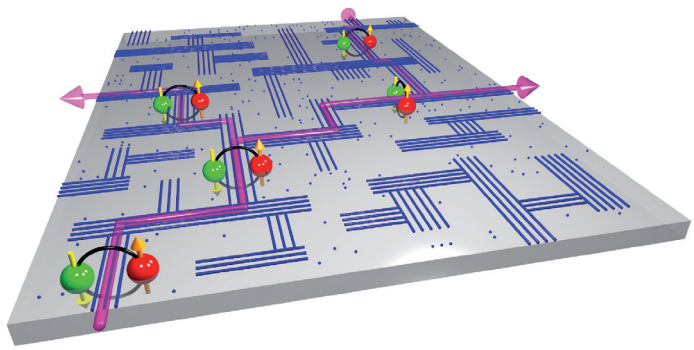
QUANTUM PHENOMENA IN COMPLEX MATTER 2011



edited by
N.L. Saini – A.R. Bishop – A. Bianconi

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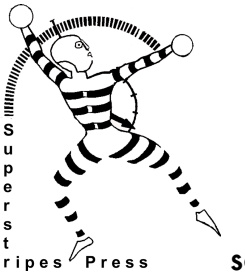

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Abstracts of selected advanced
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of the series on Stripes and High T_c
Superconductivity,

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CONTENTS

Preface

How to evade the temperature decoherence effects in a macroscopic quantum condensate is a major topic of modern physics. For 75 years from the discovery of superconductivity in Leiden in 1911 to 1986 the macroscopic quantum condensates in Fermi liquids "BCS condensates" and in Bose liquids "Bose-Einstein condensates" have been considered to be confined near zero temperature. The quantum mechanics world was considered to be confined at subatomic dimensions or at very low temperature. The macroscopic world of the life on the earth at the length scale ranging from nanometers to meters and in the temperature range between 270K and 370K was considered to be driven by classical mechanics.
The 1986 the discovery of high temperature superconductivity has falsified the assumption that a coherent macroscopic condensate cannot survive at high temperature opening a new road for the search of the Holy Grail: room temperature superconductors (RTS). The community looks for RTS to solve energy transport problems and for new quantum computers. Scientists search for the physical quantum laws giving macroscopic quantum phenomena at high temperature. Some scientists think that the new physical laws for high temperature superconductivity will help to elaborate new quantum theories for the emergence of coherence in living matter i.e. for a new Quantum Physics of Living Matter. The theoretical problem is so difficult that in spite of the large number of theoretical works they have not been able to provide predictions or to give directions or roadmaps for the experimental discoveries.
Beautiful inventions of new quantum matter have been made in these last 25 years. The quantum world emerges from deep low temperature to high temperatures by going from simple materials to complex materials.
Today after 25 years of experimental research the two Interlaken Dogmas assumed by the majority of scientists at the Interlaken first M^2S conference in 1988.

First Dogma*: "A single effective band"*
Second Dogma: *"Lattice effects are non relevant extrinsic effects"*
have been falsified by experimental facts.
A minority of scientists (few heretics that have not been accepting the Dogmas of the majority) has continued for 25 years their research show accumulating experimental facts that HTS is generated by the control of essential terms for developing the new general theory of HTS:
multiple electronic components,
proximity to a Bose condensation,
time fluctuations of the charge, spin and lattice degrees of freedom.
space fluctuations of the charge, spin and lattice degrees of freedom,
multiscale phase separation
unconventional multigap superconductivity,
the role of quantum size effects in the particular lattice architecture of the heterostructures at atomic limit
the shape resonances between different condensates proposed in 1993
Following this alternative views the electrons organize into collective textures (called stripes), which cannot be 'mapped' onto the electrons in ordinary metals. Understanding the properties of the material would then need quantum field theories of objects such as textures and strings, rather than point-like electrons. The local lattice distortions give large space and time scale deviations from the average crystalline structure ranging in the space scale from atomic scale to nanoscale to micron scale and in the time scale from fentaseconds to persistent out-of-equilibrium phases. These fluctuations can get self organized providing a complex rough energy

landscape for the multicomponet electronic systems driving the physics if high temperature superconductors close to the problems to be faced by a recent group of scientists aiming at developing a new Physics of Living Matter. For this reasons we have organized the 8th conference of the series of conferences on "Stripes and High T_c superconductivity" together with the symposium on "Quantum Physics of Living Matter".

The first international conference on "Stripes and High Temperature Superconductivity" was organized in December 1996 in Rome and the international scientific committee proposed to start a regular series of conferences on this topic in Rome. After 15 years we are at the 8th international conference of this series "Stripes 11" and the wide program of the conference shows the growing the scientific interest in the intrinsic complexity on high temperature materials. The main topics is the complexity of the electronic magnetic and lattice structure in these complex heterostructures at atomic limit (cuprates, borides, iron arsenide's and the very recently discovered iron calchogenides), and their common features with manganites, nikelates, and other complex materials. The unconventional multigap superconductivity in systems with multiscale phase separation appears to be a key feature reported by different experiments showing a complexity scenario.
Antonio Bianconi

The conference has been possible thanks to help of the Program Committee:

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I

L. H. Greene
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Detecting electronic order with point contact spectroscopy: Heavy-fermions to Fe-based superconducting and related materials

Laura H. Greene

Department of Physics and Frederick SeitzMaterials Research LaboratoryUniversity of Illinois at Urbana-Champaign, Urbana, IL, 61801 USA

lhgreene@illinois.edu

Point contact spectroscopy (PCS) has proven to be a powerful probe of the superconducting order parameter in conventional, novel, and unconventional superconductors. We have expanded this technique to detect other strongly-correlated states. In the Kondo lattice URu_2Si_2 we detect the Fano resonance and hybridization gap as a distinct double-peaked structure. In underdoped $Ba(Fe_{1-x}Co_x)2As2$ and $Fe_{1-y}Te$, PCS reveals a novel ordered region well above the magnetic and structural transition temperatures. The temperature onset of this gap-like feature in the conductance allows us to identify a new region in the underdoped side of the Co:Ba122 phase diagram. We relate our results to recent studies of electronic nematicity observed in these materials [1]. In honor of this centenary, I will start with a short history, and future prospects, of superconducting materials discovery. Then I will present an introduction to PCS, including how this versatile technique can be used to detect electronic structure, beyond the well-understood Andreev reflection in the superconducting state [2].

This work is in collaborationwith W.K. Park, H.Z. Arham, C.R. Hunt, Z.J. Xu, J.S. Wen, Z.W. Lin, Q. Li, G. Gu, P. H. Tobash, F. Ronning, E.D. Bauer, J.L. Sarrao, J.D. Thompson, J. Gillett, S. Sebastian, A. Thaler, S.L. Bu'dko, P.C. Canfield and is supported by the U.S. DOE: DE-FG02-07ER46453 and DE-AC02-98CH10886

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Electric Field Control of Interface Quantum Phases

Yoshi Iwasa
Quantum-Phase Electronics Center and Department of Applied Physics,
University of Tokyo, Tokyo 113-8656, Japan
Correlated Electron Research Group, RIKEN-ASI, Wako 351-0198, Japan
E-mail: iwasa@ap.t.u-tokyo.ac.jp

Heterogeneous interfaces are attracting growing interest as a platform for creation and control of novel properties and functions of materials. In this presentation, we discuss on the electric field control of superconductivity, spin states, and ferromagnetism at electrochemical interfaces formed of electrolyte liquids and solids, called electric double layer (EDL).
The EDL is regarded as a capacitor with nano-scaled thicknesses, where a large electric field exceeding 10 MV/cm = 1 V/nm can be generated. Because of this electric field, the amount of accumulated charges can be extremely high in comparison to the solid capacitor, and thus, the electric double layer capacitor is practically applied to charge accumulation devices. On the other hand, this high density charge accumulation may induce not only the conductivity change but also electronic phase transitions in solids. When additional electrodes are attached to the solids, one is able to monitor the electronic states through measurements of electrical conductivity. This device is a kind of field effect transistor, named as an electric double layer transistor (EDLT).
With the EDLT configurations, we have demonstrated electric field induced insulator-metal transition in ZnO, and superconductivity in $SrTiO_3$, ZrNCl, and $KTaO_3$. In addition to superconductivity, we show that EDLT can induce ferromagnetism at room temperature in magnetic semiconductor Co doped TiO_2. This work has been carried out in collaboration with H. T. Yuan, J. T. Ye, Y. Kasahara, M. Kawasaki, K. Ueno, A. Tsukazaki, T. Fukumura (University of Tokyo), H. Shimotani, T. Nojima, and S. Nakamura (Tohoku University).

Quantum Criticality and Superconductivity in Spin and Charge Systems

Siddharth Saxena [1,2,]
[1]*Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, Great Britain,*
[2]*Centre for Materials and Micro-systems, FBK, Trento, Italy*
email:montusaxena@gmail.com

This talk will focus on experimental search and discovery of novel forms of quantum order in metallic and insulating magnets, intercalated compounds, ferroelectric systems and multi-ferroic materials. Particularly discussed will be the pressure-induced superconductivity and critical phenomena in the vicinity of quantum phase transitions.
Materials tuned to the neighbourhood of a zero temperature phase transition often show the emergence of novel quantum phenomena. Much of the effort to study these new emergent effects, like the breakdown of the conventional Fermi-liquid theory in metals has been focused in narrow band electronic systems. Spin or Charge ordered phases can be tuned to absolute zero using hydrostatic pressure. Close to such a zero temperature phase transition, physical quantities like resistivity, magnetisation and dielectris constant change into radically unconventional forms due to the fluctuations experienced in this region giving rise to new kind superconductivity and other possible ordered states. Extension of this methodology to dipole-ordered insulating materials provides an interesting departure and new opportunities for both new physics and applications.

II

A. Bansil
A. Lanzara
S. Ming
D. Le Boeuf

A New Generation of Modeling Highly Resolved Spectroscopies: Cuprates, Pnictides and Topological Insulators

Arun Bansil
Physics Department, Northeastern University, Boston, Massachusetts
Email:bansil@neu.edu

I will discuss how as we move to model spectroscopic data from a qualitative to a quantitative level, surprising new insights into the nature of electronic states and correlation effects are obtained in high-temperature cuprate superconductors and other complex materials.[1-8] For example, in order to obtain a realistic description of various spectroscopies of the cuprates, one must include not only the effects of matrix elements but also of self-energy corrections beyond the LDA-based conventional picture, so that spectral features such as the high- and low-energy kink and the pseudopgap are accounted for properly. In this connection, we have developed a self-consistent, intermediate coupling scheme based on first principles band structures where effects of Hubbard U and d-wave superconductivity are included. The underlying spectrum is found to describe quite well the key doping and energy dependencies of ARPES, neutron scattering, inelastic x-ray scattering, STM and optical spectra of the cuprates. Illustrative examples in cuprates will be discussed. I will also comment on our recent work on the manganite, pnictides and topological insulators.

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A Pump Probe Angle-Resolved Photoemission Study of high temperature superconductors.

Alessandra Lanzara
Physics Department - University California, Berkeley
Materials Science Division, Lawrence Berkeley National Laboratory
alanzara@lbl.gov

Angle resolved photoemission spectroscopy (ARPES) has been a powerful tool in the study of high temperature superconductivity. Adding a new dimension, the time resolution, to these types of experiments will enable to study how the electronic structure evolves as the system re-equilibrates on femtosecond time scales.
Here we present one of the first experiments using ultra-high resolution angle-resolved photoemission spectroscopy to optically pump and probe an optimally doped $Bi_2Sr_2CaCu_2O_{8+x}$ superconductor. An unexpected suppression of the spectral weight following the pump laser excitation is observed. Its peculiar temperature dependence and the implication of this finding for superconductivity are discussed.

ARPES Studies of High-Temperature Superconductors

Ming Shi
Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland
Email: ming.shi@psi.ch

Angle-resolved photoemission spectroscopy (ARPES) has been proven to be a powerful tool for the investigation of electronic structure and energy gaps in high-temperature superconducting materials. In this talk I will present some of our recent ARPES results on cuprate and iron-based high-temperature superconductors. For cuprates, I shall show how the underlying Fermi surface, the superconducting and pseudogaps evolute from a highly underdoped samples to overdoped ones. I will also show that the superconducting transition temperature (T_c) is not related to the shape and size of the energy gap in the electronic excitation spectrum, but it controls the spectral weight of the coherence peaks at the gap edge. For pnictides, I will focus on high-resolution measurements of the superconducting gap, as a function of crystal momentum. Our results strongly suggest that the pairing mechanism of the pnictides is mainly driven by the short-range antiferromagnetic fluctuations, similar to the case of high-T_c cuprate superconductors.

The rise and fall of the electron pocket in hole-doped cuprates

D. LeBoeuf [1, 2*]N. Doiron-Leyraud[2], B. Vignolle[1], M. Sutherland[3], B. J. Ramhaw[4], J. Levallois[1], R. Daou[2], F. Laliberté[2], O. Cyr-Choinière[2], J. Chang2, Y. J. Jo5, L. Balicas[5], R. Liang[4], D. A. Bonn[4], W. N. Hardy[4] and L. Taillefer[2]

[1]*Laboratoire National des Champs Magnétiques Intenses, CNRS-INSA-UJF-UPS, Toulouse, France*
[2]*Département de Physique, Université de Sherbrooke, Sherbrooke, QC, Canada*
[3]*Department of Physics, University of Toronto, Toronto, ON, Canada*
[4]*Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada*
[5]*National High Magnetic Field Lab., Florida State University, Tallahassee, FL, USA*

D. LeBoeuf
[*]*email : david.leboeuf@lncmi.cnrs.fr*

The discovery of quantum oscillations in high-Tc cuprates both in the overdoped and underdoped regime revealed the dramatic evolution of the Fermi surface across the phase diagram. In the overdoped regime, the Fermi surface is found to be a large hole cylinder occupying 65 % of the first Brillouin zone. In contrast, the dominant frequency found in quantum oscillation experiments in the underdoped regime is small, indicating the presence of a Fermi pocket. The fact that this low frequency quantum oscillations were observed in a metallic state characterized by a negative Hall coefficient demonstrated that this pocket is electron-like. A Fermi surface reconstruction, occuring at a critical hole concentration between $p \sim 0.25$ and $p \sim 0.14$, where a translationnal symmetry breaking oreder sets in, is the standard mechanism to produce such a Fermi surface transformation.
I will present a study of the normal-state Hall effect measured in magnetic fields up to 60 T for dopings $0.078<p<0.152$, that brings new insights about the origin of the Fermi-surface reconstruction. For $p>0.08$, the Hall coefficient features a sign change as a function of temperature due to the emergence of an electron pocket. Below $p\sim0.08$, the Hall coefficient is positive down to the lowest temperature. We attribute this change of behaviour to the loss of the electron pocket through a possible Lifshitz transition at $p=0.08$. This Lifshitz transition is shown to trigger a sudden drop in the conductivity, reflecting the loss of the high-mobility sheet of the Fermi surface. The in-plane resistivity anisotropy also jumps at the Lifshitz transition. All these findings are consistent with a Fermi-surface reconstruction caused by a stripe order.

III

N. Hussey
M. Kartsovnik
U. Bovenspielen
T. Maier

Quantum oscillations in overdoped $Tl_2Ba_2CuO_{6+\delta}$ implications.

Nigel Hussey
University of Bristol niversity of Bristol, H. H. Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL , United Kingdom
Email: N.E.Hussey@bristol.ac.uk

We report a detailed quantum oscillation study of the overdoped cuprate $Tl_2Ba_2CuO_{6+\delta}$ at two different doping levels (T_c = 10 and 26 K). The derived Fermi surface size and topology complement earlier angle-dependent magnetoresistance studies and confirm the existence of a large quasi-cylindrical hole- doped Fermi surface with a small, but finite, c-axis warping. An accurate determination of the hole concentration reveals that superconductivity in $Tl_2Ba_2CuO_{6+\delta}$ does not follow the universal $T_c(p)$ parabola for cuprate families and survives up to a larger doping of pc = 0.31. The observation of quantum oscillations for both dopings demonstrates that Fermi-liquid behaviour is not confined to the edge of the superconducting dome, but is robust up to at least $0.3T_{cmax}$. Moreover, the observation of such well-resolved oscillations implies that the physical properties of overdoped $Tl_2Ba_2CuO_{6+\delta}$ are determined by a single, spatially homogeneous electronic ground state. Finally, analysis of the different quasiparticle masses points towards a purely magnetic or electronic pairing mechanism.

Magnetic Quantum Oscillations and the Fermi Surface in $Nd_{2-x}Ce_xCuO_4$

M. V. Kartsovnik[1*], T. Helm[1], C. Putzke[2], F. Wolff-Fabris[2], C. Proust[3], S. Lepault[3], I. Sheikin[3], A. Kiswandhi[4], E.-S. Choi[4], J. S. Brooks[4], and A. Erb[1]
[1]*Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany,*
[2]*Hochfeld-Magnetlabor Dresden, Dresden-Rossendorf, Germany,*
[3]*Laboratoire National des Champs Magnétiques Intenses, CNRS, Toulouse,*
[4]*National High Magnetic Field Laboratory, Tallahassee, USA*

M. V. Kartsovnik
[*]*e-mail: mark.kartsovnik@wmi.badw.de*

We present the current status of the Fermi surface studies using the Shubnikov-de Haas (SdH) effect in the electron-doped superconductor $Nd_{2-x}Ce_xCuO_4$. The SdH oscillations are observed in the interlayer magnetoresistance of optimally doped and overdoped crystals. The most prominent oscillatory component has a low frequency, between 250 and 300 T, depending on the doping level. It reveals cyclotron orbits enclosing ~ 1% of the first Brillouin zone area and is attributed to a small hole pocket produced by folding the original large Fermi surface due to a (π/a, π/a) superlattice potential. The persistence of the slow oscillations all the way up to x = 0.17 implies that the reconstructed Fermi surface survives over the whole superconducting doping range. However, the relevant energy gap is very small, ~10-20 meV, extrapolating to zero right at the edge of the superconducting dome. This is indicated by the presence of fast magnetic-breakdown oscillations detected at the highest fields for doping levels down to x = 0.15. Interestingly, the SdH effect is rapidly suppressed, as Ce concentration is reduced below the optimal level. This suggests that the Fermi surface undergoes a further transformation associated with a formation of a large gap closing the small hole pockets.

