanied by drastic changes in the Fermi surface and the spin fluctuations in contrast to experimental observations. In the successive papers, [3,4] we have investigated this problem in detail and proposed an *ad hoc* procedure, subtraction of a static part of the self-energy. With this modification, we can apply the FLEX approximation over wide ranges of carrier doping without any drastic changes mentioned above.

Here we employ the modified FLEX scheme to study the doping dependence of the electron correlation and spin fluctuations, and also the superconducting pairing mechanism. The obtained tendencies in the spin fluctuation and the electron correlations with the carrier doping qualitatively agree with the overall features observed in the $Ba_{1-x}K_xFe_2As_2$, $Ba(Fe_{1-x}Co_x)_2As_2$, and $LaFeAsO_{1-x}F_x$ systems. For instance, Figure 1 shows the T-dependence of NMR-$1/T_1T$ for vaious carrier dopings. It indicates suppressions like the pseudo-gap behavior on the electron-doped side, and remarkable growth by the enhanced AF spin fluctuations in $n=5.92$ and 5.80, and then suppression of such enhancement with further the hole doping. Figure 2 indicates the corresponding phase diagram. For a moderate hole doping, $n=5.92$-5.80, the strong AF spin fluctuation with the stripe-type $Q=(\pi,0)$ dominates, and in the proximity of the AF phase, the $s_{\pm}$-wave superconductivity appears. In addition, for the electron doping $n>6.16$, where the $\Gamma'(\pi,\pi)$ hole surface is absent, the d_{x2-y2}-wave solution competes with the nodal $s_{\pm}$-wave one.

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Figure 1

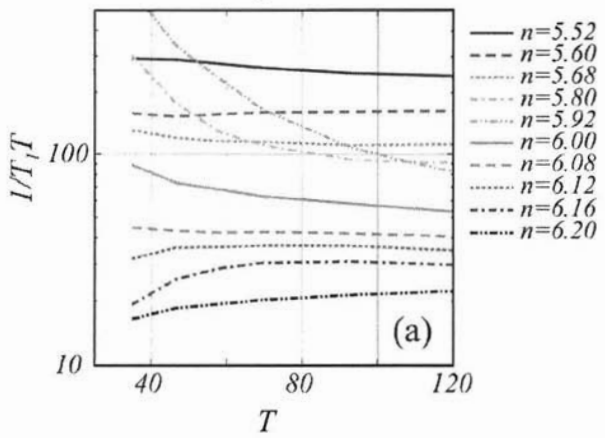
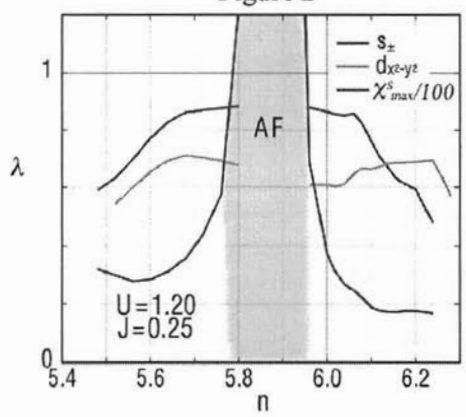


Figure 2



Bulk and edge of Z_2 topological insulator

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A topological insulator has a remarkable property of being metallic on the surface albeit insulating in the bulk. Recently much focus is on a specific type of topological insulators, which is said to be *Z_2-nontrivial*, and realized as a consequence of interplay between spin-orbit coupling and a band structure with effective relativistic dispersion (electrons satisfy a Dirac equation). Such systems are invariant under time reversal and shows Kramers degeneracy.

Graphene is a two-dimensional (2D) implementation of such Dirac electron system, which also realizes a prototype [1] of Z_2 topological insulator, in the presence of intrinsic and extrinsic (Rashba) spin-orbit interactions. Recently, we were able characterize specific localization properties of this system, in the presence of weak disorder and under doping [2]. We have shown in particular that localization symmetry class is determined by the parity of the total number N_s of "activated" effective spins in the system. Our diagnosis provides a contemporary version of the weak localization theory.

The correspondence between the physics of bulk and of the edge highlights the physics of a topological insulator [3]. To demonstrate, we make a close comparison between the continuum Dirac theory and the square lattice tight-binding model [4] for a Z_2-topological insulator in 2D. It is naturally shown that not only *explicit*, but also *hidden* Dirac cones in the high-energy spectrum, contribute to and ensure the integral quantization of spin Hall conductance. The nature of gapless edge modes in the lattice model under different (straight vs. zigzag) boundary conditions is extensively studied. We demonstrate that the edge modes of a Z_2-topological insulator are susceptible of various finite size effects, in comparison with chiral edge modes of quantum Hall insulator. By comparing the behavior of gapless edge modes in real and momentum spaces, we show that localizability of edge mode is intricately related to level crossings due to projection of 2D bulk spectrum onto the 1D edge.