Keywords: electron-doped cuprate superconductor; Fermi surface; magnetotransport; Shubnikov-de Haas effect

III

Femtosecond time- and angle-resolved photoelectron spectroscopy of high-*T*c superconductors

U. Bovensiepen
Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany
uwe.bovensiepen@uni-due.de

Femtosecond laser pulses in the infrared and the ultraviolett spectral range were used as pump and probe pulses, respectively, and combined with angle-resolved photoelectron spectroscopy to time-resolved ARPES. This approach facilitates experimental information complementary to conventional ARPES because (i) it is sensitive to the optically excited state and (ii) scattering processes active in the relaxation of the excited state are probed in the time domain. In this talk recent experiments on superconducting optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and antiferromagnetic $EuFe_2As_2$ will be presented. In BSCCO we analyze the momentum-dependence of optically excited quasiparticles as a function of electron momentum. We find metastable quasiparticles in the antinodal region of the superconducting gap, which is explained by blocking of inelastic electron-electron scattering due to restriction in the scattering phase space in consequence of energy and momentum conservation. We conclude that quasiparticle relaxation is dominated by recombination into Copper pairs. In $EuFe_2As_2$ we focussed our attention on the antiferromagnetic phase and find momentum dependent scattering which is anisotropic for excited electrons and holes in the vicinity of the Fermi momentum. Above the Neel temperature this anisotropy vanishes which led to the conclusion that the essentially nesting of electron and hole pockets is probed in the antiferromagnetic state.

keywords: femtosecond laser pulses, angle-resolved photoemission, quasi-particle relaxation

Superconductivity in striped and multi-Fermi-surface Hubbard models: From the cuprates to the iron-based superconductors

T.A. Maier
Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, Oak Ridge National Lab, Oak Ridge, TN 37831, USA
maierta@ornl.gov

Hubbard models have been found to describe many of the complex phenomena that are observed in the cuprate and iron-based high-temperature superconductors. Simulations of these models therefore provide an ideal framework to study and understand the superconducting properties of these systems and the mechanisms responsible for them. Here, I will present dynamic cluster quantum Monte Carlo simulations of these models, which provide an unbiased view of the leading correlations in the system. In particular, I will discuss what these simulations tell us about superconductivity in the homogeneous 2D single-orbital Hubbard model, and how inhomogeneity in form of charge stripes affects this behavior. I will then describe recent simulations of a Hubbard model with multiple Fermi surface sheets similar to the iron-based superconductors, and conclude with a discussion of how to optimize electronic pairing in the search for room-temperature superconductors.

IV

I. Martin
G. Seibold
Y. Li
S. Ishihara

Spontaneous non-coplanar magnetism and anomalous Hall effect in itinerant magnets

Ivar Martin
Los Alamos Natl. Laboratory, Theoretical division, MS B262, Los Alamos NM ,USA
i-martin@lanl.gov

When electrons move in a magnetic material, their transport properties can be strongly affected by scattering off magnetic ions. Converse is also true: Itinerant electrons, through their interaction with magnetic ions, themselves can define the magnetic state into which the system orders at a low enough temperature. The resulting states are typically simple ferromagnetic, antiferromagnetic, or spiral, even though more complex states are known to emerge in the presence of spin-orbit interaction.
In this talk I will present several examples of two- and three-dimensional itinerant models that exhibit complex non-coplanar magnetism even in the absence of spin-orbit interaction. One of the most interesting manifestations of these states is a coherent topological effect of the non-coplanar magnetic orderings on electrons – similar to the Aharonov-Bohm effect – which leads to spontaneous Hall effect and ground-state electrical and spin currents. The equivalent strength of the orbital magnetic field can exceed 10^4 Tesla. Some examples of materials where these effects may be realized will be discussed.

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Magnetic structure of electronic inhomogeneities in cuprates Competition between stripes and spirals

G. Seibold[1], R. S. Markiewicz[2] and J. Lorenzana[3]
[1]*Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany*
[2]*Physics Department, Northeastern University, Boston MA02115, USA*
[3]*ISC-CNR and Dipartimento di Fisica, Università di Roma ``La Sapienza'', P. Aldo Moro 2, 00185 Roma, Italy*
G. Seibold
goetz@physik.tu-cottbus.de

The formation of spin and charge stripes is one of the scenarios in order to account for the formation of the pseudogap in cuprate superconductors. Whereas this kind of electronic inhomogeneity is now well established in lanthanum based cuprates the experimental situation in other compounds is less evident. Here we argue that the magnetic structure is strongly influenced by the next-nearest neighbor hopping parameter t' which distinguishes different families of cuprates. In particular our investigations, based on the unrestricted Gutzwiller approximation of the extended Hubbard model, indicate that uniform spirals get favored by a large t'/t ratio but are unstable at small doping towards stripes and checkerboard textures with spin canting. The structure of these inhomogeneities also depends on t'/t and the
associated spin currents may induce a small lattice distortion associated with local dipole moments.
We discuss a new kind of stripe which appears as a domain wall of the antiferromagnetic (AF) order parameter with a fractional change of the phase of the AF order. For large |t'/t| spirals can be stabilized under certain conditions in the overdoped regime which may explain the elastic incommensurate magnetic response recently observed in iron-codoped Bi2201 materials.
Keywords: stripes, spirals, cuprate superconductors

Unusual magnetic excitations in the pseudogap phase of a high-Tc superconductor

Yuan Li[1,2], V. Balédent[3], G. Yu[4], Yangmu Li[4], N. Barišić[4,5], K. Hradil[6], Ra.Mole[7], Y. Sidis[3], P. Steffens[8], X. Zhao[4,9], P. Bourges[3], M. Greven[4]
[1]*Max Planck Institute for Solid State Research, Stuttgart, Germany*
[2]*Department of Physics, Stanford University, Stanford, USA*
[3]*Laboratoire Léon Brillouin, CEA-CNRS, CEA-Saclay, Gif sur Yvette, France*
[4]*School of Physics and Astronomy, University of Minnesota, Minneapolis, USA* [5]*Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany*
[6]*Institut für Physikalische Chemie, Universität Göttingen, Göttingen, Germany*
[7]*Forschungsneutronenquelle Heinz Maier-Leibnitz, Garching, Germany*
[8]*Institut Laue Langevin, Grenoble CEDEX 9, France*
[9]*State Key Lab of Inorganic Synthesis and Preparative Chemistry, Jilin University, Changchun, China*

Yuan LI
Yuan.Li@fkf.mpg.de

Magnetic fluctuations might be essential to the mechanism of high-temperature superconductivity in the cuprates. For a long time, such fluctuations have been regarded as arising from the antiferromagnetic spin correlations within the copper-oxygen layers, and neutron scattering studies have mainly been carried out near the wave vector (1/2, 1/2). Following the recent demonstration of a universal "$q = 0$ antiferromagnetic order" in the pseudogap phase by spin-polarized neutron diffraction [1], our recent inelastic neutron scattering experiments on the model compound $HgBa_2CuO_{4+x}$ (Hg1201) revealed the existence of unusual magnetic excitations that weakly disperse throughout the entire Brillouin zone [2,3]. Like the $q = 0$ antiferromagnetic order, the new excitations are observed in the pseudogap phase and therefore appear to be associated with the order. The excitations have well-defined characteristic energies that are comparable to the resonance energy [4] and to those of electron-boson-coupling features observed in a wide range of cuprates, highlighting their possible influence on the electronic structure. These findings demonstrate that the pseudogap state is a distinct phase of matter rather than a mere crossover. They furthermore have the profound implication that a single-band description of the cuprates is insufficient.

Key words: HTSC, magnetic excitations, pseudogap

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Stripe-type charge order and electric polarization in complex oxides

Sumio Ishihara, M. Naka, and H. Takashima
Department of Physics, Tohoku University, Sendai, Japan
Sumio Ishihara
ishihara@cmpt.phys.tohoku.ac.jp

Ferroelectric material has spontaneous electric polarization induced by displacement of ion and electronic clouds. When electronic charges are ordered without inversion symmetry, a macroscopic electric polarization appears in a crystal. This new class of ferroelectricity is examined recently in a wide variety of the charge-ordered transition metal oxides and low-dimensional organic salts.

I will present recent our theoretical studies for the stripe-type charge order in polar complex oxides [1-4]. In particular, we focus on the electronic structure and dielectric properties in the rare-earth iron oxides $LuFe_2O_4$. This material is recognized as one of the charge-order type ferroelectric materials. We construct the electronic model Hamiltonian and analyze this by the numerical methods. It is shown that a three-fold stripe-type charge order associated with the electric polarization is stabilized by the thermal fluctuation at finite temperature and quantum fluctuation. This polar charge-order phase is more stabilized by the ferrimagnetic order. I will also talk about the charge dynamics in this novel charge ordered complex oxides and compare the recent x-ray scattering experiments.

key words: charge order, multiferroics, frustration
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V

G. Le Lay
C. Berger
L. Boeri
B. M. Andersen

Silicene epitaxial sheets

G. Le Lay[1,2*], P. Vogt[1,3], P. De Padova[2], C. Quaresima[2], B. Olivieri[4], J. Avila[5], E. Franzetzeskatis[5] and M.-C. Asensio[5]
[1]*CINaM-CNRS, Campus de Luminy, Case 913, F-13288 Marseille Cedex 09, France*
[2]*CNR-Istituto di Struttura della Materia, via Fosso del Cavaliere 100, 00133 Rome, Italy*
[3]*Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany*
[4]*CNR, Istituto di Scienze dell'Atmosfera e del Clima, via Fosso del Cavaliere, 00133 Rome, Italy*
[5] *Synchrotron SOLEIL - L'Orme des Merisiers Saint-Aubin - BP 48 91192 GIF-sur-YVETTE CEDEX*

G. Le Lay
**guy.lelay@univ-provence.fr*

The first synthesis of silicene, the all silicon analogue of graphene, theoretically conjectured recently [1], has just been reported upon *in situ* silicon deposition onto silver surfaces [2]. Graphene has not only unprecedented electronic properties but also a wealth of promising potential applications. Silicene, its sp^2-like hybridized silicon counterpart [3], might well be a challenger with the advantage of more easily fitting into the silicon based micro/nano- electronics industry. Indeed, silicene has essentially the same electronic properties as graphene, with, typically, the occurrence of massless Dirac fermions and a very high Fermi velocity [4]. Its robustness toward oxidation [5] reflects the stability of silicon nanotubes in air [6]. Prospects for the epitaxial growth of silicene on insulating substrates have been given [7]. The implications of these novel results for new physics and applications will be discussed.

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High mobility epitaxial graphene for graphene nanoelectronics

Claire Berger[1, 2], Ming Ruan[1], James Palmer[1], John Hankinson[1], Yike Hu[1], Edward Conrad[1], Walt A. de Heer[1]
[1] *CNRS- Institut Néel, Grenoble, France*
[2] *School of Physics, Georgia Institute of Technology, Atlanta GA 30332*
Claire Berger
claire.berger@physics.gatech.edu

Epitaxial graphene has demonstrated a great potential for novel electronic devices [1], with high electronic mobility (high speed transistors), good conductivity (interconnects), and conductance modulation by an electrostatic gate. High quality graphene on a scalable platform is a prerequisite. Here we show that high quality seamless epitaxial graphene layers can be grown on the entire surface of SiC substrates by thermal decomposition of the SiC crystal (Silicon Confinement Controlled method) [2]. A new structure is produced on the SiC(000-1) surface (C-face), that consists of a non-graphitic commensurate rotated stacking of the graphene layers. Transport (quantum Hall effect) and spectroscopy (Raman, ARPES and magneto-infra red) demonstrate that the integrity of the individual graphene layers is preserved due to an effective decoupling of the adjacent layers.
Planar graphene being a gapless semimetal, the opening of a band gap is required for digital electronics that calls for large switching ratios. Transport gaps have been demonstrated in chemical functionalized graphene or in narrow ribbons. But patterning techniques severely degrade graphene transport. We will present results on very narrow graphene ribbons down to 10 nm wide directly grown on silicon carbide substrate step edges at high temperature [3]. Evidence for ballistic transport on micron length scales is presented that opens the way to EG device architectures that rely on wave properties of the electrons, beyond diffusive electronics.
key words: graphene – nanoelectronics – transport

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Exotic Electron-Phonon Superconductivity in Solid Picene and Intercalated Hydrocarbons

A. Subedi[1], L. Boeri[1]
[1] *Max-Planck-Institute for Solid State Research, Stuttgart, Germany*

L.Boeri
L.Boeri@fkf.mpg.de

Carbon-based compounds offer many interesting examples of diverse superconducting behaviour, ranging from the conventional electron-phonon (ep) mechanism in intercalated graphites, to the much richer physics of alkali-intercalated fullerides. Recenlty, superconductivity with Tc's up to 18 K was reported in two alkali-doped polycyclic aromatic hydrocarbons: picene ($C_{22}H_{14}$), and phenanthrene ($C_{14}H_{10}$),[1] which can be seen as small fragments of graphene sheets.
In this work, we study the nature of superconductivity in doped solid picene, with linear response calculations of the phonon spectrum and electron-phonon (ep) interaction. [2]
We show that the coupling of the high-energy C bond-stretching phonon to the molecular orbitals is high enough to reproduce the experimental Tc within Migdal Eliashberg theory, for the experimental doping of 3 electrons/molecule. However, due its molecular nature, picene most likely belongs to the same class of strongly correlated ep superconductors as the fullerenes.[3]

Keywords: Carbon, new superconductors, electron-phonon interaction

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Disorder-induced stripes in the high-Tc superconductors

Brian Møller Andersen
Niels Bohr Institute University of Copenhagen Universitetsparken 5 DK-2100 Copenhagen Denmark
bma@fys.ku.dk

The cuprates materials are prone to exhibit inhomogeneous ground states due to strong electronic correlations. In addition, they can be made to superconduct by chemical doping which also disorders the samples. Modelling these complex materials therefore necessarily calls for inclusion of both correlations and random impurity potentials, leading to various theoretical real-space methods. In this talk I will review some of our recent work in understanding neutron and tunneling experiments based on such modelling. Also I will discuss the implications for the elusive pseudogap state and the emerging nematicity of these materials

VI

M. Oda
B. Fine
A. Piriou
T. Hasegawa
D. Popovic

Dichotomy of the Fermi surface in Bi2212: STM/STS and pump-probe optical experiments

M. Oda*[1], T. Kurosawa[1], Y. Toda[2], Y. H. Liu[1], Y. Kitajima[1], N. Momono[3] and M. Ido[1]
[1]*Department of Physics, Hokkaido University, Sapporo 060-0810, Japan*
[2]*Dpartment of Applied Physics, Hokkaido University, Sapporo 060-8628, Japan*
[3]*Department of Applied Sciences, Muroran Institute of Technology, Muroran 050-8585, Japan*

M. Oda
**moda@sci.hokudai.ac.jp*

The superconducting (SC) gap (SCG) and pseudogap (PG), which are formed mainly on the nodal and antinodal parts of the Fermi surface (FS), respectively, were examined by STM/STS and time-resolved optical pump-probe technique in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212). In STM/STS experiments, we observed an electronic charge order (ECO) accompanied by spatially inhomogeneous gap structure in the nanometer scale. For the spatial dependence of energy gap in STS spectra of the SC state, the high-bias gap, reflecting the PG on the antinodal part of the FS near (π, 0), is strongly inhomogeneous, while the low-bias bottom part of gap, reflecting the SCG on the Fermi-arc around the node point of the *d*-wave gap near ($\pi/2$, $\pi/2$), is very homogeneous; the inhomogeneous PG and homogeneous SCG coexist in the real space. The coexistence of PG and SCG was also revealed by the time-resolved optical pump-probe technique (Y. H. Liu *et al*., Phys. Rev. Lett. **101**, 137003 (2008)). From systematic STM/STS studies on the hole-doping (*p*) dependences of energy gaps, we also demonstrated the following results. 1) The SCG size Δ_{sc} at the edges of the Fermi-arc, which can be estimated from the bias voltage (energy) range of the homogeneous bottom part in STS spectra, follows the BCS relation between SCG and T_c for *d*-wave superconductors (T. Kurosawa *et al*., Phys. Rev. B **81**, 94519 (2010)), which is consistent with recent ARPES studies by Yoshida *et al*. (Phys. Rev. Lett. **103**, 37004 (2009)). 2) The gap inhomogeneity tends to be weaker with the increase of *p*. We will discuss the role of PG/ECO in the occurrence of the high-T_c cuprate superconductivity.

Implications of the spin vortex lattice scenario for muSR and NQR experiments in 1/8-doped lanthanum cuprates.

Boris Fine
University of Heidelberg Institute for Theoretical Physics Philosophenweg 19, 69120 Heidelberg, Germany
B.Fine@thphys.uni-heidelberg.de

Spin vortex lattice was proposed in [1] as a possible alternative to the stripe interpretation of spin and charge modulations in 1/8 doped lanthanum cuprates. We demonstrate that the spin vortex scenario leads to a singularity in the distribution of local magnetic fields, which should have observable implications for muSR and NQR experiments. The presence of this singularity is consistent with the strong oscillations of the muSR signals. These oscillations were previously considered as a strong indication in favor of the stripe interpretation. The NQR lineshapes predicted on the basis of the spin vortex scenario exhibit certain sharp features which, so far, have not been observed experimentally, but a similar discrepancy is even larger for the stripe interpretation. [1] B. V. Fine, Phys. Rev. B 75, 060504 (2007).

First direct observation of the Van Hove Singularity in the tunnelling spectra of cuprates

A. Piriou, C. Berthod, N. Jenkins, I. Maggio-Aprile, and Ø. Fischer.
Départment de la Matière Condensée, University of Geneva, Geneva, Switzerland.

A. Piriou
alexandre.piriou@unige.ch

In two-dimensional (2D) lattices, the electronic levels are unevenly spaced, and the density of states (DOS) displays a logarithmic divergence known as the Van Hove singularity (VHS). This is the case in particular for the layered cuprate superconductors. The scanning tunnelling microscope (STM) probes the DOS, and is therefore the ideal tool to observe the VHS. No STM study of cuprate superconductors has reported such an observation so far giving rise to a debate about the possibility of observing directly the normal state DOS in the tunnelling spectra. I will show that the VHS is unambiguously observed in our STM measurements performed on the cuprate $Bi_2Sr_2CuO_{6+\delta}$ (Bi-2201). I will analyse the behavior of parameters governing the shape of tunnelling spectra and its relation with what has been observed in other cuprates.
key words : cuprates, scanning tunnelling microscopy, Van Hove Singularity

Vortices in nano-size superconductors studied by low-temperature scanning tunneling microscopy / spectroscopy

Yukio Hasegawa*, Takahiro Nishio, T. Tominaga, T. An, and T. Eguchi
The Institute for Solid State Physics, the University of Tokyo *

Yukio Hasegawa
Email address: hasegawa@issp.u-tokyo.ac.jp

Vortices in mesoscopic superconductors, whose lateral size are in the same order as the coherence length, have attracted lots of attention as they show various unique configurations, such as a giant vortex and an anti-vortex, depending on their size and shape. In order to investigate their behaviors directly we have used ultrahigh vacuum low-temperature scanning tunneling microscopy / spectroscopy (STM/S) which works under high magnetic fields.
As a sample, we use nanometer-size Pb island structures formed on a Si(111) substrate whose typical sizes are 25-75 nm in radius, comparable with the coherence length (~ 30 nm), and 3 nm in thickness with an atomically flat-top surface. Spatial profiles of superconductivity and the vortex penetration / expulsion into / from the islands were directly observed through measurements of tunneling conductance at the zero bias voltage (ZBC), that is, one at the bottom of the superconducting gap. All processes including sample preparation/ characterization and the superconductivity measurements were performed *in situ* under UHV conditions, so that we can eliminate unwanted influences such as oxidation, contaminations or unknown structures.
We examined the lateral size dependence of critical magnetic fields for vortex penetration / expulsion and transition between the superconducting and normal states for various sizes of islands. It turned out that there is a minimum lateral island size for the vortex penetration. The experimentally obtained size dependences are consistent with that estimated by a theoretical analysis using the Ginzburg-Landau equations.