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Electronic band gaps in graphene-based quasi-periodic superlattices

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Recently, a monolayer of carbon atoms arranged in a honeycomb pattern called graphene has attracted people's great interest due to its unique electronic properties [1]. For a graphene sheet, it possesses a Dirac point in which the valence and conduction bands touch each other. Moreover, superlattices based on graphene sheets can be realized by introducing electrostatic potentials or magnetic barriers [2,3]. Graphene-based superlattices, as other superlattices composed of conventional semiconductors, provide us more freedom to tune the electronic structures. For example, strong anisotropy for the group velocities of electrons can occur in graphene-based superlattice [4]. Most recently, electronic band gaps in graphene-based superlattices with periodic potentials has been studied [5]. By tuning the voltage of gate electrode, in one kind of layer the direction of wave vector of electrons can be in opposite to that of group velocity of electrons while in the other kind of layer both directions are the same. Therefore, at some electronic energy, the phases of electrons in two kinds of layers can be cancelled out, leading to the zero (volume) averaged wave number (zero <k>) gap. The zero <k> gap possesses some unusual properties compared to the Bragg gap coming from the Bragg scattering. For example, the zero <k> gap is invariant with the scaling change of the widths of the potential barriers. Here, we further confirm that zero <k> gap not only occurs in graphene-based periodic superlattices, but also exists in graphene-based quasi-periodic superlattices, such as superlattices with Fibonacci sequences. In Fig. 1(a), the zero <k> gap is indicated while the other gaps are Bragg gaps. It is found the zero <k> gap exists for all Fibonacci levels. Moreover, in contrast to Bragg gaps, the center of zero <k> gap remains invariant with the scaling change of the widths of the potential barriers. Self-similar property of band splitting is also found in Fig. 1.

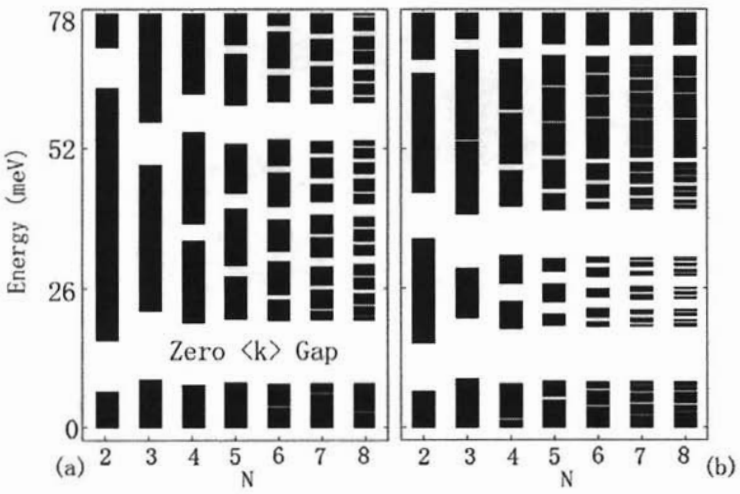

Fig. 1. The electronic energy versus Fibonacci level. The voltages in A and B layers are 0 and 20 mev, respectively. The widths of A and B layers are identical. The width of A layer is 20 nm in (a) and 40 nm in (b), respectively.

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Fulde-Ferrell-Larkin-Ovchinnikov phase in correlated electron systems

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The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) unconventional superconducting state has suddenly gained renewed interest recently because of its possible realization in the heavy fermion superconductor $CeCoIn_5$ [1], as well as in organic superconductors, and optical lattices. In $CeCoIn_5$ spin dependence of quasiparticle masses has also been observed recently by means of the de Haas-van Alphen measurements [2]. Therefore, the question arises as to what extent these two basic phenomena are interconnected. Here we show that the appearance of the spin-split masses essentially extends the regime of temperature and applied magnetic field, in which FFLO state is stable, and thus, it is claimed to be very important for the phase detectability [3]. Furthermore, we analyze the Andreev reflection from the FFLO superconductor and provide conductance spectra for a normal metal – FFLO superconductor junction, which could lead to experimental verification of the presented results.

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METAL-INSULATOR PHASE TRANSITION IN AN EXACT SOLVABLE MODEL OF NONDEGENERATE INTERACTING FERMION CHAINS

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The metal-insulator transition in strongly correlated materials remains a central problem of modern condensed matter physics. The quantum critical point separating different phases is a topic of great current interest. The nondegenerate strongly interacting fermion systems have been subject of intensive investigation. Localized and itinerant electrons and their correlations in multiorbital systems seem to play an important role in the formation of heavy fermion states in the transition metal oxides and rare-earth compounds. One typical example of transition metal oxide LiV_2O_4, in which heavy fermion-like behavior was observed. Mostly models of strongly interacting electron systems describing subbands with different bandwidths are used for description of such compounds, they permit to describe explicitly both the localized orbitals, such as the d in transition metal oxides or the f in heavy fermion systems, and their hybridization to an itinerant electron bands (p-orbitals of oxygen in transition metal oxides). The minimal model consists of a regular array of sites, each accosiated with nondegenerate f-electron orbital coupled to a delocalized conduction electron orbital. The Kondo lattice and periodic Anderson model should be specially noted.

We have discussed in depth the model of two coupled nondegenerate free fermion chains interacting via the correlated hopping and interchain Coulomb interaction. A two parametric family of the models is solved by the means of the Bethe ansatz. The model has a rich ground-state phase diagram at half-filling: the 'intermadiate metallic' state separates the insulator and 'inter-chain ferromagnetic' phase states, the curves of the phase transitions are defined by the parameters of the interactions. The phase diagram is characterized by the tricritical point, where these three phase states coexist. The critical fluctuations are described by a conformal field theory with the central charge c=1. In the tricritical point the critical exponents of a marginal Luttinger liquid are characterized by abnormal strong density-density correlations and correlations of the field operator.

Electronic properties of (111) oriented CeO_2 thin film grown by pulsed laser deposition

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Abstract

Ceria (CeO_2) has drawn considerable interest due to its technological importance in oxygen storage capacity, catalytic and electrochemical properties and its application in solid oxide fuel cells and has interesting physical properties, inherent to the Ce f-electron system. Most of the applications of CeO_2 strongly depend on the electronic properties, which involve largely localized or delocalized 4f electronic state of Ce. We have deposited the thin film of CeO_2 on Si (100) substrate using pulsed laser deposition and studied the chemical state and electronic structure of Ce using XPS and RPES measurements. XPS study divulges that in the film Ce is in 3+ and 4+ valence states. Appearance of 3+ valence state of Ce could be due to oxygen vacancy in the film. The RPES measurement confirms that VB spectra of the studied CeO_2 thin film contain Ce^{3+} and Ce^{4+} states. We observe three dominant bands of energy 2.1 eV, 4.4 eV and 6.9 eV in the valence band spectra of CeO_2 thin film, which are mainly derived from Ce-4f, Ce-5d states and O-2p states, respectively. Further, to understand the dependence of VBS on incident photon energy and individual contributions to the O-2p emission from the 5d and 4f bonding orbitals and emission from the localized 4f orbital of Ce, we have plotted the constant initial state (CIS) intensity plots for different features of VBS spectra. Constant Initial State (CIS) plot versus photon energy for 2.1 eV feature of VBS reveals resonance at photon energy 122 eV confirming it to be due to Ce^{3+} state. We also find that the resonance energy value Ce^{4+} state is 125 eV, O-2p also show resonance at that energy, suggesting Ce^{+4} hybridized with oxygen.

Calculation of magnetocaloric effect in GdGa and some related compounds

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The intermetallic compound GdGa is reported to be ferromagnet [1] with two magnetic order transitions; a spin reorientation transition at $T_{SR} \sim 100$ K [2] and a ferromagnetic-paramagnetic transition at $T_C \sim 180$ K [3]. It also showed a magnetocaloric effect (MCE) which is of potential interest in magnetic refrigeration study [4].

Substitution of Ga with some nearby elements (Ge, Zn, Cu) can strongly infuence the magnetic order, and therefore the thermodynamic properties of the prototype compound. The influence of substitution in tuning such properties is useful in studying the MCE and the mechanism of mediating exchange interactions through nonmagnetic atoms.

In this work we presented preliminary results of calculations of the MCE, in terms of the isothermal magnetic entropy changes ΔS_{mag} and the adiabatic temperature changes ΔT_{ad}, in GdGa, $GdGa_{1-x}Ge_x$, $0 < x < 1$, and in Gd(Zn,Cu) compounds, under the magnetic field changes from 0->5T. Calculations are based on the mean-field model of coupled magnetic lattices [5] combined with the density functional theory (DFT) [6]. Lattice contribution to total entropy is added in Debye approximation.

In brief, we wanted to show how mean-field model accompanied with DFT calculation of exchange coupling constants could be used in prediction of the transition ordering temperature and the MCE. Results of the calculations are compared with experimental values [1,4,7,8]. The role and dependence of conduction electron mediated exchange on chemical composition is discussed.