Key words: scanning tunneling microscopy, nano-size superconductors, vortices

Noise and Memory Effects in the Charge Response of Lightly Doped $La_{2-x}Sr_xCuO_4$

I. Raičević [1], *[1], C. Panagopoulos [2,3], T. Sasagawa [4]
[1]*National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, FL 32309, USA*
[2]*Division of Physics and Applied Physics, Nanyang Technological University, Singapore*
[3]*Department of Physics and FORTH, University of Crete, Greece*
[4]*Materials and Structures Laboratory, Tokyo Institute of Technology, Kanagawa, Japan*

Dragana Popović
**email :dragana@magnet.fsu.edu*

We present a study of the in-plane magnetotransport and resistance noise on lightly doped $La_{2-x}Sr_xCuO_4$ single crystals. Our data have revealed a number of glassy features in the charge response, such as hysteresis and memory effects in the magnetoresistance at temperatures well below the spin-glass transition temperature. The noise spectroscopy, performed also in the presence of the in-plane and out-of-plane magnetic fields, has revealed the onset of non-Gaussianity deep inside the spin-glass phase, suggesting that the charge dynamics becomes increasingly slow and correlated as temperature T approaches zero. The analysis of the higher order noise statistics provides evidence for the existence of a collective ground state of charge clusters ("cluster charge glass") located in CuO_2 planes, which seem to coexist with charge-poor antiferromagnetic domains that are frozen at such low T. The hysteresis and memory exhibited by the magnetoresistance are further used[†] as a practical tool to detect the underlying charge glassiness in $La_{2-x}Sr_xCuO_4$ thin films as a function of doping x that extends into the superconducting region. The evolution of the charge glass ground state with doping will be discussed.

[†]Work by X. Shi, D. Popović, C. Panagopoulos, G. Logvenov, A. Bollinger, and I. Bozovic.

Keywords: charge dynamics, complexity, cuprates

VII

S. Brazowski
T. Örd
M. Y. Kagan
G. A. Ummarino

Modeling of the ground state reconstruction by vortexes in nano-junctions of Charge Density Waves

Tianyou Yi[1], A. Rojo-Bravo[2], and S. Brazovskii[3*]
[1] *LPTMS, University Paris-Sud, Orsay, France* [2]*Boston University, USA* [3]*LPTMS, CNRS, Orsay, France*

S. Brazowskii
brazov@lptms.u-psud.fr

In charge density waves (CDW), the ground state can be adjusted by absorbing or ejecting pairs of electron or holes. The reconstruction proceeds via topologically nontrivial configurations: solitons and dislocations – the CDW vortexes. A recent experimental access to those states came from studies of nano-fabricated mesa-junctions, from the STM and from the coherent X-ray micro-diffraction. Following these requests, we performed a program of modeling stationary states and their transient dynamic for the CDW in restricted geometries. The model takes into account multiple fields in mutual nonlinear interactions: the phase and the amplitude of the CDW order parameter, distributions of the electric field, of the density and the current of normal carriers. Following events of creation and the subsequent evolution of dislocations, we find that vortexes are formed in the junction when the voltage across, or the current through, exceed a threshold. The number of vortexes remnant in the reconstructed ground state increases stepwise - in agreement with experiments. The vortex core concentrates the voltage drop across the junction giving rise to observed peaks of the inter-layer tunneling. The studied reconstruction in junctions of CDWs may be relevant to modern efforts of the field-effect transformations in other correlated electronic systems.
Key words: electronic crystal, CDW, nano-junction, field-effect, dislocation, vortex

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Correlation lengths in a two-band superconductor with intra- and interband couplings

T. Örd[*], K. Rägo
Institute of Physics, University of Tartu, Tartu, Estonia
[*]*teet.ord@ut.ee*

We study the peculiarities of correlations in superconducting ordering of a two-band system. The both intraband couplings, inducing superconductivity in the independent bands, and interband pair-transfer interaction have been taken into account. On the basis of the Ginzburg-Landau equations derived from the Bogoliubov-de Gennes equations and the relevant self-consistency conditions for a two-gap superconductor, one can distinguish two characteristic length scales in the correlation of superconducting fluctuations. One of these lengths as a function of temperature behaves critically diverging at the phase transition point. The other one remains finite and its temperature dependence is weaker. The formation of these length scales is caused by the interband interaction mixing the fluctuations of the superconducting order parameters of initially autonomous phase transitions in the non-interacting bands. The dependencies of the correlation lengths of the normal-phase fluctuations of order parameters on intra- and interband interactions have been analyzed.

Keywords: two-band superconductors, fluctuations, correlation lengths, intra- and interband interactions

Anomalous Resistivity and the electron-polaron effect in the two-band Hubbard model with one narrow band

M. Yu. Kagan[1], V.V. Val'kov[2]
[1]*P.L. Kapitsa Institute for Physical Problems, Kosygina st. 2, 119334 Moscow, Russia*
[2]*Kirenskii Institute of Physics, Akademgorodok 50, building 38,*
660036 Krasnoyarsk, Russia

M. Yu. Kagan
kagan@kapitza.ras.ru

We search for marginal Fermi-liquid behavior in the two-band Hubbard model with one narrow band. We consider the limit of low electron densities in the bands and strong intraband and interband Hubbard interactions. We analyze the influence of electron polaron effect and other mechanisms of mass-enhancement on effective mass and scattering times of light and heavy components in the clean case. We find the tendency towards phase-separation in a 3D case for large mismatch between the densities of heavy and light bands in a strong coupling limit. We also observe that for low temperatures and equal densities the resistivity in a homogeneous state $R(T) \sim T^2$ – behaves in a Fermi-liquid fashion both in 3D and 2D cases. For temperatures higher then effective bandwidth for heavy electrons $T > W_h^*$ the coherent behavior of heavy component is totally destroyed. The heavy particles move diffusively in the surrounding of light particles. At the same time the light particles scatter on the heavy ones as if on immobile (static) impurities. In this regime the heavy component is marginal, while the light one is not. The resistivity goes on saturation for $T > W_h^*$ in the 3D case. In 2D the resistivity has a maximum and localization tail due to weak – localization corrections of Altshuler – Aronov type. Such behavior of resistivity in 3D could be relevant for some uranium-based heavy-fermion compounds like UNi_2Al_3 and in 2D for some other mixed-valence compounds possibly including the layered manganites. We also consider the superconductive (SC) instability in the model. The leading instability is towards p-wave pairing and is governed by enhanced Kohn – Luttinger mechanism of SC at low electron density. The critical temperature is mostly governed by the pairing of heavy electrons via polarization of the light ones in 2D. However the two SC gaps in heavy and light bands are opened simultaneously below this temperature.

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Multiband *s*± Eliashberg theory and temperature-dependent spin-resonance energy in iron pnictide superconductors

G.A. Ummarino

Dipartimento di Fisica and CNISM, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

G.A. Ummarino

giovanni.ummarino@infm.polito.it

The phenomenology of iron pnictide superconductors can be explained in the framework of a three-band $s\pm$ wave Eliashberg theory with only two free parameters plus a *feedback effect*, i.e., the effect of the condensate on the antiferromagnetic spin fluctuations responsible for the superconductivity in these compounds. I have examined the experimental data of four materials, $LaFeAsO_{1-x}F_x$, $SmFeAsO_{1-x}F_x$, $Ba_{1-x}K_xFe_2As_2$, and $Ba(Fe_xCo_{1-x})_2As_2$,and I have found that it is possible to reproduce the experimental critical temperature and gap values in a moderate strong-coupling regime, $\lambda_{tot} \approx 1.7 - 2.0$.

key words multiband Eliashberg theory, iron pnictide, spin-resonance energy

VIII

P. Carretta
H. Julien
S. D. Conradson
B. Sacépé
L. Baldassarre

Frustration in spin-diluted pnictides, vanadates and cuprates

P.Carretta[1], G.Prando[1], P.Bonfà[1], L.Bossoni[1], S.Sanna[1], R.De Renzi[2]
[1] *Department of Physics "A. Volta", University of Pavia-CNISM, I-27100 Pavia, Ital*
[2] *Department of Physics, University of Parma-CNISM, I-43124 Parma, Italy*

P.Carretta
e-mail: pietro.carretta@unipv.it

The theoretical modelling of iron pnictides is presently attracting significant debate. One of the crucial aspects that has been realized since the early days is that in these systems comaprable nearest and next-nearest neighbour hopping integrals could lead to the frustration of the exchange coupling among the iron magnetic moments. Accordingly, the J_1-J_2 model on a square lattice has been tentatively used to describe the magnetic ground-state of these materials [1]. Here, by means of NMR, μSR and magnetization measurements, we show that the main properties of the spin-density-wave phase in spin-diluted $LaFe_{1-x}Ru_xAsO$ can be suitably described by the S=1/2 J_1-J_2 model on a square lattice (QJ1J2SL) and that many similarities with the behaviour observed in $Li_2V_{1-x}Ti_xSiO_4$ [2], a prototype of spin-diluted QJ1J2SL, are found. Moreover, we will show that in S=1/2 systems on a square lattice where frustration is absent a priori, as it is the case of La_2CuO_4, spin dilution can give rise to frustration [3].

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keywords: frustration, pnictides, quantum spin systems

Magnetic-field-induced stripe order in $YBa_2Cu_3O_y$

T. Wu[1], H. Mayaffre[1], S. Krämer[1], M. Horvatic[1], C. Berthier[1], W.N. Hardy[2], R. Liang[2], D.A. Bonn[2], M.-H. Julien*[1]
[1]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France. [2]University of British Columbia, Vancouver, Canada.
M.-H. Julien
marc-henri.julien@lncmi.cnrs.fr

In the search of the broken-symmetry state inferred from quantum oscillation and other transport measurements, we undertook high magnetic field NMR experiments in ultra clean, oxygen-ordered, untwined single crystals of $YBa_2Cu_3O_y$. We find that the translational symmetry breaking does not arise from the magnetic order anticipated by most of us, but from a unidirectional charge-ordered state. Because it occurs only in strong magnetic fields oriented along the crystalline c-axis, this charge order appears to compete with superconductivity. While two (orthogonal) ordered patterns are technically compatible with NMR spectra, we argue that the charge ordered state is most likely the 4a-periodic stripe phase. Nevertheless, we provide evidence that the stripe order remains partly fluctuating down to low temperatures. While the charge order is visibly pinned here by CuO chains, its occurrence at doping levels near 1/8 hole/Cu in a noticeably cleaner cuprate than e.g. $La_{2-x}Ba_xCuO_4$, strengthens the idea that stripe correlations are a generic propensity of charges in the CuO_2 planes of hole-doped cuprates.

Key words : stripes, NMR, high fields, quantum oscillations, competing order

Dynamical Processes in Hypervalent Urania

Steven D. Conradson,[1] A. David Andersson,[1] Francisco J. Espinoa-Faller,[2] Mary B. Martucci,[1] Jose Mustre de Leon,[3] Gerald T. Seidler[4]
[1]*Material Science and Technol. Div., Los Alamos National Lab-, Los Alamos, NM 87545 USA*
[2]*Department of Engineering, University Marista de Merida, Merida, Yucatan, Mexico*
[3]*Department of Physics, CINVESTAV-IPN, Universidad Merida, Merida, Mexico*
[4]*Physics Department, University of Washington, Seattle, WA 98105 USA*

Steven D. Conradson
conradson@lanl.gov

One of the more intriguing aspects of high temperature superconductors and related complex correlated materials was the observation of intrinsic dynamics: their polarons involved multiple atoms in degenerate arrangements and the charge and coupled lattice distortion tunneled between these equivalent configurations so that they were always in motion. This was originally contentious because at that time the extent to which experimental results – and certainly not direct structural measurements – reflected the time and energy domain of the measurement was not yet fully realized, so there was substantial controversy about the different structures measured by diffraction, pair distribution function analysis, and XAFS.[1] This phenomenon is now at least documented[2] if still not universally appreciated and understood. Using a combination of XAFS and x-ray and neutron scattering, we have now identified this process in hypervalent urania, UO_{2+x}, over its full fluorite rangea through U_3O_7. However, relative to cuprates, the charge inhomogeneity here is a "superpolaron." The differ-ence in the U-O bond between its two modes is >30% in comparison with the 6% found for cuprates, most likely because it also involves a complete change in the bonding and two electrons. Furthermore, because of the nature of the uranyl species, the spatial extent and the number of atoms involved in should be much larger than in the polarons in first row transition metal compounds. This difference and the simplicity of the structure and compo-sition of UO_2 provide an opportunity to better elucidate the intrinsic dynamics process. One previously neglected aspect in the structure measurements that is quite prominent for UO_{2+x} is the changes in the anharmonicity, reflected in the widths and areas of the peaks and possible interchange between the peaks and a more diffuse atom density component. The x-ray measurements that exhibit the multisite U-O distributions also display much greater increases in the widths of the U-U pairs, while in contrast the neutron pdfs show a much larger increase in the baseline.

However, the most potentially exciting characteristic is the electronic structure. The description of polaron tunneling[2] predicted that some of the electronic states would be modified by the retardation of the electronic motion because of its strong coupling to the atomic motion. The O K XAS of these materials shows no evidence of inhomogenous broad-ening, suggesting the paradox of disorder in the crystal structure but fully ordered electronic states. This is substantially different from the original predictions, which only found a tendency in the lower energy excited states to form polarons spontaneously, and therefore points to new physics. The increase in the excited state lifetimes with increased pump power in time resolved pump-probe reflectivity measurements is, however, consistent with interactions between the polarons. It is therefore possible that the electronic structure is modified not only by the tunneling but also by collective and cooperative effects. Real space calculations do show binding of mobile charges by charge inhomogeneity aggregates, and we are currently evaluating the local densities of electronic states in these types of systems.

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Localization of preformed Cooper-pairs in disordered superconductors

B. Sacépé[1*], T. Dubouchet[2], C. Chapelier[2], M. Sanquer[2], M. Ovadia[3], D. Shahar[3], M. Feigelman[4], L. Ioffe[5]

[1]*Institut Néel, CNRS & Université Joseph Fourier, Grenoble, France*

[2]*SPSMS, CEA-Grenoble, Grenoble, France*

[3]*Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel*

[4]*L.D. Landau Institute for Theoretical Physics, Moscow, Russia*

[5]*Department of Physics and Astronomy, Rutgers University, Piscataway, USA*

B. Sacépé

**Benjamin.sacepe@cnrs.grenoble.fr*

The concept of localized Cooper pairs in disordered superconducting films close to the Superconductor-Insulator Transition (SIT) has intrigued scientists for several decades both theoretically and experimentally. Although the interplay of localization and superconductivity has been clearly evidenced on the macroscopic scale by transport measurements, very little is known about the microscopic details of the strong disorder limit. In this talk I will present tunneling measurements of the local density-of-states on amorphous indium oxide films close to the SIT [1]. Our results show that disorder fluctuations lead to a mixture of superconducting and insulating regions that distinguish themselves by the presence or absence of coherence peaks at the gap edges. This finding as well as other striking anomalies such as the presence of a strong pseudogap above T_c will be discussed regarding recent theories of superconductivity close to the mobility edge that interpret such a gapped state without coherence peak as the spectral signature of localized Cooper pairs.

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Metal to Insulator Transition and Phase separation in Cr-doped V_2O_3

L. Baldassarre[1], A. Perucchi[1], D. Nicoletti[2], B. Mansart[3], E. Papalarazou[3], M. Marsi[3] and S. Lupi[2]

[1]*Sincrotrone Trieste S.C.p.A., Area Science Park, I-34012 Basovizza, Trieste, Italy*
[2]*CNR-IOM and Dipartimento di Fisica, Università di Roma 'La Sapienza', Piazzale A. Moro 2, I-00185 Roma, Italy.*
[3]*Laboratoire de Physique des Solides, CNRS-UMR 8502, Université Paris-Sud, F-91405 Orsay, France.*

L. Baldassarre
leonetta.b@gmail.com

The spontaneous emergence of phase separation, and the existence of many competing states are often associated with complex matter such as soft or biological systems. Recently, an increasing number of investigations showed that several transition metal oxides also form electronic non-homogeneous states, in particular when competing interactions - charge, spin, lattice- take place. Intriguing examples include CMR effect in manganites, or the spin and charge stripes in cuprates.
Here we report on the showcase-system for the Mott transition, Cr-doped V_2O_3, where temperature or pressure induce a first-order transition between a paramagnetic insulator (PI) to a paramagnetic metal (PM).
We have studied the MIT in Cr-doped V_2O_3 with submicron lateral resolution: We show that with decreasing temperature, microscopic domains become metallic and coexist with an insulating background. This explains why the associated PM phase is actually a poor metal. The phase separation can be associated with a thermodynamic instability near the transition. This instability is reduced by pressure, that promotes a genuine Mott transition to an eventually homogeneous metallic state.

key words: Phase Transition, Mott Insulator, Phase Separation

IX

J. E. Hirsh
P. Phillips
A. Chubukov
A. Bianconi

Correcting 100 years of misunderstanding: electric fields in superconductors, hole superconductivity, and the Meissner effect

J.E. Hirsch
Department of Physics, University of California San Diego
jhirsch@ucsd.edu

From the outset of superconductivity research it was assumed that no electrostatic fields could exist inside superconductors, and this assumption was incorporated into conventional London electrodynamics. Yet the London brothers themselves initially (in 1935) had proposed an electrodynamic theory of superconductors that allowed for static electric fields in their interior, which they unfortunately discarded a year later. I argue that the Meissner effect in superconductors *necessitates* the existence of an electrostatic field in their interior, originating in the expulsion of negative charge from the interior to the surface when a metal becomes superconducting. The theory of hole superconductivity predicts this physics, and associated with it a macroscopic spin current in the ground state of superconductors ("Spin Meissner effect"), qualitatively different from what is predicted by conventional BCS-London theory. A new London-like electrodynamic description of superconductors is proposed to describe this physics. Within this theory superconductivity is driven by lowering of quantum kinetic energy, the fact that the Coulomb repulsion strongly depends on the character of the charge carriers, namely whether electron- or hole-like, and the spin-orbit interaction. The electron-phonon interaction does not play a significant role, yet the existence of an isotope effect in many superconductors is easily understood. In the strong coupling regime the theory appears to favor local charge inhomogeneity. The theory is proposed to apply to all superconducting materials, from the elements to the high T_c cuprates and pnictides, is highly falsifiable, and explains a wide variety of experimental observations.