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Paramagnetic-ferromagnetic transition in a double-exchange model

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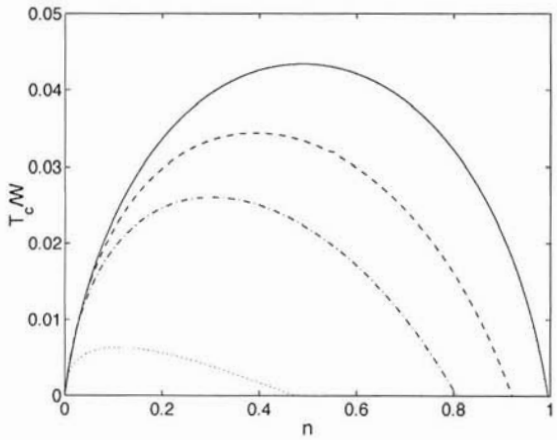

FIG. 1. T_c as a function of electron concentration n for different relative strengths of the exchange (exchange integral times spin divided by the band width W): $JS/W = .25$ (dotted line), $JS/W = 1$ (dash-dotted line), $JS/W = 2$ (dashed line), and $JS/W = 20$ (solid line).

We study paramagnetic - ferromagnetic transition due to exchange interaction between classical localized magnetic moments and conduction electrons. We formulate the Dynamical Mean Field Approximation equations for arbitrary electron dispersion law, concentration and relation between exchange coupling and the electron band width. Solving these equations we find explicit formula for the transition temperature T_c. We present the results of calculations of the T_c for the semi-circular electron density of states.

MAGNETIC COMPENSATION AND EXCHANGE BIAS BEHAVIOR OBSERVED IN $Sm_{1-x}Gd_xNi_2$

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Keywords: spin-orbital compensation, Exchange bias

We report the observation of a compensation point in the temperature dependence of magnetization data of polycrystalline $Sm_{0.97}Gd_{0.03}Ni_2$ alloy. Magnetization measurements show that this compound magnetically orders at about 25 K. Below this temperature, the magnetization data shows a compensation point. When the cooling field is below 5 kOe, the alloy exhibits a large negative magnetization below the compensation temperature (T~18 K). However, for the higher cooling fields, a spin flip takes place which aligns the total magnetic moment along the field direction leaving a dip in the *M(T)* curve at the compensation point. Field cooled hysteresis loops obtained below the compensation temperature show that the compound possesses exchange anisotropy. Both the exchange anisotropy field and the coercive field are found to be quite large and a peak at the compensation temperature for temperature dependence of exchange bias field is detected. These results are similar to those of the well known and classical spin-orbit compensated ferromagnet $(Sm,Gd)Al_2$ [1,2,3]. Resistivity data indicates that the material remains in the ferromagnetic phase even at the compensation temperature and below it. This peculiar magnetic property is attributed to the different temperature dependencies of the spin and orbital magnetic moments due to the complex thermal admixture of nearly degenerate *J* multiplets of Sm^{+3} ions[1]. A detailed discussion on the nature of the compensation in this alloy will be presented.

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Magnetoelastic study of the incommensurate phase in $TiOCl$

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We present a phase diagram for the spin-Peierls compound $TiOCl$ based on an XY model coupled to adiabatic phonons. It is obtained through a minimization of the free energy with respect to the lattice distortions at different temperatures. We are able to find the experimental phase transitions and obtain a transition between a sinusoidal pattern and a soliton lattice for the distortions inside the incommensurate phase. Furthermore, we calculate spin-spin correlations in the incommensurate phase and compare them with the ones obtained through DMRG calculations in a Heisenberg model with modulated exchange couplings.

Revisiting The Criteria

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Metal-insulator transitions (MIT) are widely observed in condensed-matter systems and are quite studied as well [1]. Especially important are the transitions resulting from electron-electron interaction, giving rise to the so called Mott-insulators. We study the repulsive fermionic Hubbard model on a two-dimensional square lattice using determinantal quantum Monte Carlo (DQMC) simulations [2] and make a review on the different quantities that are frequently used to infer the metallic/insulator ground-state of these systems. For this purpose we calculate the electronic compressibility, the optical conductivity, the density of states, the dc conductivity and the density of states at the Fermi energy and we see that all those quantities are subject to finite size problems and agree with the gaps in the energy spectrum of the noninteracting Hubbard model. These gaps appear as a direct consequence of the finite square lattice treated. Motivated by this problem we analyze the Drude weight, a quantity fully scrutinized in the seminal paper of Scalapino [3], and we see that it gives response that is not susceptible to finite size problems. We also make comparisons relating the densities in which is evident the issue of finite systems and see that there is no sign problem at such densities.

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Spontaneous translational symmetry breaking associate magnetization plateaus in one-dimensional spin systems with Ising and Heisenberg bonds

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Abstract

There are well known examples of integrable many-particle systems solvable within the Bethe ansatz technique, like 1d Heisenberg chain, Hubbard model, e.t.c. Though, Bethe ansatz, being a paradigm in modern theoretical and mathematical physics, is very important by itself, its application in condensed matter physic is still very restricted. Particularly, in the physics of magnetism one usually needs to describe thermodynamic properties of certain quantum spin-lattice models at finite temperature. At the moment exact treatment of this problem is feasible only for very limited number of model within rather complicated and sophisticated techniques like quantum transfer matrix and non-liner integral equation. However, majority of real magnetic materials (even one-dimensional) has lattice structure which corresponds to no known integrable models. Thus, numerical calculations are almost the only way to shed a light into their thermodynamic properties. However, one can change a little underlying spin system to get the model, which can be easily solved exactly within classical transfer-matrix technique. Namely, if one change some interaction bonds with Ising ones in such a way that Hamiltonian of the emergent system be a sum of commuting operator, then one can expand the exponential in the partition function and get the formal structure which is suitable to applying the classical transfer matrix method. Thus, one will obtain a one-dimensional spin system with clusters of quantum spins and intermediate "classical" spins between them. The problem of calculation the partition function of the system yield the problem of diagonalization of the small quantum spin clusters which in most cases are feasible and further calculation of the eigenvalues of classical transfer matrix which is also straightforward. A various spin systems with Ising and Heisenberg bonds have been considered recently, e.g. diamond-chain, alternating linear chain, chains of triangle quantum cluster, sawtooth chain, orthogonal-dimer chain, e.t.c. Here we would like to emphasize one particular phenomena which is inherent to such a systems where left and right side neighboring of each cluster of quantum spins are non equivalent to each other. On the example of two systems, the sawtooth chain with quantum clusters of two spins and orthogonal-dimer chain with quantum cluster of three spins in triangular topology, we demonstrate the appearance of magnetization plateau at $M/M_{sat} = 1/4$ which is connected with breaking of translational symetry of the lattice, more precisely with the doubling of unit cell. Solving the problem of partition function calculation exactly we also obtain analytic expressions for free energy and all thermodynamic function, presenting the plots of magnetization processes for finite temperature displaying magnetization plateaus at $M/M_{sat} = 0, 1/4, 1/2$. Analyzing ground states properties we obtain $T = 0$ ground states phase diagrams with exact description of all transition lines and triple points.

Quantum criticality in multi-band superconductors

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In multi-band metals quasi-particles arising from different atomic orbitals coexist at a common Fermi surface. Superconductivity in these materials may appear due to interactions within a band (intra-band) or among the distinct metallic bands (inter-band). The orbitals are in general hybridized but the resulting bands keep the main features of the original orbitals. We introduce a new method to study this problem beyond the mean-field approximation. We calculate the response of the system to a fictitious space and time dependent field which couples to the superconducting order parameter. The appearance of superconductivity is related to the divergence of a generalized susceptibility. For a single band superconductor this coincides with the *Thouless criterion*. We show that for intra-band interactions a sufficiently strong hybridization (pressure) can destroy superconductivity at a SQCP. For inter-band interactions we found a zero temperature instability of the normal system as the Fermi wave-vectors mismatch of the bands is reduced, obtaining a continuous quantum phase transition to a PDW superconducting state. From the fluctuations close to the SQCP we obtain the dynamic critical exponent which control the power law behavior of the main thermodynamic and transport properties at the SQCP.

Financial Support: CNPQ, FAPERJ.

Bose-Einstein condensation in magnetic systems under strong field

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Abstract

At zero temperature and strong applied magnetic fields the ground sate of an anisotropic antiferromagnet is a saturated paramagnet with fully aligned spins. We study the quantum phase transition as the field is reduced below an upper critical H_{c2} and the system enters a XY-antiferromagnetic phase. Using a bond operator representation we consider a model spin-1 Heisenberg antiferromagnetic with single-ion anisotropy in hyper-cubic lattices under strong magnetic fields. We show that the transition at H_{c2} can be interpreted as a Bose-Einstein condensation (BEC) of magnons. The theoretical results are used to analyze our magnetization versus field data in the organic compound $NiCl_2$-$4SC(NH_2)_2$ (DTN) at very low temperatures. This is the ideal BEC system to study this transition since H_{c2} is sufficiently low to be reached with static magnetic fields (as opposed to pulsed fields). The scaling of the magnetization as a function of field and temperature close to H_{c2} shows excellent agreement with the theoretical predictions. It allows to obtain the quantum critical exponents and confirm the BEC nature of the transition at H_{c2}.

Superconducting Fluctuations, Pseudogap and Phase diagram in Cuprates

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We report transport measurements using pulsed magnetic fields to suppress the superconducting fluctuations (SCF) conductivity in a series of $YBa_2Cu_3O_{6+x}$ single crystals [1, 2]. These experiments allow us altogether to measure the temperature T'_c at which SCF disappear, and the pseudogap temperature T^*. While the latter are consistent with previous determinations of T^*, we find that T'_c is slightly larger than similar data taken by Nernst measurements. A careful investigation near optimal doping shows that T^* becomes smaller than T'_c, which is an unambiguous evidence that the pseudogap cannot be assigned to preformed pairs. Studies of the incidence of disorder on both T'_c and T^* allow us to propose a phase diagram including disorder which explains most observations done in other cuprate families, and to discuss the available knowledge on the pseudogap line in the phase diagram.