Mottness and Holography

P. Phillips, M. Edalati, S. Hong, R. Leigh, and Ka-Wai Lo
Department of Physics, Univ.Illinois, Urbana-Champaign, Il.

Twentyfive years the discovery of superconductivity in the copper-oxide ceramics (hereafter cuprates), the central problem remains the anomalous properties of the normal state. The key anomaly is the strange metal in which the resistivity scales as a linear function of temperature rather than the characteristic quadratic dependence of Lev Landau's standard theory of metals. I will present two approaches to this problem. In the first, I will show that correctly integrating out the high-energy physics results in a new degree of freedom at low energies that mediates T-linear resistivity and is also capable of describing the evolution from Fermi arcs at low doping to a big Fermi surface at high doping. In the second, I will show that a class of bottom-up gravitational models exhibits some of the key ingredients of cuprate physics, including UV-IR mixing, thye dynamical generation of a gap and strange metal behaviour. The latter opens the possibility that holography can uncloak the nature of strong correlations in the Mott state. [1]

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Symmetry and structure of the superconducting gap in Fe-based superconductors

Andrey Chubukov
The University of Wisconsin, Madison, Department of Physics, 1150 University Ave., Madison WI 53706-1390, USA
chubukov@physics.wisc.edu

Lattice complexity and shape resonances in multigap superconductors: chalcogenides, pnictides, diborides and cuprates

Antonio Bianconi
Department of Physics, Sapienza University of Rome, 00185 Rome, Italy

The shape resonance provides a possible mechanism for evading temperature decoherence effects in a quantum condensate [1-4]. The shape resonance in the superconducting gaps is basic quantum phenomenon determined by interference between quasi-bound and continuum states introduced by Majorana-Fano-Feshbach theories popular in Bose or BCS condensation in ultra-cold gases. In multigap superconductors the shape resonances provide an exchange pairing mechanism (a contact non retarted interaction) mixing a Bose condensate with a BCS condensate in different real and/or k-space locations that could coexist with intraband electron-phonon mechanisms. The shape resonance mechanism for the amplification of the critical temperature appears to be common in cuprates [5,6] pnictides, [7,8] diborides [9] and recently in chalcogenides although the large differences between these materials. Shape resonances appear in systems made of multiple components, where the Fermi level is tuned near a Lifshitz critcal point in one of the bands. The complexity of the electronic and lattice phase of these materials arises because the system is in the verge of a catastrophe i.e. near a critical point for an arrested first order phase transition as shown in superoxigenated La_2CuO_{4+y} [10,11] showing scale free structural organization and dynamics of percolating striped domains of oxygen interstitials favoring the high T_c phase. Recent results in KFeSe superconductors: evidence of frustrated phase separation, percolating superconductivity, competing with percolating magnetism and shape resonances in the superconducting gaps in concentric Fermi surfaces will be reported.

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X

A.R. Bishop
M. Arndt
A. Patel

Gene Sequence Control of Conformational Structure and Functions in DNA

Alan Bishop
Los Alamos National Laboratory, P.O. Box 1663, MS-B210, Los Alamos, NM 87545 USA
Email: arb@lanl.gov

Establishing the general and promoter-specific mechanistic features of gene transcription initiation requires improved understanding of the sequence-dependent structural/dynamic features of promoter DNA. Experimental data suggest that a spontaneous DNA strand separation at the transcriptional start site is likely to be a requirement for transcription initiation in several promoters. We describe our progress in using simulations of an effective nonlinear model to analyze the strand separation (bubble) dynamics of certain promoter DNA sequences. We argue that three dynamic criteria, bubble probability, bubble lifetime, and average strand separation, are needed to characterize bubble formation at the transcriptional start sites of a set of mammalian gene promoters. We observe that the most stable (longer lifetime) DNA openings do not necessarily coincide with the most probable openings and the highest average strand displacement, underscoring the advantages of accurate molecular dynamic simulations. The dynamic profiles of the tested mammalian promoters differ significantly in overall profile and bubble probability, but the transcriptional start site is typically distinguished by large (longer than 10 base pair) and long-lived transient openings in the double helix. In strong support of our simulation based arguments, our experimental transcription data demonstrate that an artificial bubble-containing DNA template is transcribed bidirectionally by human RNA polymerase alone, in the absence of any other transcription factors. We also describe recent extensions of our approach to very large DNA sequences, and to the potential effects of THz radiation on DNA conformations and expressions.

Work performed with B Alexandrov and K Rasmussen (Los Alamos), A Usheva (Harvard Medical School)

Macroscopic coherence of large organic molecules: from fundamental quantum phenomena to measurements of molecular properties

Arndt Markus
University of Vienna, A-1090 Wien , Austria
markus.arndt@univie.ac.at

I shall present recent advances in experiments on quantum interferometry with large organic molecules. They demonstrate that even complexes composed of several hundred atoms, delocalized over several hundred nanometers can maintain center-of-mass coherence over more than one millisecond when appropriately prepared and protected from the environment. The instruments used in demonstrating the quantum wave nature of large organic molecules can now also be used to measure internal molecular properties, too.

A Wave Model for Efficient Energy Transport in Photosynthesis

Apoorva Patel
CHEP and SERC, Indian Institute of Science, Bangalore-560012, India
E-mail: adpatel@cts.iisc.ernet.in

Recently it has been discovered—contrary to expectations of physicists as well as biologists— that the energy transport during photosynthesis, from the chlorophyll pigment that captures the photon to the reaction centre where glucose is synthesised from carbon dioxide and water, is highly coherent even at ambient temperature and in the cellular environment. By looking at the process from the computer science view-point, we can analyse what has been optimised and how. The hardware needs to be stable against environmental decoherence, a.nd the software corresponds to the spatial search algorithm. Both of these can be realised in the framework of wave computation. The physical properties of the light harvesting antennae that can implement wave computation are described.
As a concrete example, a coupled oscillator model based on robust features of wave dynamics is presented. It implements the spatial search algorithm with nearest neighbour coupling and a reflection oracle. In analogy with Grover's algorithm, its dynamics concentrates the energy of the system at the target location. Furthermore, the trapping mechanism of a resonating cavity increases the duration of the energy peak at the target location. Geometry and connectivity of the coupled oscillators are the features to be optimised, while the resonance condition has tobe met to make the process highly efficient.
These algorithmic requirements can be tested against what is observed in case of the light harvesting antennae.

Keywords: Light harvesting antenna, Decoherence, Spatial search, Wave computation, Coherent state, Resonating cavity.

XI

H. Takahashi
V. Hinkov
H. Aoki
J. Lorenzana

High- pressure studies for hydrogen substituted $CaFeAsF_{1-x}H_x$, and $SmFeAsO_{1-x}H_x$

H.Takahashi,[1,2], T. Tomita[1,2], H. Soeda[1], M. Ebata[1], T. Hanna[3], Y. Muraba[3], S. Matsuishi[3], H. Hosono[3,4]

[1]*Department of Physics, College of Humanities and Sciences, Nihon University, Tokyo, Japan*
[2]*Transformative Research-Project on Iron Pnictides (TRIP), Japan Science and Technology Agency (JST), Tokyo, Japan*
[3]*Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Japan*
[4]*Frontier Research Center, Tokyo Institute of Technology, Yokohama, Japan*

H.Takahashi
hiroki@chs.nihon-u.ac.jp

Hydrogen substituted $CaFeAsF_{1-x}H_x$ and $SmFeAsO_{1-x}H_x$ have been successfully synthesized very recently[1]. Neutron diffraction measurements demonstrated that these hydrogen atoms are incorporated as H^- ions at the F^- sites in $CaFeAsF_{1-x}H_x$ and the O^{2-} sites in $SmFeAsO_{1-x}H_x$, respectively. CaFeAsF is a semimetal and exhibits structural and magnetic phase transitions at ~110 K. These phase transitions are suppressed with Co substitution for Fe and the superconductivity appears at 22 K with Co concentration of 10%. Co doping is considered to be electron doping. In $CaFeAsF_{1-x}H_x$, those phase transitions are suppressed a little with H substitution from x = 0 to 1. Superconductivity does not appear with H substitution, because the isovalent substitution does not affect largely the electronic state. However, for CaFeAsF structural and magnetic transitions are suppressed by pressure and pressure-induced superconductivity appears at 28 K at ~5 GPa. In this study electrical resistivity measurements under high pressure were carried out, in order to investigate the superconducting properties for H substituted materials. High-pressure experiments for CaFeAsH revealed that the structural and magnetic transitions were suppressed rather steeply by pressure and pressure-induced superconductivity was confirmed at 28 K at 3 GPa. The pressure where the pressure-induced superconductivity appears is smaller than the case of CaFeAsF. High-pressure x-ray diffraction is now in progress to decide the crystal structure under high pressure. Pressure effect for $SmFeAsO_{1-x}H_x$ will be also presented.

(keyword: high pressure, H^- ions, $CaFeAsF_{1-x}H_x$, $SmFeAsO_{1-x}H_x$)

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Universal correlation between the pairing strength and T_c in iron-arsenide and cuprate superconductors

V. Hinkov[1,2], D. S. Inosov[1], J. T. Park[1], B. Keimer[1], Y. Li[1]
[1] *Max-Planck-Inst. for Solid-State Research, Heisenbergstr. 1, Stuttgart, Germany*
[2] *Department of Physics, University of British Columbia, Vancouver, Canada*

V. Hinkov
Email: hinkov@fkf.mpg.de

Superconductors are classified by their pairing mechanism and by the pairing strength, measured as the ratio of the superconducting gap, 2Δ, and the critical temperature, T_c. Conventional phonon-mediated superconductors are characterized by relatively weak pairing and low critical temperatures, whereas in layered high-T_c cuprates much stronger pairing is mediated by alternative, most likely magnetic, interactions. Therefore, we usually consider these two classes of materials as clearly distinct. Recently, a constant $2\Delta/T_c$ ratio, independent of the transition temperature, has been suggested for the newly discovered iron pnictides.

In my presentation I will first discuss an extensive comparison of previously published pairing strengths among many single- and multiband superconductors, encompassing simple metals, high-T_c cuprates and Fe-based compounds. For Fe- and Cu-based materials, our analysis [1,2] shows that $2\Delta/k_BT_c$ *does* depend on the transition temperature, and it reveals a universal *correlation* between the gap ratio and T_c which is not found in conventional superconductors and therefore supports a common unconventional mechanism for Cooper pairing in both families. The gap ratio in ferropnictides ranges from weak, near the limit predicted by the Bardeen-Cooper-Schrieffer theory, to strong, like in cuprates. Ferropnictides therefore bridge the gap between these two extremes. Our comparison emphasizes the internal differences within the Fe-based family and places it as a "missing link" between conventional and high-T_c superconductors.

Then I will point out the connection of these findings with the doping and momentum dependence, as well as the dimensionality, of the neutron magnetic resonance in the iron arsenides.

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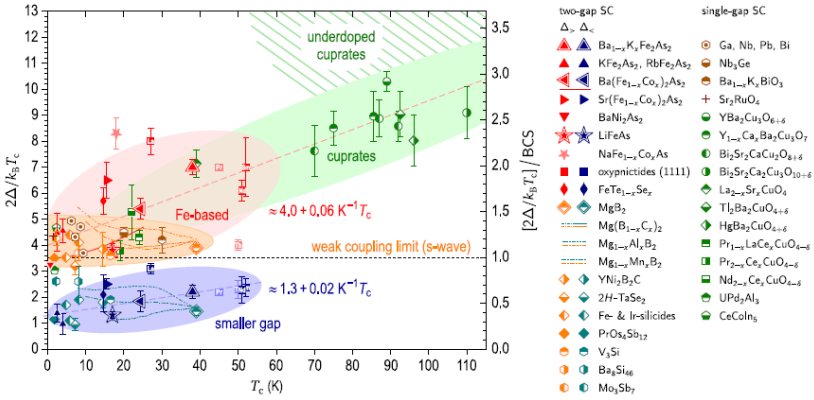
Fig. 1: Gap ratios $2\Delta/k_BT_c$ for different families of single- and two-gap superconductors.



A perspective of superconductivity as multiband phenomena: Cuprate, iron and aromatic systems

Hideo Aoki
Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan
Email:aoki@phys.s.u-tokyo.ac.jp

This talk will give a theoretical overview of the classes of superconductors encompassing **(a)** the iron-based, **(b)** the aromatic and **(c)** the high-Tc cuprate super- conductors (Fig. below, from left to right). The iron-oxypnictides superconductor is a multi-d-band system, with three of them primarily involved in the gap function as revealed from a microscopic model construction[1]. A pairing symmetry, sign-reversing but nodeless "s±" where each Fermi pocket is fully gapped while different pockets have opposite signs, is suggested from the viewpoint of the spin-fluctuation mediated pairing, which can depend on materials[1]. Hence this is a prototypical *multiband superconductor*. More recently, an aromatic superconductivity was discovered in K-doped picene for the first time, and the first-principles band structure indicates that the conduction band comprises multibands originating from multiple molecular orbitals, with the Fermi surface consisting of multiple sheets that have different dimensionalities[2]. Now, we can revisit the cuprate afresh, which has conventionally been viewed as a single($d_{x^2-y^2}$)-band system. We reveal [3] that, in the electronic structure and superconductivity for $La_{2-x}Sr/Ba_xCuO_4$ (T_C = 40 K) and $HgBa_2CuO_{4+\delta}$ (T_C = 90 K), the effect of d_{z^2} orbital is so significant as to supersede the effect of the Fermi surface shape, which resolves the long-standing puzzle. Thus all of iron, aromatic and cuprate superconductors have to be conceived as mutliband systems, with some important differences among them, and such an observation gives a renewed perspective on how superconductivity can dramatically depend on elements/crystal structures, and provides a guiding principle for searching new high-Tc superconductivity for the decades to come.

Keywords: High-Tc cuprates, iron-based superconductor, aromatic superconductor, multiband superconductivity

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Quantum tricriticality in FeAs layers

J. Lorenzana*[1,2]
[1] *Dipartimento di Fisica, "Sapienza", University of Rome, Italy.*, [2] *Istituto dei Sistemi Complessi, CNR, Rome, Italy.*

J. Lorenzana
**jose.lorenzana@romal.infn.itj*

Magnetism in FeAs superconductors appears some times through a first-order transition and some times through a second order transition which suggest that these systems are close to a tricritical point where a line of first order phase transitions continue in a line of second order character. A Landau analysis close to the tricritical point identifies all possible phases competing with superconductivity [1]. Apart from the well know columnar phase we find a non-collinear phase and a spin and charge ordered phase, all states that have been identified letter by other approaches. In order to locate the position of the tricritical point in the phase diagram we have made constrained magnetization computations in LaOFeAs [2] .Our results show that the system is remarkably close to a tricritical point at zero temperature, i.e. a quantum tricritical point. In addition the computation determines the Landau coefficients and the zero temperature phase diagram. Schemes to tune the materials exactly at the quantum tricritical point and the consequences for the normal and superconducting properties will be analyzed. We also compare with the effective field theory and discuss the experimental consequences.

Key words : quantum criticality, competing orders, high-Tc superconductivity

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XII

A. Perali
A. A. Shanenko
S. Bose
A. M. García-García

Pseudogap phase and remnant Fermi surface in ultracold Fermi gases and comparison with the pseudogap phase of cuprates.

Andrea Perali
Physics Unit of the School of Pharmacy, University of Camerino, Italy
andrea.perali@unicam.it

The origin of the pseudogap is widely debated for cuprate superconductors. The main controversy concerns whether superconductivity and the pseudogap phase are competing with each other or are manifestations of the same phenomenon. In the latter case, pairing fluctuations would extend above T_c the effects of the pairing gap below T_c.

A contribution to settle this controversy can be obtained by ultracold fermions, which are free of the structural complications of cuprates and where only pairing fluctuations are present. In these systems, the inter-particle attraction can be varied by Fano-Feshbach resonances as to amplify the effects of pairing fluctuations.

In this context, wave-vector resolved radio frequency spectroscopy data for an ultracold trapped Fermi gas are reported for several couplings at T_c , and analyzed by a pairing-fluctuation theory. We show that the non-Fermi-liquid behavior associated with the presence of a pseudogap coexists with a robust remnant Fermi surface over a wide coupling range, which sets the boundary of the pseudogap phase [1,2].

Once the pseudogap has been characterized in ultracold fermions, we compare the temperature dependence of the spectral intensity suppression obtained within our theory with the one recently measured in cuprates by ARPES [3].

key words: pseudogap, non-fermi-liquid, ultracold fermions, fano-feshbach resonances

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Cascade superconductor-to-normal transition in metallic nanowires.

A. A. Shanenko, Y. Chen, M. D. Croitoru, and F. M. Peeters
A. A. Shanenko
arkady.shanenko@ua.ac.be

It is well-known that size quantization can result in quantum oscillations of the critical temperature (and other basic quantities) in low dimensional superconducting systems like, e.g., superconducting nanofilms or superstripes. Here we report about a new quantum-size phenomenon, i.e., cascade superconductor-to-normal transition. The effect of a parallel magnetic field on the orbital motion of electrons in superconducting metallic nanowires results in a decay of the superconducting states through a cascade of jumps in the order parameter as function of the magnetic field. It is a direct consequence of splitting the conduction band into a series of single-electron subbands due to quantization of the perpendicular electron motion. Numerically solving the Bogoliubov-de Gennes equations, we investigate how such cascades depend on the confining geometry, temperature and spin-magnetic interactions. We also demonstrate that the quantum-size cascades survive in the presence of surface roughness and, so, can be observed experimentally in high-quality superconducting metallic nanowires.

Quantum size effects in nanoscale superconductors

Sangita Bose
CEBS (UM-DAE), Mumbai. INDIA
sangita.bose@gmail.com

Technological developments in the synthesis and characterization of high quality nano-structures have revealed novel physical phenomena in low dimensional superconductors when the system size is reduced below the bulk characteristic length scales. I will present our results of finite size effects on the superconducting properties in nanostructured thin films of Nb and Pb as a function of particle size size [1,2]. In addition I will demonstrate that the measurement of single, isolated superconductors by scanning tunneling spectroscopy (STS), opens up the possibility to explore interesting effects, hitherto inaccessible in ensemble averaged systems. These include the role of thermal fluctuations on superconductivity and the occurrence of shell effects which cannot be observed from bulk measurements [3].

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Enhancement of the critical temperature in iron-pnictide superconductors by finite size effects

M. A. N. Araújo[1,2], Antonio M. García-García,[2,3] and P. D. Sacramento[2]
[1]*Departamento de Física, Universidade de Évora, P-7000-671, Évora, Portugal*
[2]*CFIF, Instituto Superior Técnico, Universidade Técnica de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa,*
[3]*Portugal Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE, UK*

Antonio M. García-García
amg73@cam.ac.uk

Recent experiments [1] have shown that, in agreement with theoretical results [2], superconductivity in metallic nanostructures can be enhanced with respect to the bulk limit. Motivated by these results we study [3] finite size effects (FSE) in an iron-pnictide superconductor. For realistic values of the bulk critical temperature 20 ~ 50K, we find that, in the nanoscale region L ~ 10 nm, the critical temperature has a complicated oscillating pattern as a function of the system size L. A substantial enhancement of T_c ($\leq$ 50%) with respect to the bulk limit is observed for different boundary conditions, geometries and two microscopic models of superconductivity. Thermal fluctuations, which break long range order, are still small in this region. Finally we show that the differential conductance, an experimental observable, is also very sensitive to FSE.

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XIII

W. Lang
P. Raychaudhury
S. Haddad
A. Salleo

Non-Ohmic electrical transport properties in the pseudogap regime of underdoped $YBa_2Cu_3O_{6+x}$

W. Lang,[1] I. Puica[1], K. Siraj[2], J.D. Pedarnig[2]
[1]University of Vienna, Faculty of Physics, Boltzmanngasse 5, A-1090 Wien, Austria [2]Johannes-Kepler-University Linz, Institut of Applied Phyiscs, A-4040 Linz, Austria.