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Multiband character of the electronic structure and transport properties in the iron pnictides

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Multiband effects due to the presence of several small hole and electron pockets in the Fermi surface of Fe-pnictides are of prime importance to understand the evolution of their transport properties. We will present results of systematic Hall effect and resistivity studies in the $BaFe_2As_2$ system where Fe is substituted either by Co which results in electron doping [1] or by isovalent Ru which is expected not to change the ratio between electrons and holes [2]. We will show that electrons always dominate the transport properties in undoped and Co-doped materials, while contribution of the two types of carriers are clearly evidenced in Ru-substituted $BaFe_2As_2$. Using ARPES data obtained on the same samples [3,4], we are able to propose a coherent picture of the charge transport at low T in these compounds.

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Nanoscale electromechanical resonators as probes of the charge density wave transition in $NbSe_2$

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$NbSe_2$ undergoes an incommensurate charge density wave (CDW) phase transition around 35 K. Electron-phonon coupling leads to a distortion of the electron density and the lattice also undergoes a periodic deformation in the CDW state. Elastic and electronic aspects of this transition are studied at nanoscale using nanoelectromechanical (NEM) resonators. Suspended $NbSe_2$ flakes in field-effect transistor geometry are used as heterodyne mixers[1,2]. The output mixing current contains information about the resonant frequency (which depends upon the elastic modulus) of the device. Induced charges (q) modulate the conductance (G). The mixing current also depends upon the response of conductance to electrostatic gating, i.e., the factor dG/dq.

Thin flakes of $NbSe_2$ (thickness 35-50 nm) are obtained by mechanical exfoliation. Fig. 1a shows the scanning electron microscope image of a suspended flake, clamped by metallic electrodes which are made using electron beam lithography. A resonance-measurement plot is shown in Fig. 1b.

Detailed measurements were done by varying the temperature around 35 K to observe the characteristics of the CDW phase transition. The highlights of our observations (Ref. 3) are:

- Elastic modulus changes by 10 per cent at the CDW transition (Fig. 1c). This is an enormous change, exceeding by far the value reported in earlier studies of bulk $NbSe_2$ crystals[4].
- There is also a sharp change in elastic modulus at 18 K. No such anomaly had been reported in earlier experiments on bulk crystals.
- dG/dq reduces remarkably as the system crosses over from the CDW to the normal phase (Fig. 1d). This quantity can be related to the order parameter (energy gap at Fermi surface) which is non-zero in the CDW state. Power law fit to $dG/dq \sim (T_c - T)^{\beta}$ gives $\beta = 0.47$. This is very close to 0.5, the critical exponent of the order parameter in Ginzburg-Landau theory.
- dG/dq remains prominent and does not show any change at 7.2 K, when $NbSe_2$ becomes superconducting.

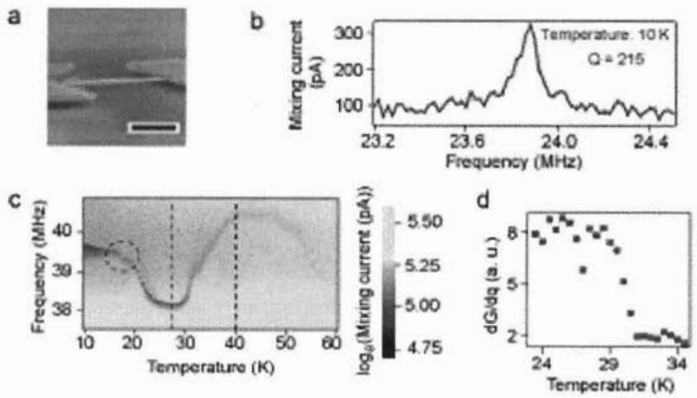

Fig. 1. a) Scanning electron microscope image of a suspended flake. Scale bar: 1μm. b) Plot of mixing current versus driving frequency at 10 K. Mechanical resonance is seen at 23.9 MHz with a quality factor of 215. c) Colourscale plot of mixing current as a function of driving frequency at temperatures near the CDW transition. d) dG/dq in arbitrary units near the CDW transition.

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Magnetic edge states in 2D metals.

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The structure of real 2D finite metallic systems (inversion layers, heterostructures etc) is investigated. The existence of so called static skin-layer along the sample border in practically all these systems is demonstrated. In presence of normal magnetic field the corresponding soft edge electron states (SES) along skin-layer area are developed. The properties of SES are discussed in front of the traditional edge states (ES) [1,2]. The applications of this activity to point contact [3] and Quantum Hall Effect problems [4] are proposed.

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Calculations of upper critical fields in strong-coupling superconductors near quantum criticality

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Several heavy fermion superconductors are located near magnetic quantum critical points (QCP) and the superconductivity can exhibit very interesting phenomena. For example, in noncentrosymmetric superconductors $CeRhSi_3$ and $CeIrSi_3$ near antiferromagnetic QCPs, very high upper critical fields H_{c2} up to 30 (T) are observed [1][2]. Such a value is surprisingly large compared to their transition temperature at zero field, $T_c \sim 1$ (K) . Unusual behaviors in H_{c2} are also seen in recently discovered ferromagnetic superconductor UCoGe [3][4]. There, H_{c2} along the a-axis is huge up to 15 (T), while the transition temperature is merely 0.6 (K). Another key property of H_{c2} in UCoGe is that H_{c2} along c-axis is lower than 1 (T), in spite of the fact that the easy axis of the magnetization is c-axis.

In this study, we examine H_{c2} near magnetic QCPs. For $CeRhSi_3$ and $CeIrSi_3$, we explain quantitatively the observed unusual behaviors in H_{c2}, and clarify the relation between the quantum criticality and the superconductivity [5]. For UCoGe, we use a simple model and show some properties in H_{c2} near a ferromagnetic QCP. With regard to the ferromagnetic spin fluctuations, it has been pointed out that there exist nonanalytic corrections in the susceptibility and the ferromagnetic phase transition is largely affected by them. Thus, we also investigate the effects of the nonanalytic corrections on the superconductivity.

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Magnons of the CE ordered phase of half-doped manganites

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Abstract

In 1955, Goodenough proposed the combined spin+charge+orbital ordering known as "CE"-arrangement as ground state for the perovskite Mn-oxides [1]. Here, planes with ferromagnetically ordered Mn ions along zig-zag chains couple antiferromagnetically, as do consecutive chains in a plane. The charge ordering of Mn^{3+}-Mn^{4+} ions is 2D-checkerboard in the planes, with identically charged planes stacked along the direction normal to them.

Colossal magnetoresistance and other applications of technological interest of these compounds, are thought to be related to the richness of their phase diagrams. Due to the strong competition between different phases, many questions remain open. Near half-doping, as in $Pr_{0.6}Ca_{0.4}MnO_3$, neutron diffraction results led to the proposal of dimer formation in the planes, periodically arranged along the chains [2], as an alternative to the CE phase.

One way to probe the magnetic ordering is to measure the magnetic excitations (such as magnons, by inelastic neutron scattering) and compare them with those characteristic of each proposed phase. In this work, describing the half-doped manganites in terms of a localized spin model, we calculate the magnon excitations of the CE phase for 3D-manganites, like $La_{1-x}M_xMnO_3$ where $M = Ca, Sr, Ba$, and for their 2D-laminar version $La_{0.5}Sr_{1.5}MnO_4$. We compare our results with the dimer phase magnons and with available experimental data on these compounds [3].

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How electronic correlations make Na_xCoO_2 a better thermoelectric

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Abstract — *In materials such as sodium cobaltate disorder and electron-electron correlation affect the electronic structure in a non-trivial manner. With the aim of treating both effects simultaneously, we develop an algorithm where disorder and correlation are considered on the same footing. Dynamical mean field theory (DMFT) models electron-electron correlation and the coherent potential approximation (CPA) is applied to describe a system with two non-equivalent and stochastically distributed lattice sites. The algorithm is then employed to compute the resistivity and the high thermopower of Na_xCoO_2. Understanding the reason for the thermoelectric properties of this material leads the way to new technical applications.*

1. LDA+DMFT+CPA Approach

For the computation of the non-interacting electron structure the local density approximation (LDA) is employed. The LDA bandstructure $\varepsilon_n(k)$ provides a first information of the transport properties, such as the group velocity $\nabla\varepsilon_n(k)$.

To account for correlation effects dynamical mean field theory (DMFT) is applied. In this scheme, the lattice problem is replaced by one site surrounded by a self-consistently determined electron bath, cf. Figure 1. In the picture of Feynman diagrams, DMFT corresponds to the inclusion of all irreducible local diagrams for the self energy which is therefore local in space $\Sigma(k,\omega) = \Sigma(\omega)$. To include correlations *and* disorder, we expanded the (existing) DMFT algorithm by means of coherent potential approximation (CPA), where the single site in the dynamic bath is replaced by two sites α, β with a difference $\Delta\varepsilon$ in on-site potentials connected to the same self-consistently determined dynamic mean field, cf. Figure 1. In the first step of the algorithm, two electronic propagators G_α, G_β corresponding to the two different sites are computed. Then, the total (frequency-dependent) Greens function reads

$$G(\omega) = x_\alpha G_\alpha(\omega) + (1 - x_\alpha) G_\beta(\omega). \qquad (1)$$

where $x_\alpha, x_\beta = 1 - x_\alpha$ is the stoichiometric occurrence of the sites α, β, respectively.