W. Lang
e-mail: wolfgang.lang@univie.ac.at

The energy gap between the superconducting pairs of charge carriers and the normal-state quasiparticles is considered the fundamental parameter for characterizing the superconducting state. In underdoped cuprate high-temperature superconductors, a markedly robust additional gap-like feature opens up at a temperature $T^* > T_c$. This so-called pseudogap manifests itself in a variety of experimental probes in the normal state, with smooth crossover from the pseudo- to superconducting gap. In order to explain the pseudogap a wide variety of models have been evoked, like a dilute pair condensate without long-range phase coherence, correlated states independent or even competing with superconductivity, and fluctuating stripes.

Recent experimental findings, like Nernst effect and diamagnetism, as well as novel angle resolved photoemission data have revealed a second, possibly independent, temperature scale with a different doping dependence than T^*. These various and partially contradicting experimental findings and their theoretical interpretation demonstrate vividly the need for additional experimental probes. We explore a novel experimental approach, the investigation of resistivity and Hall effect in the normal state of underdoped $YBa_2Cu_3O_{6+x}$ (YBCO) beyond the weak electric field limit and the search for possible non-ohmic effects.

The in-plane longitudinal and transverse (Hall) conductivities in thin films of YBCO are reduced in intense current densities of 2.6 $MAcm^{-2}$ in the temperature range from T_c = 53 K to ~150 K. In optimally-doped pristine and ion irradiated (defect rich) samples, however, this non-ohmic effect is limited to temperatures below 100 K. The onset temperatures follow the trend of the pseudogap opening at T^* but do not scale with T_c, excluding classical amplitude fluctuations of the superconducting order parameter as possible origin. The results may provide novel constraints for the various models that are competing to explain the origin of t he pseudogap in cuprate superconductors.

Phase-Fluctuations Driven Pseudogap State in a Strongly Disordered Conventional Superconductor: NbN

Pratap Raychaudhuri

Tata Institute of Fundamental Research

pratap@tifr.res.in

In a superconductor, the "super-current" is carried by weakly bound pairs of electrons, called Cooper pairs, which condense into a phase coherent quantum macro-state. The formation of these pairs induces a gap in the electronic energy spectrum, which appears in conventional superconductors, such as Pb and Nb, at the same temperature where the phase-coherent state forms, leading to zero resistance.

We have recently shown [1] that this scenario is no longer valid when strong disorder is introduced in the superconductor. Using scanning tunneling spectroscopy measurements on strongly disordered NbN thin films, we show that the gap in electronic spectrum associated with superconductivity persists up to temperatures many times higher than T_c, suggesting that Cooper pairs continue to exist in the system even after the zero resistance state is destroyed. The clue to the origin of this unusual behavior comes from complementary penetration-depth measurements, which show that thermal fluctuations of phase are the primary excitations responsible for destruction of the superconducting order, even when Cooper pairs themselves survive in the system above the critical temperature for zero resistance.

These experiments also provide a new perspective to the physics of High Temperature Cuprate Superconductors, where tunneling data show a striking similarity with the pseudogap state of disordered NbN. Our work suggests that a similar comparative analysis between tunneling and penetration-depth measurements in these materials can shed light on a possible common origin of the pseudogap state in both systems, namely, that Cooper pairs survive even after global superconductivity is destroyed by strong phase fluctuations.

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Enhancement of upper critical fields and Nernst effect by superconductingfluctuations in organic superconductors

S. Haddad, B. Bellafi and S. Charfi-Kaddour
Department of Physics, Faculty of Sciences of Tunis, University of Tunis El Manar 1060, Tunisia
S. Haddad
Email: sh_sonia@yahoo.fr

Based on the time dependent Ginzburg-Landau theory we study the effect of superconducting fluctuations on layered conductors showing a slab structure where superconducting domains are sandwiched between non-superconducting regions. This structure has been reported in the case of $(TMTSF)_2PF_6$ [1,2] in the vicinity of the critical pressure where the spin density wave transition line collapses. We show that the upper critical fields and the Nernst coefficient are strongly enhanced by the superconducting fluctuations. The latter may be at the origin of the controversy between thermodynamics and transport measurements in organic superconductors [3,4].

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Neither crystalline nor amorphous: transport in organic semiconductors

A. Salleo[1], J. Rivnay[1], R. Noriega[1], L. Jimison[1], C. Wang[1], M. F. Toney[2]
[1] *Department of Materials Science and Engineering, Stanford University, Stanford CA 94305*
[2] *Stanford Synchrotron Radiation Laboratory, Menlo Park, CA 94025*
A. Salleo
asalleo@stanford.edu

The promise of organic electronics is to dial in desirable properties (emission wavelength, mobility, chemical sensitivity) and use the power of organic chemistry to rationally design new synthetic semiconductors without being limited by Nature and the periodic table.
From the fundamental standpoint, these materials are fascinating as they are neither crystalline nor amorphous and their microstructure plays a central role in governing charge transport. We apply classical Materials Science concepts towards understanding how organic semiconductors "work". Using advanced synchrotron-based X-ray characterization techniques we are able to define and measure structural order at different length-scales. I will show that understanding disorder is the key to determining charge transport mechanism. For instance, static cumulative disorder (e.g. paracrystallinity) –which we devised how to measure quantitatively in soft materials– provides a fundamental justification to using a mobility edge model with an exponential distribution of trap states in the gap. Furthermore, we are able to provide a structural interpretation of these trap states, which for instance manifest themselves as a broad sub-threshold region in transistors or recombination centers in solar cells. Paracrystalline disorder allows to rank organic semiconductors thereby allowing to determine whether shallow traps or grain-boundaries limit transport. In this regard, I will show that engineering the microstructure of organic semiconductors leads to new insights in the role of grain-boundaries in charge transport. Understanding the relationship between microstructure and transport is of fundamental importance for the rational design of new synthetic semiconductors.

XIV

K. Koepernick
R. Gonnelli
P. Samuely
A. Marcelli
D. Louca

Photoemission in iron pnictides, a DFT perspective.

Klaus Koepernik*[1], Alexander Lankau[1], Helmut Eschrig[1], Jeroen van den Brink[1], Sergey Borisenko[1], Volodymyr Zabolotnyy[1], Bernd Buechner[1], Erik van Heumen[23], Mark S. Golden[2]
[1]*Institute for Theoretical Solid State Physics, IFW Dresden, D-01171 Dresden, Germany*
[2]*van der Waals–Zeeman institute, University of Amsterdam, 1018 XL Amsterdam, the Netherlands*
[3]*Department of Physics, Tampere University of Technology, PO Box 692, FIN-33101 Tampere, Finland*

Klaus Koepernik
email: k.koepernik@ifw-dresden.de

The iron pnictide superconductors are the second large class of unconventional superconductors with a promisingly high T_c and potential technical applicability. This makes the understanding of the electronic structures and mechanism of superconductivity a hot topic. Among the experimental tools to study these compounds some are potentially surface sensitive, like scanning tunneling microscopy and angle resolved photo emission spectroscopy. In order to help to determine the nature of the electronic structure seen in those experiments, we performed density functional studies with the focus on cleavage behavior and possibly emerging surface states. We can conclude that the 111 family behaves differently from the 122 and 1111 family in being most likely free of any surface related complications.

Key words: ARPES, iron pnictides, surface states

The symmetry of order parameter(s) in Fe-based superconductors: The point-contact Andreev-reflection approach

R.S. Gonnelli,*[1] M. Tortello,[1] D. Daghero,[1] G.A. Ummarino,[1] V.A. Stepanov,[2] Z. Bukowski,[3] N. D. Zhigadlo,[3] J. Karpinski,[3] J. Jiang,[4] P. Reuvekamp,[5] and R.K. Kremer[5]
[1]*Dipartimento di Fisica, Politecnico di Torino, 10129 Torino, Italy.*
[2]*P. N. Lebedev Physical Institute,RAS, Moscow, Russia.*
[3]*Laboratory for Solid State Physics, ETHZ, CH-8093 Zurich, Switzerland*
[4]*Applied Superconductivity Center, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA*
[5]*Max-Planck Institute for Solid State Research, Stuttgart, Germany*

R.S. Gonnelli
renato.gonnelli@polito.it

One of the hottest debates of the last two years in the physics of Fe-based superconductors has to do with the number, the amplitude, and, in particular, the symmetry of the superconducting order parameter(s) (OPs). Thus the precise determination of these quantities is a necessary step to understand the details of how superconductivity occurs in these compounds. Despite its apparent simplicity, point-contact Andreev-reflection (PCAR) spectroscopy is one of the techniques that have been more useful in the investigation of the OPs in these materials. Nevertheless, early PCAR measurements indeed suffered from the unsatisfactory quality of the first samples and gave contradicting results. We will show here that, instead, when PCAR experiments in good-quality samples are carried out with all the necessary cautions by different groups and even in samples of different forms (single crystals, polycrystals, films) they do provide surprisingly consistent results. In fact, in the most studied La 1111, Sm 1111, Co-doped and K-doped Ba 122 compounds, the available PCAR results agree rather well on the presence of two OPs, on their amplitude and temperature dependence and on their symmetry (the s± one, with isotropic OPs with sign reversal between holelike and electronlike FS sheets, at least at optimal doping).
In addition we will also present and discuss our recent directional PCAR results on single crystals of the Ca 122 family, which are consistent with at least one nodal (or strongly anisotropic) OP.
These findings can be a crucial test for the theories that predict the occurrence of anisotropic or nodal symmetries in suitable conditions, related to fine details of the lattice structure.
We also demonstrate that, if properly extended theoretical models for Andreev reflection are used, directional PCAR spectroscopy can even provide information about the shape of the Fermi surface.

key words: Point-contact Andreev-reflection spectroscopy, symmetry of the order parameter, nodal and strongly anisotropic pair symmetry

Scanning Tunneling Spectroscopy of Superconducting Energy Gap in $SrPd_2Ge_2$ Single Crystal, Isostructural with 122 Iron Pnictides

T. Samuely[1], P. Szabó[1], J.G. Rodrigo[2], D. S. Inosov[3], J. T. Park[3], N. H. Sung[4], B. K. Cho[4], P.Samuely[1]
[1] *Centre of Ultra Low Temperature Physics at the Institute of Experimental Physics of the Slovak Academy of Sciences and P.J. Šafárik University, Watsonova 47, 04001 Košice, Slovakia*
[2] *Laboratorio de Bajas Temperaturas, Instituto N.Cabrera, Univesidad Autonoma de Madrid, Spain*
[3] *Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[4] *School of Material Science & Engineering,Institute of Science and Technology, Gwangju, Korea*

T. Samuely
samuely@saske.sk

Iron pnictides, become superconducting when the parental itinerant antiferromagnetic semimetals are doped, which also gradually suppresses their magnetism. The systems have revealed a strong multiband character and a hot debate is held on the multiple superconducting energy gaps which can be open with an opposite phase on separated sheets of their Fermi surface. Then, the exotic *s*+- superconductivity can be realized due to magnetic interactions. Our point-contact measurements performed on the iron pnictides have indeed shown a presence of multigap superconductivity. On the hole doped $Ba_{1-x}K_xFe_2As_2$ ("122" type) single crystals two *s*-wave gaps have been found where the smaller gap has a size below the BCS value while the large gap reveals much higher coupling strength [1]. Angular dependence of the upper critical field in $Ba_{1-x}K_xFe_2As_2$ measured near T_c shows also significant deviations from the Lawrence-Doniach prediction for a single-gap superconductor, presumably due to effect of two distinct gaps. The recent discovery [2] of a new low-temperature (T_c = 3 K) superconductor $SrPd_2Ge_2$ isostructural with the group of 122 iron pnictides can shed a light on the role of magnetism in pnictides because this compound is not only pnictogen-free, but also has the magnetic metal (Fe) completely replaced by the non-magnetic one (Pd) and is stoichiomety rich. In this contribution we will show that $SrPd_2Ge_2$ is, in fact, very different from 122 pnictides. Its electronic structure reveals, in contrast to basically 2D pnictides, a much more pronounced three-dimensional character. Three-dimensional topology of $SrPd_2Ge_2$ Fermi surface is confirmed by experimentally measured momentum distribution maps by ARPES and supported by the LDA calculations [3]. The superconducting density of states have been measured by the Kosice home-built STM in helium-3 refrigerator. There the superconducting Pb tip has been applied to acquire a high resolution of the sample gap measurements. This configuration allows also for a direct determination of the temperature dependence of the gap. As a result a single s-wave superconducting energy gap is obtained in $SrPd_2Ge_2$ with the strong coupling strength $2\Delta/kT_c=4$ and following the standard BCS-like temperature dependence. No multigap features have been observed. All these findings indicates that in the isostructural 122 iron arsenides different physics is related to magnetism absent here.

Keywords: Iron based superconductors, superconducting gap structure, STM/S

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Interplay between local structure and electronic and magnetic properties of F-dopedoxypnictides

A. Marcelli,[1,2] D. Di Gioacchino,[1] A. Puri,[1,3] J. Cheng[2,4] W.S. Chu,[2,4] W. Xu,[4] and Z.Y. Wu[2,4]
[1]*Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, 00044 Frascati (RM), Italy*
i[2]*National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P.R. China*
[3]*Dipartimento di Scienze Geologiche, Università degli Studi Roma Tre, Largo S.Leonardo Murialdo 1, 00146 Roma, Italy*
[4]*Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, P.R. China*

A. Marcelli
marcelli@lnf.infn.it wuzy@ustc.edu.cn

The interplay between the local structure and the electronic properties is a key issue in many condensed matter phenomena. The ReFeAsO (Re = rare earth) has a layered structurewith an insulating layer (ReO) and a conducting slab (FeAs). Replacing oxygen with fluorine atoms or generating oxygen deficiency or vacancies, ReFeAsO compounds becomesuperconducting. Moreover, in these systems the superconducting critical temperature iscorrelated with the RE ion size. We present here an investigation of the local lattice and theelectronic structure of the high-T_c superconductor $SmO_{1-x}F_xFeAs$ as a function of F-doping by means of Sm L_3-edge X-ray absorption near edge structure (XANES) and multiplescattering (MS) calculations. A correlation emerges between F doping, oxygen vacanciesand local empty density of states at the RE edge in agreement with the occurrence in $SmO_{1x}F_xFeAs$ at $x \sim 0.14$ of a quantum critical point. In these oxypnictides XANES spectra at the As K-edge may explore also the local structure around the pnictogen site. These data pointout differences among light and heavy rare earth compounds and point out a reduced interlayer disorder in the LaFeAsO in comparison to heavier oxypnictides. The higher disorder in the SmFeAsO system probably due to a higher interlayer coupling and a smaller misfit strain lead to a higher T_c after doping inside the ReO layer. As a consequence theinterlayer order/disorder affects XANES spectra and plays a significant role in the coupling between FeAs and the ReO layers and control electronic and magnetic properties in these materials.
Keywords: $ReO_{1-x}F_xFeAs$; XANES; oxygen vacancy; doping; superconductivity

Suppression of superconductivity in Fe chalcogenides by annealing: a reverse effect to pressure

Despina Louca,[*1] J. Yan,[2] A. Llobet,[3] and R. Arita[4]
[1] *Department of Physics, University of Virginia, Charlottesville, VA 22904-4714, USA.*
[2] *Ames Laboratory, Iowa State University, Ames, IA 50011, USA.*
[3] *Lujan neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.*
[4] *Department of Applied Physics, University of Tokyo, and JST TRIP, Tokyo 113-8656, JAPAN.*

Despina Louca
Louca@virginia.edu

A common route to controlling the superconducting transition temperature (T_C) in the iron pnictides and chalcogenides is to introduce charge carriers via chemical substitution or to apply pressure. Extensive experimental and theoretical works have revealed important traits of these itinerant magnets. In particular, their Fermi surface topologies are remarkably similar except for the recently discovered $A_xFe_2Se_2$ (A-alkali) system, and both classes exhibit a superconducting spin resonance. In the pnictides it was shown that the anion height from the Fe basal plane and the tetrahedral bond angle reach optimal values, 1.38 Å and ~109^o respectively, on approaching the maximum T_C. These structural features show a similar dependence to both pressure and doping. Remarkably, very little is known of the mechanism that suppresses T_C and of the changes brought upon the electronic structure, as is the case of overdoping in $BaFe_2As_2$ or impurity doping in LaFeAsO. Using neutron scattering we find that superconductivity in $FeSe_{1-x}Te_x$ can be suppressed by annealing, in the absence of extrinsic influences. With annealing, the height of the Se ion from the basal plane increases while that for Te decreases. The angle between Se and Fe decreases while that between Te and Fe increases. In contrast, under pressure, the height of the Se ion decreases while that for Te increases and the bond angle between Se and Fe increases while the angle between Te and Fe decreases. T_C sensitively depends on the local atomic configuration of Te and Se, and on their degree of hybridization with Fe.

Key words: Superconductivity in pnictides, local structure, pressure

XV

W. D. Schneider
M. D. Croitoru
G. E. Johnston
D. Innocenti

Quantum oscillations, superconductivity, zero-bias anomalies, and Coulomb blockade in supported nanoscale lead islands

Wolf-Dieter Schneider
Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Wolf-Dieter Schneider
wolf-dieter.schneider@epfl.ch, christof.schneider@physik.uni-augsburg.de

Using scanning tunneling spectroscopy down to a temperature of 3 K, we studied the linewidth of unoccupied quantum-well states in ultrathin Pb islands, grown on Si(111) on two different Pb/Si interfaces. A quantitative analysis of the differential conductance spectra allowed us to determine the electron- electron (e-e), electron-phonon (e-ph), and the interface contributions to the lifetime. Layer-dependent ab initio calculations of the e-ph linewidth contribution are in excellent agreement with the data. Importantly, the sum of the calculated e-e and e-ph lifetime broadening follows the experimentally observed quadratic energy dependence [1].

The energy gap of these superconducting Pb islands, in a thickness range between 60 and 5 monolayers, was found to decrease from its bulk value as a function of inverse island thickness. Corresponding values of the critical temperature T_c, estimated using the bulk gap-to-T_c ratio, are in quantitative agreement with *ex-situ* magnetic susceptibility measurements, however, in strong contrast to previous scanning probe results. Layer-dependent *ab initio* density functional calculations for free-standing Pb films show that the e-ph coupling constant, determining T_c, decreases with diminishing film thickness [2].

By reducing the lateral dimensions of these nano-islands to a few nm^2, we show that the charge transport between metallic nanocontacts and various types of materials varies strikingly with diminishing contact area, manifesting itself by the subsequent appearance of zero-bias anomalies and Coulomb blockade phenomena in the differential conductance spectra [3].

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In-plane magnetic field anisotropy in FFLO state in layered superconductors.

M.D. Croitoru[1]*, M. Houzet[2], and A. Buzdin[1]
[1]*Université Bordeaux I, LOMA, F33405 Talence Cedex, France*
[2]*CEA, Grenoble, DRFMC/SPSMS/LCP, F38054 Grenoble Cedex 9, France*

M.D. Croitoru
mikhail.croitoru@uni-bayreuth.de

During the last 40 years a lot of theoretical and experimental studies have been devoted to layered superconductors. In particular in some organic layered superconductors the in-plane critical field is mainly determined by the paramagnetic limit. This feature favours the formation of the Fulde-Ferrell-Larkin-Ovchinnikov state (FFLO state). There have been observed several hints indicating the experimental realization of the FFLO state in organic superconductors. In this work we provide the quasi-classical description of the anisotropy of the in-plane critical field in uniform and non-uniform (FFLO) phases of layered superconductors, taking into account the interlayer Josephson coupling. Near TC we generalize the Lawrence-Doniach model for the case of high magnetic fields. We show that the anisotropy of the onset of superconductivity may change dramatically in the FFLO state as compared with the uniform superconducting phase. The study of the character of this anisotropy gives important information on the orientations of the FFLO modulation vector. Our results can qualitatively describe the recent experimental data. [1]

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Determining the Electronic Ground State in a Bilayer Manganite

G. E. Johnstone[1], T. G. Perring,[2] O. Sikora,[3] D. Prabhakharan,[1] A. T.Boothroyd,[1]
[1] *Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, UK,* [2]*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK.* [3]*Department of Physics, University of Bristol, Bristol, UK.*

G. E. Johnstone
g.johnstone1@physics.ox.ac.uk

There has been a debate in recent years as to the true electronic ground state in the CE-type antiferromagnetic phase in materials related to the colossal magnetoresistive manganites. Two possible models have been suggested, the first is the truly charged ordered CE-phase model with a checkerboard lattice of Mn^{3+} and Mn^{4+} ions, based on the Goodenough-Kanamori rules. The second proposed model is known as the Zener polaron model, where two neighbouring manganese ions are tied together ferromagnetically by the Zener double exchange interaction and the lattice is made up of these Zener polarons. I will report inelastic neutron scattering measurements on $Pr(Sr_{0.1}Ca_{0.9})_2Mn_2O_7$ that show the Zener polaron model is incompatible with the spin wave dispersion measured for this material. The measured dispersion agrees with that predicted for the CE-phase model, but also reveals some interesting competing interactions within the antiferromagnetically ordered layers.
Key words: Colossal magnetoeresistance, CE-type order, bilayer manganite

Shape resonance and crossover phenomena at a Lifshitz transition in multiband superconductor

D. Innocenti[1]*, A. Ricci[2], N. Poccia[2], A. Valletta[3], S. Caprara[2], A. Perali[4] and A. Bianconi[2]
[1] *Dipartimento di Ingegneria Meccanica, University of Roma 'Tor Vergata', 00133 Rome, Italy*
[2] *Department of Physics, Sapienza University of Rome, 00185 Rome, Italy*
[3] *Inst. for Microelectronics and Microsystems, IMM CNR, 00133 Roma, Italy*
[4] *School of Pharmacy, Physics Unit, University of Camerino, 62032 Camerino, Italy*

D. Innocenti
E-mail: innocenti1@libero.it

We investigate the shape resonance -belonging to the class of Feshbach-like resonances- in the superconducting gaps of a two-band superconductor, modulated by quantum confinement effects in a superlattice of quantum wells, by tuning the chemical potential near a Lifshitz topological transition. The high Tc superconducting scenario shows the coexistence of a first BCS condensate made of Cooper pairs in the first band and a second boson-like condensate made of bosons like bipolarons, in the second band. The interband coupling controls the shape resonance in the pair exchange between the condensates. We discuss the response of the condensates in the particular BCS–Bose crossover that occurs at the shape resonance tuning the Lifshitz parameter like tuning the external magnetic field for the Feshbach resonances in ultracold gases.

keyword: Lifshitz transition, shape resonance, BCS-Bose crossover, multiband superconductivity

XVI

A. Kanigel
T. R. Lemberger
P. Armitage
H. Iwasawa
D. Di Gioacchino

Square-root Scaling of T_c vs. Superfluid Density near the Underdoped and verdoped Quantum Phase Transitions in Cuprate Superconductors

J. Yong[1], A. McCray[1], T.R. Lemberger*[1], M. Randeria[1], M. Naamneh[2], A. Kanigel[2], A. Tsukada[3], and M. Naito[3]
[1]*Dept. of Physics, The Ohio State University, Columbus, OH, USA.*
[2]*Dept. of Physics, Technion - Israel Institute of Technology, Haifa 32000, Israel.*
[3]*Dept. of Appl. Phys., Tokyo Univ. of Agriculture and Technology, Tokyo, Japan*

T. R. Lemberger
**TRL@physics.osu.edu*

Superfluid density (N_s) measurements have been made on several cuprate families - $YBa_2Cu_3O_{7-\delta}$ (YBCO), $La_{2-x}Sr_xCuO_4$ (LSCO), and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212)- near their quantum phase transitions from superconducting to insulating or from superconducting to normal-conducting. In underdoped YBCO and LSCO, despite the increase in *ab*-plane vs. *c*-axis anisotropy with underdoping, the super-to-insulator transition is characterized by 3D quantum critical fluctuations, with T_c scaling as square-root of $N_s(0)$. In overdoped LSCO, square-root scaling is observed near the super-to-normal transition, but this scaling may be due to the disappearance of disordered *d*-wave superconductivity as cooper pairing weakens, rather than a quantum critical point. Bi-2212 is interesting because it is much more anisotropic than YBCO and LSCO, and STM measurements show strong inhomogeneity in the superconducting gap. We find that T_c scales with $N_s(0)$ in Bi-2212 very much like it scales in ultrathin 2D YBCO films – scaling is 2D (linear) as the underdoped QCP is approached. In all underdoped samples other than the ultrathin YBCO films, $N_s(T)$ shows an interesting evolution with underdoping – the strong downward curvature seen in samples near optimal doping disappears, and $N_s(T)$ is nearly linear from low-T to T_c. This anomalous feature may point to the nature of quantum fluctuations that dominate the physics near the underdoped QCP.

Key Words: Cuprates, Quantum Critical Points, Superfluid Density.

Fast vortices in the Cuprates? A vortex plasma model analysis of the THz conductivity and diamagnetism in $La_{2-x}Sr_xCuO_4$

L. S. Bilbro[1], R. Valdés Aguilar[1], G. Logvenov[2], O. Pelleg[2], I. Bozovic[2] and N. P. Armitage[1*]
[1]*The Institute for Quantum Matter, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218, USA*
[2]*Brookhaven National Laboratory, Upton, New York 11973, USA.*

P. Armitage
**e-mail: npa@pha.jhu.edu.*

The nature of the underdoped pseudogap regime of the high-temperature copper oxide superconductors has been a matter of long-term debate. On quite general grounds, we expect that, owing to their low superfluid densities and short correlation lengths, superconducting fluctuations will be significant for transport and thermodynamic properties in this part of the phase diagram. Although there is ample experimental evidence for such correlations, there has been disagreement about how high in temperature they may persist, their role in the phenomenology of the pseudogap and their significance for understanding high-temperature superconductivity. Here we use THz time-domain spectroscopy to probe the temporal fluctuations of superconductivity above the critical temperature (Tc) in $La_{2-x}Sr_xCuO_4$ (LSCO) thin films over a doping range that spans almost the entire superconducting dome (x=0.09–0.25). Signatures of the fluctuations persist in the conductivity in a comparatively narrow temperature range, at most 16 K above Tc. We compare our results with measurements of diamagnetism in a similarly doped crystals of LSCO and show through a vortex-plasma model that if the fluctuation diamagnetism solely originates in vortices, then they must necessarily exhibit an anomalously large vortex diffusion constant, which is more than two orders of magnitude larger than the Bardeen-Stephen estimate. This points to either the extremely unusual properties of vortices in the under-doped d-wave cuprates or a contribution to the diamagnetic response that is not superconducting in origin.

Angle-resolved photoemission studies of cuprate and ruthenate superconductors

H. Iwasawa*
Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima, Japan.
**h-iwasawa@hiroshima-u.ac.jp*

Knowledge on the electronic structure is indispensable to understand various unusual physical properties of strongly correlated electron systems. The macroscopic physical properties of solids are closely related to the electrons near the Fermi level, which are more or less renormalized by many-body interactions. It is, therefore, important to clarify the origin and magnitude of the renormalization. In this talk, we characterize the renormalization effects in cuprate and ruthenate superconductors using high-resolution ARPES.

This work has been done in collaboration with Y. Aiura, Y. Yoshida, H. Eisaki, K. Sato, H. Bando, I. Hase, S. Koikegami, T. Saitoh, J. F. Douglas, N. C. Plumb, Z. Sun, D. S. Dessau, T. Masui, S. Tajima, S. Uchida, H. Hayashi, J. Jiang, D. Hirayama, T. Habuchi, A. Ino, M. Arita, K. Shimada, H. Namatame, and M. Taniguchi

Keywords: ARPES, cuprate, ruthenate, renormalization

Coexistence of a superconducting and a magnetic phase in $NdFeAsO_{1-x}F_x$ and $FeSe_xTe_{1-x}$ systems

D. Di Gioacchino[1], A. Marcelli[1,2], A. Puri[1,3,4], N. Poccia[4], A. Ricci[4] , N.L. Saini[4] and A. Bianconi[4]
[1]*Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, 00044 Frascati (RM), Italy*
[2]*Chinese Academy of Science, University of Science and Technology of China, Hefei, Anhui 230029, P.R. China*
[3]*Dipartimento di Scienze Geologiche, Universita` degli Studi Roma Tre, Largo S. Leonardo Murialdo 1, 00146 Roma, Italy*
[4]*Dipartimento di Fisica, Università degli Studi di Roma "La Sapienza", Piazzale Aldo Moro 5, 00185, Roma, Italy*

D. Di Gioacchino
daniele.digioacchino@lnf.infn.it

Since the discovery of superconductivity, the simultaneous occurrence of superconducting and magnetic phenomena has been considered each other exclusive. Although pointed out in 1958 by Matthias et al. [1] a possible correlation between the magnetism in some rare earth compounds and the superconductivity in other closely related alloys, has been matter of debate until today. Also in the newly discovered iron-based superconductors the subject remains an open issue.
In this contribution we show that in these new systems the AF magnetic phase is not suppressed and a magnetic phase may coexist with superconductivity. By means of ac multi-harmonic susceptibility and dc susceptibility measurements we show in $NdFeAs_{1-0.14}F_{0.14}$, $FeSe_{0.25}Te_{0.75}$ and in the $FeSe_{0.5}Te_{0.5}$ superconductors the presence of interplay between magnetism and superconductivity.

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Keywords: $NdO_{1-x}F_xFeAs$; $FeSe_xTe_{1-x}$; magnetic and superconductive phases; ac multi-harmonic susceptibility.

XVII

H. Hosono
Y. J. Uemura
D. Mihailovic
S. V.Borisenko

Recent Advances in Iron Pnictide Superconductors and Relevant Materials

Hideo Hosono
Frontier Research Center, Tokyo Institute of Technology,Yokohama 226-8503, JAPAN
hosono@msl.titech.ac.jp

More than 3,000 papers have been published since the paper reporting $LaFeAsO_{1-x}F_x$ with T_c=26K in early 2008. Six kinds of parent materials containing a common building structural unit of a square lattice of Fe^{2+} are found and many derived superconductive materials are reported to date. In this talk, I talk on progress of iron pnictide superconductors emphasizing on our recent works on the bulk and thin films of these materials and relevant superconductors with a similar structure.
The focuses are placed on:

- Indirect electron doping to 122 to induce superconductivity
- Hydrogen and superconductivity in 1111
- Epitaxial thin films in Ba122:Co and device application
- Non-Iron based Superconductors with 1111 and 122 structures

Keywords: Iron pnictides, Hydrogen, Thin Films

Energy-scale Phenomenology of Uconventional Superconductors: Comparable Charge and Spin Energies

utomo J. Uemura
Physics Department, Columbia University, New York, USA
tomo@lorentz.phys.columbia.edu

In unconventional suprconductors, including high-Tc cuprates, FeAs, organic BEDT, A_3C_{60} and heavy-fermion $CeCoIn_5$ systems, we notice a few common behaviors which point towards novel condensation and pairing mechanisms. They include: (1) superconducting phase emerging adjacent to the competing antiferromagnetic / SDW states; (2) scaling of resonance-mode energy with T_c analogous to rotons in superfluid He; (3) scaling of the spin fluctuation energy scale with T_c; (4) scaling of the superfluid density with Tc in the underdoped region; (5) scaling of the superfluid density with Tc in the overdoped / pressurized region; (6) scaling of the specific heat jump C/T at Tc with Tc in the overdoped / pressurized region.

While (3) is expected for a BCS-like condensation, (2), (4), (5) and (6) point towards Bose-Einstein condensation where T_c is governed by the condensing boson density and mass. In particular, we notice that the spin fluctuation (mediating boson) energy scale is comparable to condensing charge energy scale (derived from superfluid density) in many of these systems, suggesting a resonant behavior in condensation and pairing. This may be a key concept to understand highly unusual non-BCS like behaviors (5) and (6) in the overdoped / pressurized regions of these unconventional superconductors. Scaling of Tc on the soft-mode energy (2), in addition to superfluid density (4) and (5), may be understood by BE condensation and BE-BCS crossover in the vicinity of magnetic competing states (1).

Recent progress of ARPES, Raman, neutron and STM experiments revealed details of nodal energies which scale with Tc and antinodal responses which undergo symmetry breakings at T*. These features are often taken as signatures of superconductivity due to nodal region while antinodal region being unrelated or even competing with superconductivity. However, I would like to present an opposite view point that the antinodal charges determine the main thermodynamic features of superconducting condensation and the nodal charges are simply following that physics.

Coherent dynamics through symmetry-breaking transitions in electronically ordered systems.

Dragan Mihailovic[§1], Roman Yusupov1, Tomaz Mertelj[1], Viktor V.Kabanov1, Primoz Kusar1 and Serguei Brazovskii,[2]
[1]*Dept. of Complex Mater, Jozef Stefan Institute, Jamova 39, Ljubljana, SI-1000, Ljubljana, Slovenia*
[2]*LPTMS-CNRS, UMR8626, Univ. Paris-Sud, Bat. 100, Orsay, F-91405 France*

Dragan Mihailovic
dragan.mihailovic@ijs.si

The study of system trajectories undergoing symmetry breaking phase transitions (SBTs) - whether in condensed matter physics, cosmology or finance - is difficult because they are hard to repeat, or they occur very rapidly. Here we report for the first time on a high-time-resolution study of the nonergodic evolution of bosonic and fermionic excitations through an electronic charge-ordering SBT in charge-density-wave systems using a novel multi-pulse femtosecond laser spectroscopy technique. Quenching our system with intense optical pulses, we subsequently detect hitherto unrecorded coherent aperiodic undulations of the order parameter, critical slowing down of the collective (Higgs) mode, and evolution of the particle-hole gap as the system evolves through the transition (see figure for a summary of observed events). Modeling based on Ginzburg-Landau theory is used to reproduce the observations without free parameters1. Of particular interest is the observation of spectro-temporal distortions arising from spontaneous annihilation of topological defects, analogous to those discussed by the Kibble-Zurek cosmological model and the incoherent annihilation at long times.
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Superconductivity and magnetism in iron pnictides.

Sergy V. Borisenko
IFW Dresden, Institute for Solid States Research, Surface and Interfaces Section, Spectroscopy Group, Helmholtzstrasse 20, 01069 Dresden , Germany

s.borysenko@ifw-dresden.de

We study various iron superconductors at ultra low temperatures by means of angle-resolved photoemission spectroscopy (ARPES). The measurements provide a direct access to the information on the low energy electronic structure, which includes the detailed knowledge of the Fermi surface, band renormalization, electronic self-energy and symmetry of the superconducting order parameter.
The results suggest a direct correlation between the fermiology and fundamental physical properties throughout the phase diagram of all iron superconductors. In particular, the Van Hove singularity is identified as playing a primary role for the superconductivity.
The project was supported, in part, by the DFG under Grant No. BO 1912/3-1 within the framework of the priority program SPP1458.

XVIII

G. Deutscher
H. Keller
A.Bussmann-Holder
J.Mustre de Leon
N. Poccia

Inhomogenous Superconductivity and the role of Cu-O bond length fluctuations in the high tc mechanism

Guy Deutscher
Department of Condensed Matter Physics, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv , Israel
guyde@post.tau.ac.il

We review three different kinds of experiments that emphasize the non-BCS, inhomogeneous aspects of superconductivity in the High Tc cuprates: the existence of two different energy scales in the superconducting state; EXAFS measurements of the Cu-O bond length distribution, which have shown that below a temperature $T^*>T_c$ it becomes broader than expected from the Debye-Waller broadening; and the effect of frozen lattice disorder on critical current and vortex pinning, which profoundly affects the pairing landscape. We then discuss how these results fit with models in which the electron-lattice interaction plays a leading role,possibly in the context of a Quantum Critical Point at the edge of the superconducting dome.

From cuprate to iron-based superconductors – key elements of high-temperature superconductivity

H. Keller[1] and A. Bussmann-Holder[2]
[1]*Physik-Institut der Universität Zürich, CH-8057 Zürich, Switzerland*
[2]*Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany*
H. Keller
keller@physik.uzh.ch

Cuprate and the recently discovered iron-based high-temperature superconductors (HTSs) appear to have some features in common: 1) they have unusually high transition temperatures T_c, 2) they have layered structures with strongly anisotropic normal state and superconducting properties, 3) they exhibit a rich doping dependent phase diagram with coexisting or non-coexisting magnetic and superconducting phases (with the exception that for cuprates the undoped mother compound is an isolator, whereas in the iron-based systems the mother compound is metallic), 4) there exist hole doped and electron doped variants of these HTS, 5) they show a pronounced isotope effect on T_c (for the cuprates isotope effects on various quantities, including the in-plane penetration depth and the pseudogap temperature, were observed, whereas in iron-based compounds at present controversial results have been reported for the isotope effect on T_c), and 6) they are multi-band superconductors with (eventually) mixed order parameters.
In this talk some common and unlike properties of cuprate and iron-based HTSs will be discussed and also compared to those of the “non-magnetic” layered two-band superconductor magnesium diboride. Furthermore, it is shown that pronounced lattice and multi-band effects are essential to achieve the high transition temperatures in the cuprate and iron-based HTSs.

Key signatures of multi-band and polaronic superconductors

Annette Bussmann-Holder[1] and Hugo Keller[2]
[1]*Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany*

[2]*Physik-Institut der Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich, Switzerland*

Annette Bussmann-Holder
a.bussmann-holder@fkf.mpg.de

Multi-band superconductivity has been predicted to be realized in many systems shortly after the BCS theory. The experimental confirmation followed, however, more than 20 years later with a disappointing low value of T_c of 3K. Another 10 years later, one of the discoverer of high temperature superconductivity in copper oxides suggested multi-band superconductivity also for this novel material class based on the observation that the copper oxides are intrinsically inhomogeneous and that many experiments are incompatible with a pure d-wave order parameter. An unambiguous verification of this scenario has been obtained by various experimental probes, however, not being overall accepted by the community. With the discovery of MgB_2 the multiband aspects of superconductivity became more popular and have been confirmed to be realized also in the new high temperature superconducting pnictides. While for conventional superconductors the isotope effect on T_c is known to stem from electron-phonon interactions, this is no more clear for multiband systems, where different pairing glues may combine and change the isotope exponent gravely. In addition, strong local electron-lattice coupling may lead to polaron formation thereby introducing novel isotope effects.
The implications of multiband superconductivity for isotope effects, coherence factors, local lattice distortions are discussed and compared to experimental results.