2. Numerical Results for Na_xCoO_2

Sodium cobaltate, which consists of trigonal sodium and cobaltate layers where oxygen atoms coordinate the Co atoms in distorted octahedra, shows a very large thermopower $\mathcal{O}(100\ \mu V/K)$ at room temperature in experiment [1]. The partial occupation of the Na sites gives rise to two inequivalent sites Co^{+3} (x_{Na}=x_α) and Co^{+4} (1-x_{Na}=x_β). From the LDA [2] we expect that the a_{1g} band is mainly responsible for transport which is modeled by a tight-binding approximation. In our analysis, we compare the resistivity ρ and the thermopower S for Na_xCoO_2 computed by our LDA+DMFT+CPA scheme with $U = 3.5$ eV and $\Delta\varepsilon = 0.55$ eV to experiment. To investigate the importance of disorder and correlation in this system, we expanded our study fixing $T = 290$ K and vary U and $\Delta\varepsilon$. The thermopower for $[U = 0, \Delta\varepsilon = 0]$ declines by 50 % when the disorder $\Delta\varepsilon$ is increased to 0.55 eV with no correlation U=0. A stronger disorder leads to an insulating phase due to alloy band splitting. On the other hand, increasing the disorder potential $\Delta\varepsilon$ for non-zero correlation $U = 3.5$ eV recovers the large thermopower with the maximal value at [U=3.5 eV,$\Delta\varepsilon = 0.8$ eV]. Thus, the combined effect of disorder and correlation appears essential for an explanation of the (thermo) electric properties in Na_xCoO_2.

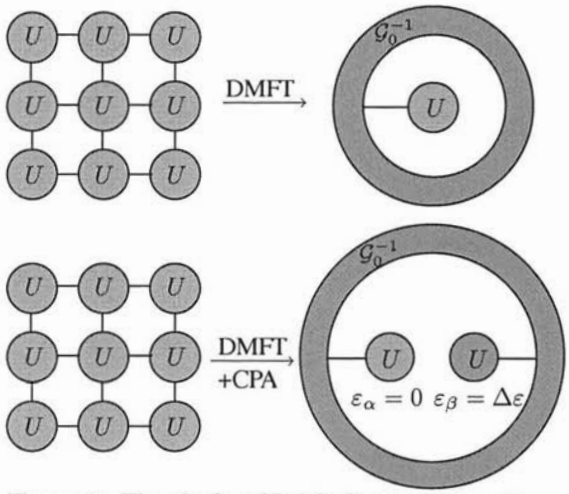

Figure 1: The single-orbital lattice problem with on-site Coulomb interaction U and the DMFT approximation (top) where one site with interaction U is coupled to a frequency-dependent and self-consistently determined mean field $\mathcal{G}_0^{-1}$ and the Coherent potential expansion of DMFT (bottom) where two sites α, β with on-site potential $\epsilon_\alpha = 0$ and $\epsilon_\beta = \Delta\varepsilon$, respectively, are coupled to the same dynamical bath $\mathcal{G}_0$.

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Magnetic properties of the Falicov-Kimball model with Hund coupling at half filling

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Abstract

A strongly correlated electron system was investigated where localized and itinerant electrons are interacting with the on-site Coulomb repulsion and the first Hund's rule force in an external magnetic field. The generalized Falicov-Kimball model with Hund coupling was used. The calculations were performed on the two-dimensional cluster of size 4x4 at half filling (one conduction electron per site) and two cases were considered: pure magnets and diluted magnets. By applying an external magnetic field and temperature both metamagnetic and order-disorder transformations were obtained for different model parameters. It appears that for the diluted system smaller values of magnetic field are needed to polarize spins of ions than conducting electrons. The magnetic transition temperature strongly depends on the Hund's coupling parameter and is much lower in diluted magnets than in pure magnets.

The Electronic Structure of low dimensional 3d transition metal systems

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The d-electrons have wave functions more localized near the atomic core, experience a larger correlation effect, and have much smaller energy dispersions and group velocities, exhibiting heavier electron masses. As the dimensions of samples decrease down to nanoscale, the study of electronic structure 3d electrons will shed light on expositing the correlated effect and understanding the relevant properties such as magnetism and superconductivity. In this poster, we will present the observations of 3d electrons structure of Fe impurities atoms and Cu atomic chains with angle-resolved photoemission. These investigations are compared and analyzed with *ab initio* calculations in the frame of electrons hybridization and correlation effect.

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