Effect of rare earth substitution in the density of electronic states of LnOFeAs

J. Mustre de León[1]*, A. García Saravia Ortiz de Montellano[1], N. L. Saini[2], A. Bianconi[2]
[1)] *Departamento de Física Aplicada, Cinvestav-Mérida, Carretera Antigua a Progreso Km. 6.5, A.P. 73, 97310 Mérida, Yucatán, Méxic*

[2)] *Dipartimento di Fisica, Universitá di Roma "La Sapienza", Piazzale Aldo Moro 2,00185 Roma, Italy*

J. Mustre de León
• *e-mail: mustre@cinvestav.mx*

Measurements of the Fe K-edge x-ray absorption near edge (XANES) spectra of LnOFeAs (Ln being a lanthanide) high Tc superconductors exhibit significant changes in the pre-edge peak region upon rare earth substitution. Ab initio XANES calculations, based on the local structure centered at the Fe site obtained by crystallographic investigations, reproduce the observed changes in the spectra, indicating variations of the Fe d-local unoccupied electronic states. The calculated Fe density of states at the Fermi energy shows an increase of the Fe d-density of states with increasing height of the arsenic atomic position with respect to the iron plane, similar to that observed for the superconducting transition temperature, Tc. These calculations show that not only the atomic position variations of the Fe-As layers induced by the rare earth substitution is relevant in the increase of the DOS at the Fermi-level, but the actual change in electronic configuration of the rare earth also plays a role in the increase of Fe d-density of states at the Fermi energy.

XVIII

Space-time imaging the non-equilibrium state of a cuprate high temperature superconductor.

Nicola Poccia
Department of Physics, Sapienza University of Rome, P. le A. Moro 2, 00185 Rome, Italy
nicola.poccia@roma1.infn.it

All high temperature superconductors are complex materials far from equilibrium. We present the imaging of the defects real space organization in a cuprate superconductor. We have used the space resolved scanning micro x-ray diffraction. We have discovered a noised environment with power law correlations[1]. Dynamics of microscopic objects immersed in noisy environments belongs to the domain of non-equilibrium thermodynamics. The time resolved evolution of the defects nucleation, growth and organization have been investigated by x-ray diffraction under continuous x-ray illumination[2].
While it seems unlikely that macroscopic entanglement could exist at 300 K, interacting shape resonances are suitable in a non-equilibrium system and have been proposed for achieving room temperature superconductivity and for the unexplained robustness of living matter[3].

This presentation is based on the work in collaboration with M. Fratini, , A. Ricci, G. Campi, M. Burghammer, L. Barba, A. Vittorini-Orgeas, G. Bianconi, G. Aeppli and A. Bianconi.

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2. N. Poccia, M. Fratini, A. Ricci , G. Campi, L. Barba, A. Vittorini-Orgeas, G. Bianconi, G. Aeppli and A. Bianconi, "Evolution and control of oxygen order in a cuprate superconductor" *Nature Materials* (2011) in press.
3. N. Poccia, A. Ricci, D. Innocenti, and A. Bianconi, "A possible mechanism for evading temperature quantum decoherence in living matter by feshbach resonance." *International Journal of Molecular Sciences* 10, 2084-2106 (2009).

XIX

C. Di Castro,
J. Zaanen
G. Aeppli
R. S. Markiewicz

Frustrated Phase Separation in Cuprates, Past and Present

Carlo Di Castro
Dipartimento di Fisica, "La Sapienza" Roma Italy

I will overeview the relevance of heterogeneity in understanding the physics of the Cuprates: difficulties, problems and solutions suggested along the years.
I will focus on the latest results related to 1) the involvment of both charge and spin critical fluctuations and the crossover of their relative weigt around optimal doping, marking quantum criticality. (S. Caprara et al.); 2) finally at low doping I will outline the nemaic stripe segment formation ending with a vortex and antivortex and showing dipolar nematic orientation. (G. Seibold et al.)

Observing the origin of superconductivity in quantum critical metals.

Jan Zaanen
Inst. Lorentz for Theoretical Physics, Leiden University, The Netherlands.
jan@lorentz.leidenuniv.nl

Despite intense efforts during the last 25 years, the physics of unconventional superconductors, including the cuprates with a very high transition temperature, is still a controversial subject. It is believed that superconductivity in many of these systems originates in the physics of quantum phase transitions in strongly correlated metallic systems, but quite diverse perspectives have emerged on the fundamentals of the electron-pairing physics, ranging from Hertz style critical spin fluctuation glue to the holographic superconductivity of string theory. We will demonstrate that the gross energy scaling differences that are behind these various pairing mechanisms are directly encoded in the frequency and temperature dependence of the dynamical pair susceptibility. This quantity can be measured directly via the second order Josephson effect and it should be possible employing modern experimental techniques to build a `pairing telescope' that gives a direct view on the origin of quantum critical superconductivity.

Simplicity and complexity of the cuprates in real and reciprocal space

Gabriel Aeppli
University College London, Department of Physics and Astronomy, 17-19 Gower Street, London, WC1H 0AH , UK

gabriel.aeppli@ucl.ac.uk

The cuprates have driven the development of experimental technology as well as ideas in condensed matter physics. Momentum and real space probes have undergone major improvements over the last 25 years, and what has emerged is that they are both necessary to obtain a description of the transition metal oxides. After reviewing some of the very simple behaviour found in reciprocal space for these complex materials, we describe some recent and arguably less simple results uncovered by mixed k-space/real-space approaches

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Origins of Stripes in Cuprates: Nesting vs Phase Separation

R.S. Markiewicz[1], G. Seibold[2], J. Lorenzana[3], and A. Bansil[1]
[1]*Physics Department, Northeastern University, Boston MA 02115, USA*
[2]*Institut Fur Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany*
[3]*ISC-CNR and Dip. di Fisica, "Sapienza" University. of Rome ,Piazzale Aldo.Moro 2, 00185 Roma, Italy*

R.S. Markiewicz
markiewic@neu.edu

Recent evidence has strongly suggested that the cuprates can best be understood as having intermediate correlation strength. In this case, the leading competing order phases should be stabilized by Fermi surface nesting, and hence phase diagrams can be constructed based on the first principles LDA band structure. We find that stripe-like charge or spin density wave phases readily form, but that the nesting vectors are different for different cuprates.
We also find that the nesting phase can become unstable with respect to a nanoscale phase separation. We illustrate this with the example of $La_{2-x}Sr_xCuO_4$, where there is considerable evidence for a phase separation regime at very low doping, with a crossover from phase separation stripes to nesting stripes as doping increases.

key words: density waves, phase separation, nesting

XX

X. Zhou
T. Mizokawa
N. Mannella
T. Yoshida

Distinct Fermi Surface Topology and nearly Isotropic Superconducting Gap in the $A_xFe_{2-y}Se_2$ (A=K, Tl, Rb and etc.) Superconductor

Xingjiang Zhou
National Lab for Superconductivity, Institute of Physics of Physics, Chinese Academy of Sciences, Beijing, China
XJZhou@aphy.iphy.ac.cn

High resolution angle-resolved photoemission measurements have been carried out to study the electronic structure and superconducting gap of the newly discovered $A_xFe_{2-y}Se_2$ [A=K, (Tl,K) and (Tl,Rb)] superconductors[1,2]. Distinct Fermi surface topology, consisting of two electron-like Fermi surface sheets around the $\Gamma(0,0)$ point and an electron-like Fermi surface sheet near the $M(\pi,\pi)$ point, was revealed in all these samples. Both the electron-like Fermi surface sheet near M point and the large electron-like Fermi surface sheet near Γ point show nearly isotropic superconducting gap without nodes. The information on the Fermi surface topology and superconducting gap of this new $A_xFe_{2-y}Se_2$ superconductor will provide key insights and constraints to understand the superconductivity mechanism in iron-based superconductors.

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Orbital degeneracy, Jahn-Teller effect, and superconductivity in transition-metal chalcogenides

T. Mizokawa[1], T. Sudayama[1], Y. Wakisaka[1], K. Ikedo[1], S. Pyong[2], M. Nohara[2], T. Noji[3], Y. Koike[3], M. Arita[4], H. Namatame[4], M. Taniguchi[4,5], N. L. Saini[6]

[1]*Department of Complexity Science and Engineering & Department of Physics,University of Tokyo, 5-1-5 Kashiwanoha, Chiba 277-8561, JP*

Department of Physics, Okayama University, Kita-ku, Okayama 700-8530, Japan

[3]*Department of Applied Physics, Tohoku University, Sendai 980-8578, Japan*

[4]*Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashihiroshima, Hiroshima 739-0046, Japan*

[5]*Graduate School of Science, Hiroshima University, Higashihiroshima, Hiroshima 739-8526, Japan*

[6]*Department of Physics, University of Roma "La Sapienza", P. A. Moro 2, 00185 Roma, Italy*

T. Mizokawa

* *mizokawa@k.u-tokyo.ac.jp*

We have studied the electronic structure of $FeSe_{1-x}Te_x$ and $Ir_{1-x}Pt_xTe_2$ using multi-orbial d-p model calculations and photoemission spectroscopy experiments. For $FeSe_{1-x}Te_x$, angle-resolved photoemission results indicate that the Fe 3d yz/zx orbital degeneracy in the tetragonal lattice plays important roles for the superconductivity. It is suggested that the Jahn-Teller instability of the yz/zx states couples with local lattice distortion derived from the Te substitution for Se and provides an inhomogenious electronic state. The model calculation shows that orbitally-deriven excitonic couping [1] is responsible for the orthorhombic distortion of FeSe and that the Te substitution supresses the excitonic effect. This situation is very similar to that of the FeAs-based superconductors. On the other hand, it is expected that the orbitally-deriven Peierls transition [2] is responsible for the structural transition in $IrTe_2$ with triangular lattice. The Pt substitution for Ir suppresses the band Jahn-Teller effect of the Ir t_{2g} states and induces an inhomogeneous electronic state which is different from that of $FeSe_{1-x}Te_x$.

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Keywords: ARPES, chalcogenides, orbital degeneracy, excitonic insulator

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Title

Normann Mannella

University of Tennessee-Knoxville, Department of Physics and Astronomy., USA

nmannell@utk.edu

Three-dimensional Fermi surfaces and nesting properties in iron pnictide superconductor revealed by angle-resolved photoemission spectroscopy

Teppei Yoshida[1,2],
[1]*Department of Physics, University of Tokyo, Japan*
[2] *JST, Transformative Research-Project on Iron Pnictides (TRIP), Japan*
yoshida@wyvern.phys.s.u-tokyo.ac.jp

Most of experimental studies on the iron-pnictide superconductors have so far indicated that the superconducting gap opens on the entire Fermi surfaces in contrast to the *d*-wave superconducting gap in the high-T_c cuprate superconductors. However, the isovalent-substituted system $BaFe_2(As_{1-x}P_x)_2$ shows signatures of superconducting gap with line nodes [1]. This fact would give critical information to clarify the pairing mechanism in the iron pnictide superconductors. According to the theory of spin-fluctuation-mediated pairing mechanism, three-dimensional nodes in the superconducting gap may appear in the strongly warped hole Fermi surface [2]. Therefore, it is crucial to reveal the three-dimensional electronic structure of the $BaFe_2(As_{1-x}P_x)_2$ superconductor in order to elucidate the relationship between Fermi surface nesting, superconductivity, and gap symmetry. By angle-resolved photoemission spectroscopy, we find that one of the hole Fermi surfaces has a highly three-dimensional shape and shows poor nesting with the electron Fermi surfaces at the optimal composition. This hole Fermi surface becomes disconnected along k_z direction for large *x* where the superconductivity disappears, which may lead to the suppression of superconductivity.

This work has been done in collaboration with I. Nishi, S. Ideta, A. Fujimori, T. Shimojima, W. Malaeb, S. Shin, Y. Nakashima, H. Anzai, M. Arita, A. Ino, H. Namatame, M. Taniguchi, M. Kubota, K. Ono, S. Kasahara, T. Shibauchi, T. Terashima, Y. Matsuda, M. Nakajima, S. Uchida, Y. Tomioka, T. Ito, K. Kihou, C. H. Lee, A. Iyo, H. Eisaki, H. Ikeda, and R. Arita

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XXI

M. Grilli
E. Carlson
B. M. Anderson
Y. Song
P. Thalmeier

Dynamical charge and spin fluctuations: is this the glue in cuprates?

S. Caprara, C. Di Castro, and M. Grilli
ISC and Dipartimento di Fisica, Università "La Sapienza"; Roma, Italy
M. Grilli
marco.grilli@roma1.infn.it

We address the s-called “glue issue” in the cuprates, investigating the effective electron-electron interaction responsible for the unusual normal state properties and the high critical temperatures of these materials. Since the electronic structure of superconducting cuprates displays a strong tendency to charge and spin inhomogeneity (possibly related to a hidden order in the underdoped region), charge and spin fluctuations have a marked dynamical character and specific momentum, frequency, doping, and temperature dependencies leaving distinct signatures in optical and Raman spectra. Our analysis of Raman spectra in $La_{2-x}Sr_xCuO_4$ identifies these dynamical modes as the relevant ingredients of the glue in cuprates, with a dominance of spin at low-intermediate dopings and with charge modes becoming prominent above optimal doping [1]. This indicates that a nearly ordered state with coexisting spin and charge order supports the superconducting pairing.
Once these relevant modes have been identified, angle-resolved photoemission spectra (ARPES) can be calculated showing that: i) charge-spin dynamical fluctuations can be responsible for the observed loss of superconducting coherence in underdoped cuprates and ii) for the appearance of shadow signatures of order at intermediate energy, while leaving the low-energy Fermi surfaces unaffected [2]; iii) “kinks” in the electronic dispersions can occur when the quasiparticles scatter with these dynamical collective excitations. In particular we find that spin modes are more visible in the kinks of the antinodal regions, while the charge fluctuations having a marked phononic character are responsible for the kink in the nodal regions [3].

Key words: cuprate superconductors; stripes; spectroscopy; quantum criticality

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Spatial Complexity Due to Incipient Electronic Nematicity in Cuprates

Erica W. Carlson
Purdue University, Dept. of Physics ,525 Northwestern Ave., West Lafayette IN 47907-2036, USA
ewcarlson@physics.purdue.edu

Surface probes such as scanning tunneling microscopy (STM) have detected complex patterns at the nanoscale, indicative of electronic inhomogeneity, in a variety of high temperature superconductors. In cuprates, the pattern formation is associated with the pseudogap phase, a precursor to the high temperature superconducting state. Rotational symmetry breaking of the host crystal (i.e. from C4 to C2) in the form of electronic nematicity has recently been proposed as a unifying theme of the pseudogap phase; however the fundamental physics governing the nanoscale pattern formation has not yet been identified.
Here we use universal cluster properties extracted from STM studies of cuprate superconductors in order to identify the fundamental physics controlling the complex pattern formation. We find that the pattern formation is set by a delicate balance between disorder, interactions, and material anisotropy, leading to a fractal nature of the cluster pattern. The method we introduce may be extended to a variety of surface probes, enabling the direct measurement of the dimension of the phenomenon being studied.

Phase separation and slow long-range magnetic order rearrangement in frustrated $Ca_3Co_2O_6$

S. Agrestini[1], M. R. Lees[2], C. L. Fleck[3], L. C. Chapon[4] and C. Mazzoli[5]
[1]*Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*
[2]*Department of Physics, University of Warwick, Coventry, UK*
[3]*ISIS facility, Rutherford Appleton Laboratory, Didcot, UK*
[4]*European Synchrotron Radiation Facility, Grenoble, France*

Stefano Agrestini
stefano.agrestini@cpfs.mpg.de

The observation of a sequence of stair-step jumps, equally spaced in magnetic field, in the magnetization of the spin chain system $Ca_3Co_2O_6$ has aroused great interest in the scientific community [1]. Nevertheless a flurry of research activities the origin of this intriguing magnetic phenomenon is still elusive. Here we present a detailed neutron diffraction study of $Ca_3Co_2O_6$ as a function of temperature [2], magnetic field [3] and time [4]. Our results have allowed us to finally clarify the actual magnetic ground state of this frustrated magnetic system and to observe a novel striking magnetic phenomenon: the first experimental evidence of an ultra-slow evolution between two long-range magnetically ordered states having completely different translation symmetry. This transition occurs over an unprecedented time-scale of several hours and is never complete. This discovery shed a complete new light on the peculiar dynamical properties of $Ca_3Co_2O_6$ and on the microscopic mechanism originating the steps in the magnetization.

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Local Disorder Effects on the Density of States and Optical Conductivity in Double-Layered Superconductors

Long He, Yun Song
Department of Physics, Beijing Normal Uinversity, Beijing 100875, China.

Yun Song
yunsong@bnu.edu.cn

The kernel polynomial method is extended to investigate the double-layered inhomogeneous superconductors by solving self-consistently the Bogoliubov-de Gennes equations under the mean-field description. The influences of Anderson disorder on the arithmetically and geometrically averaged local density of states are presented to show the localization of electronic states in the double-layered square, triangular and hexagonal lattices, respectively. Comparing with the square lattice, an extensive electron delocalization is found to closely relate to the suppression of the inter-valley scattering in hexagonal lattice. Furthermore, we provide numerical results of the local disorder effects on the behaviors of optical conductivity, which show clearly the distinct influences of the competitions between superconducting order parameter and the strength of disorder in different conditions. The present results provide new insight into the puzzling experimental observations on the superconductivity in disordered double-layered cuprate superconductors and double-layered grahene.

Key words: inhomogeneous superconductor, kernel polynomial method, Anderson localization, optical conductivity.

Quantum effects in uniform and staggered moment of frustrated quasi-2D antiferromagnets

P. Thalmeier, B. Schmidt, And M. Siahatgar
Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

P. Thalmeier
thalm@cpfs.mpg.de

We investigate the frustrated two-dimensional S=1/2 next nearest neighbor anisotropic Heisenberg antiferromagnet on a square lattice. We use spin-wave theory and exact diagonalization in a magnetic field for finite tiles [1] including a new method for the finite size scaling procedure. The induced uniform and the staggered moment in the antiferromagnetically ordered phases are calculated. They deviate strongly from classical behaviour depending on frustration ratio J_2/J_1 and the exchange anisotropy. The magnetization becomes strongly nonlinear [2] and is suppressed from the classical value. This is due to enhanced quantum fluctuations already at moderate frustration. In contrast, applying a magnetic field up to one half of the saturation field stabilizes the staggered moment in the striped columnar (CAF) and Neel (NAF) antiferromagnetic phases. This field-induced stabilization is most pronounced for frustration ratios J_2/J_1 near the edges of the phase diagram where quantum fluctuations tend to destroy NAF and CAF order. For small spatial exchange anisotropy, the field dependence of the staggered moment uniquely determines the exchange parameters. This allows to derive the frustration ratio J_2/J_1 from the field dependence of magnetic neutron diffraction data. We apply the theory to layered V oxides, quasi-2D organic Cu compounds and the anisotropic case to Fe pnictides.

keywords: quasi-2D antiferromagnets, staggered moment, exchange frustration

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XXII

J. Karpinski
E. Liarokapis
T. Perring
B. O. Wells

Doping and substitutions in LnFeAsO single crystals grown at high pressure: influence on superconducting properties and structure

J. Karpinski[1], N.D. Zhigadlo[1], S. Katrych[1], Z. Bukowski[1], P. Moll[1], R. Puzniak[1], K. Rogacki[1], B. Batlogg[1], S. Weyeneth[2], H. Keller[2]
[1]*Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland;*

[2]*Physik-Institut der Universität Zürich, 8057 Zurich, Switzerland;*

J. Karpinski
karpinski@phys.ethz.ch

An overview of the basic superconducting properties measured on single crystals of LnFeAsO (Ln = La, Pr, Nd, Sm, Gd) will be presented. LnFeAsO single crystals were grown from NaCl/KCl and NaAs/KAs fluxes at high-pressure of 30 kbar. Application of NaAs flux let to mm size of LnFeAsO crystals. Superconductivity was induced by partial substitution of O by F, Sm by Th, Fe by Co, As by P and by oxygen vacancies. By comparing our experimental data for (Sm,Th)FeAsO, SmFeAs(O,F) and SmFe(As,P)O it was found that the pnictogen height is a key factor that determines the superconducting critical temperature and thus many other properties. In all superconducting samples after doping the charge-reservoir SmO layer moves closer to the superconducting FeAs layer which facilitates electron transfer. In SmFe(As,P)O samples superconductivity appears only after high pressure treatment which generates oxygen deficiency and induces electron doping. P substituted SmFeAsO samples without O deficiencies are non-superconducting however spin density wave is suppressed. Our detailed study of the magnetic and transport properties of SmFeAs(O,F) single crystals reveals a promising combination of high and nearly isotropic critical current densities exceeding $2x10^6$ A/cm^2.

Key words: *R*FeAsO; high pressure; single crystals

Lattice Anomalies In Iron Pnictides

E. Liarokapis[1], A. Antonakos[1], N.D. Zhigadlo[2], S. Katrych[2], and J. Karpinski[2]
[1]*Department of Physics, National Technical University of Athens, Athens 15780, Greece*
[2]*Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland*

E. Liarokapis
Email: eliaro@central.ntua.gr

The discovery of superconductivity in Fe pnictides attracted the interest of scientific community since they have high T_c and a similar phase diagram with the cuprates. As in cuprates, the undoped compound is an antiferromagnet that becomes superconducting at certain doping levels. It appears that lattice effects and the geometry of the $FeAs_4$ tetrahedra are important to their properties. In an oxygen deficient $NdFeAsO_{0.85}$ sample high resolution synchrotron diffraction data[1] and Fourier Transform Infrared measurements[2] have shown lattice anomalies that start around 180K and disappear at T_c. Evidence of a similar softening at the spin density wave transition temperature ~178K and an anomaly across T_c has been observed in a Raman study of superconducting $R_{1-x}K_xFe_2As_2$ (R=Ba,Sr)[3]. In this work we present a systematic Raman investigation of phonon anomalies at low temperatures (10-300K) in single crystals of (1111) oxypnictides with various substitutions and doping levels. We find phonon modifications that begin at temperatures higher than T_c and are much stronger for the modes related with vibrations of the $FeAs_4$ tetrahedra. The dependence of these lattice anomalies on doping and their association mostly with the superconducting Fe-As planes point to their connection with the carriers and superconductivity.

Keywords: Pnictides, lattice effects, Raman spectroscopy

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Itinerant Spin Excitations in $SrFe_2As_2$ Measured by Inelastic Neutron Scattering

R.A Ewings[1], T.G. Perring*[1], J. Gillett[2], S.D. Das[2], S.E. Sebastian[2], A.E. Taylor[2], T. Guidi1, A.T. Boothroyd[3]

[1] *ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, United Kingdom.*

[2] *Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom.*

[3] *Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom.*

Perring T.G.

toby.perring@stfc.ac.uk

We report inelastic neutron scattering measurements of the magnetic excitations in $SrFe_2As_2$, the parent of a family of iron-based superconductors [1]. The data extend throughout the Brillouin zone and up to energies of ~260meV. We find that the spectrum calculated from the often-used local-moment J_1-J_2 model fails to explain the data in several key respects. At a temperate of 6 K, well below the joint magnetic and structural ordering temperature $T_{S,N}$=192 K, the data cannot be explained by a single set of parameters J_{1a} , J_{1b} and J_2 (here J_{1a} and J_{1b} are the two nearest-neighbour exchange parameters in the iron planes, with J_{1a} ⑦$|J_{1b}|$), and above ~100meV the excitations are strongly damped. Moreover, on warming above $T_{S,N}$ into the tetragonal phase, one would expect $J_{1a} \equiv J_{1b}$ and hence a soft mode at **Q**=(0.5,0.5), referenced to the Fe square lattice, due to frustration in the local-moment model. However the spectrum is largely unaltered with respect to that measured in the ordered phase.

The qualitative features of the magnetic excitation spectrum that cannot be described by the J_1-J_2 model, in particular the lack of a soft mode at **Q**=(0.5,0.5), are readily explained by calculations from a 5-band itinerant mean-field model [2] without invoking additional broken symmetry. We will discuss the implications of results for theories that do invoke additional symmetry breaking, such as electronic nematic [3] or orbital ordering [4], to explain the lack of a soft mode.

Key words: Fe-based superconductors, itinerant magnetism, nematic order

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Phase Diagram for Iron-Chalcogenide Superconducting Films

Yuefeng Nie, Donald Telesca, Joseph I. Budnick, Boris Sinkovic and Barrett O. Wells
Department of Physics, University of Connecticut, Storrs, CT 06269
Barrett O. Wells
wells@phys.uconn.edu

Fundamental to the understanding of exotic phenomena in novel superconductors is an understanding of the underlying phase diagram. For example, for cuprate superconductors, discussion of the physics is framed by the material's evolution with charge-doping from antiferromagnetic insulator to an under-doped region with a mysterious pseudo-gap and then an overdoped regime with more traditional behavior. For the Fe-based superconductors there are many phase diagrams for specific systems but a universal phase diagram is not clearly established. Our work on the contrasting behaviour of films of FeTeOx and FeSeOx provides a hint at the controlling parameters that underlie such a phase diagram.
The 11-type Fe-chalcogenide superconductors have the simplest crystal structure of the Fe-based superconductors, making it a useful model compound. In the bulk, FeTe is a non-superconducting, magnetic parent compound for this family. Typically, FeTe is made superconducting by isovalent substitution of Se or S onto Te sites. We have grown FeTe, FeSe, and $FeTe_{0.5}.Se_{0.5}$ films on MgO and $SrTiO_3$ substrates using pulsed laser deposition. The freshly grown films have essentially the same structure and resistivity profile as bulk samples. However, oxygen can easily be incorporated into these films. This oxygenation causes FeTe to become superconducting with an onset temperature is near 13 K but suppresses superconductivity in FeSe; representative resistivity profiles are shown in the left panel below. In both cases, Fe evolves to have a fairly localized Fe^{3+} configuration as measured by both XAS and XPS. A schematic low temperature phase diagram for these compounds is illustrated in the right panel below.
Key Words: Fe based superconductivity, phase diagrams, thin films
For more see *Phys. Rev. B* **82**, 020508 (2010) and http://arxiv.org/abs/1102.2155
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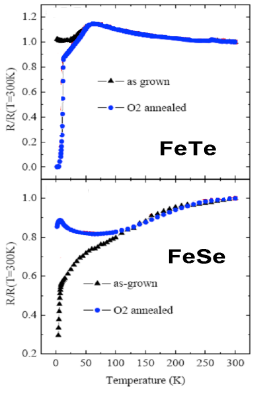

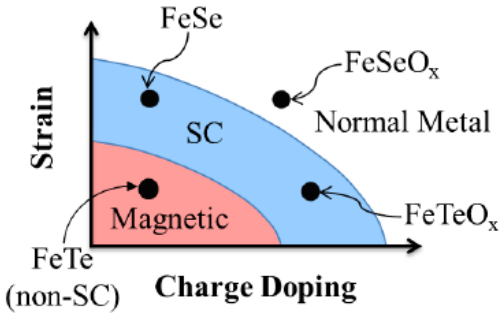

XXIII

N. Kirova
M. Salluzzo
K. Kanoda
F. Baumberger

Field-induced deformations in CDW materials revealed by the coherent X-ray micro diffraction.

D. LeBoloc'h and N. Kirova
LPS, CNRS & University Paris-Sud, Orsay, France

N. Kirova
kirova@lps.u-psud.fr

Charge density wave (CDW) is an electronic crystal typically formed in quasi one dimensional conductors; that gives rise to standard diffraction satellites. The CDW can be stressed by an electric field or a current which may give rise to local or long range modulation instabilities. The distortions' scale ~1000 of CDW periods is too long for the STM and too short to be studied by the conventional X-ray diffraction. The new method of the coherent micro diffraction provides a necessary access; this is what we shall report here together with the theoretical modeling. The experiments performed on two CDW compounds: Blue Bronze $K_{0.3}MoO_3$ and $NbSe_3$, reveal drastically different scenario of the CDW reaction to the applied electric field. $K_{0.3}MoO_3$ develops a coherent, periodic, unharmonic superstructure which develops only in the chain direction. Contrary, in $NbSe_3$ only the shift of the CDW wave number is registered along the chain direction, while a complex behavior is discovered for the inter-chain direction. Below the threshold electric field, a broad multiple peak structure appears which can be associated with the creep effects. Above the critical field, the structure evolves into two non symmetric transverse peaks which is amusing in view of the mirrow symmetry for the transverse wave number equal zero for the CDW in $NbSe_3$. We model both scenario by invoking formation of dislocations. The longitudinal structure is due to regular arrays of dislocation lines built in response to the surface charge depletion. The transverse effect is due to dislocations accumulation or the order parameter suppression at the stepwise crystal shape defects.

Keywords: CDW, coherent microdiffraction, dislocation

Signature of nanoscale modulation, charge and orbital order at the interface between $LaAlO_3$ and $SrTiO_3$ band insulators

M. Salluzzo[1]
[1]*CNR-SPIN, Complesso Universitario Monte S. Angelo, Via Cintia I-80126 Napoli, Italy*
e_mail : marco.salluzzo@spin.cnr.it

The formation of a two dimensional electron gas (2DEG) at the interface between $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) heterostructures gave rise to a huge interest since its discovery [1], because of the intriguing functionalities related to this phenomenon, including high electron mobility [2], large magnetoresistance [3], and superconductivity [4].
The mechanism behind this phenomenon have not yet fully understood and several issues, like the real ground state of the system, the presence of electron correlations and the role of defects, are strongly debate.
Here, an overview of the established results as well as of the present understanding of the phenomena of electronic reconstruction at the LAO/STO interface will be given. The fingerprints of the occurrence of an orbital reconstruction is obtained by X-ray absorption spectroscopy (XAS) [5], and consistes in the removal of the 3d orbital degeneracy and corresponding lowering of the titanium $3d_{xy}$ states at the interface.
In addition, scanning-tunneling spectroscopy shows that the interface is characterized by an ordered electronic superstructure (6x8 nm^2), incommensurate with lattice [6]. Spectroscopy maps, with nm resolution, suggests that the superstructure is due to the combination of an electronic and structural reconstruction effects. By comparing our LDOS data with the LDA+U calculations, we conclude the superstructure is associated to an ordered arrangement of the 3d orbitals. These phenomena, like orbital order and charge order, are typical of electron-correlated systems.

Key words: 2D electron gas; oxides;

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Mottness, Spin Frustration and Superconductivity in Organics

K. Kanoda
Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan
e mail:kanoda@ap.t.u-tokyo.ac.jp

Strong electron correlation is considered to mediate superconducting electron pairing. The layered organic systems κ-$(ET)_2X$ with a variety of anions, X, provide playgrounds for Mott physics in two dimensions. Because the conducting layer is modeled to triangular lattice whose anisotropy is varied by X, spin frustration as well as Coulomb repulsion plays an important role in the nature of ground state. Depending on the anisotropy of the triangular lattice, an antiferromagnic state (for $X=Cu[N(CN)_2]Cl$) or a spin liquid state (for $X=Cu_2(CN)_3$) appears in the Mott insulating phases, and both give way to superconducting state when pressurized or doped. In this conference, I review the nature of the two Mott insulators, the criticality of Mott transition, superconductive nature and pseudo-gapped behavior, shedding light on the role of electron correlation and spin frustration in the emergence of superconductivity.

This presentation is based on the work in collaboration with K. Miyagawa, Y. Shimizu, F. Kagawa, Y. Kurosaki, T. Furukawa, H. Hashiba, H. Oike, H. Kasahara, H. Taniguchi, S. Yamashita, Y. Nakazawa, M. Maesato and G. Saito.

Key words; Mott criticality, triangular lattice, spin liquid, pseudogap, nodal superconductivity

Surface 2DEGs on transition metal oxides and topological insulators

F. Baumberger[1], P.D.C. King[1], W. Meevasana[1,2,3], P. Hofmann[4], Z.-X. Shen[2]
[1]*School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, United Kingdom,*

[2]*Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA,*

[3]*School of Physics, Suranaree University of Technology, Nakhon Ratchasima, 30000 Thailand,*

[4]*Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark*

F. Baumberger[1]
felix.baumberger@st-andrews.ac.uk

Following the seminal demonstration by Ohtomo and Hwang of a high-mobility two-dimensional electron gas (2DEG) at the interface of the insulating oxides $LaAlO_3$ and $SrTiO_3$, this system rapidly became a leading contender for novel all-oxide devices. Here, we report the creation of a similar 2DEG at the bare $SrTiO_3$(100) surface and demonstrate control of its density through exposure of the surface to intense ultraviolet (UV) light. Using angle-resolved photoemission we directly image the sub-band ladder of the quantum confined Ti 3*d* states, revealing light effective masses coexisting with signatures of strong interactions. We further show that a similar approach can be used to create a 2DEG with large Rashba spin splitting in the topological insulator Bi_2Se_3. The splitting is dominated by the backside of the confining potential and reacts sensitively to the effective gating of the surface, which we control *in-situ* by adsorbing and desorbing residual gas. Such electrostatic control of the electron spin makes this system ideally suited for applications in spintronics.

Key words: transition metal oxides, topological insulators, two-dimensional electron gas, subband ladder, Rashba splitting, angle-resolved photoemission

XXIV

S. Sugai
M. Huecker
M. v. Zimmermann
G. Zheng A.
A. V. Mitin
R. Citro

Phonon-Induced Dynamical Spin Stripes and Plaquettes Observed by Raman Scattering in $YBa_2Cu_3O_y$

S. Sugai[1,2,3] and Y. Tamai[2]
[1]*Department of Physics, Arts and Science, Petroleum Institute, P.O.Box 2533, Abu Dhabi, UAE*
[2]*Department of Physics, Faculty of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*
[3]*TRIP, Japan Science and Technology Agency (JST), Chiyoda, Tokyo 102-0075, Japan*

S. Sugai
e-mail: ssugai@pi.ac.ae, sugai.shunji@h.mbox.nagoya-u.ac.jp

The cuprate high T_c superconductors have many anomalous experimental facts. The pseudo-spin-gap and the rapidly increasing isotope effect of T_c near the metal-insulator transition are two of them. Many physical quantities change at the pseudo-spin-gap transition temperature T^*, but many of them are passively induced by the opening of the pseudo-spin-gap. We took notice of the relation between the two-phonon Raman scattering peak and the pseudo-spin-gap, because both of them appear in the underdoped region. In the present Raman scattering experiment we found that the peak energy softens below T^*. This phonon mode is identified as the k=(1/8, 1/8) bond stretching mode by comparing the doping dependent phonon energy to the neutron scattering data. The anomaly at T^* is enhanced at y=6.5, because the energy coincides with the "hour-glass" dispersion of the magnetic susceptibility at (1/8, 1/8). We found that the isotope effect of the phonon energy decreases near the insulator-metal transition. So far all phonon energies are assumed to have the ideal isotope effect without deviation. If the spin system contributes to determine the phonon energy, the deviation can be induced. The spin system gets the isotope effect and can induce the anomalous isotope effect on T_c, if the spins cause the superconductivity. The stretching phonon mode at (1/8, 1/8) can create dynamical spin stripes and plaquettes, if the (1/8, 1/8) and (1/8, -1/8) modes are combined. The phonon-induced dynamical spin stripes and plaquettes may be the origin of the high T_c superconductivity.

key words: stripes, plaquettes, (1/8, 1/8) stretching phonon mode, pseudo-spin-gap, isotope effect

XXIV

Manipulating charge stripe order in $La_{2-x}Ba_xCuO_4$ in high magnetic fields

M. Hücker[1], M. v. Zimmermann[2], Z. J. Xu[1], J. S. Wen[1], G. D. Gu[1], J. M. Tranquada[1]

[1]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York, USA.*

[2]*Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany*

M. Hücker
huecker@bnl.gov

The observation of enhanced spin stripe order in the vortex cores of $La_{2-x}Sr_xCuO_4$ has been a landmark experiment that revealed the intimate connection between superconductivity and incommensurate antiferromagnetism. How exactly these phases are intertwined, whether they are interdependent or competing is still under debate. To the extent that a charge stripe order with in-plane wave vector $(2\delta,0)$ can be viewed as second harmonics of the spin stripe order with wave vector $(\delta,0)$, magnetic field enhanced charge stripes have been anticipated but not observed. Here we show by means of high energy single-crystal X-ray diffraction that in $La_{2-x}Ba_xCuO_4$ charge stripe order can indeed be enhanced in a strong magnetic field. The largest effects, however, are not observed at $x=1/8$ where stripe order is most pronounced and superconductivity strongly suppressed, but at $x\neq1/8$ where bulk superconductivity is dominant and zero field stripe order relatively weak. The results provide further evidence for electronically driven charge correlations in the vortex cores of the cuprates.

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key words: stripe order, vortex core states, high magnetic field

Competition of charge stripe order and superconductivity in $La_{1.89}Sr_{0.11}CuO_4$ tuned by a high magnetic field

Martin v. Zimmermann*[1], N. B. Christensen[2], J. Chang[3], J. Mesot[4], N. Momono[5], M. Oda[6], M. Ido[6], J. Tranquada[7] and M. Hücker[7]

[1]*Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany.*

[2]*Materials Research Division, Risø National Laboratory for Sustainable Energy, Technical University of Denmark, Roskilde, Denmark.*

[3]*Département de Physique and RQMP, Université de Sherbrooke, Sherbrooke, Québec, Canada*

[4]*Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*

[5]*Department of Materials Science and Engineering, Muroran Institute of Technology, Muroran, Japan*

[6]*Department of Physics, Hokkaido University, Sapporo, Japan*

[7]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York, USA.*

Martin v. Zimmermann
** martin.v.zimmermann@desy.de*

The role of stripe order on the physical properties of cuprate superconductors, in particular on their electronic transport and superconducting properties is still under debate. It has been shown that the application of a high magnetic field has a strong impact on the transport properties and the behavior was described by a 2-dimensional vortex glass phase. Furthermore, the field dependence of magnetic stripe order has been determined by elastic and inelastic neutron scattering for a variety of single and double layer cuprates. In several cases an enhanced magnetic stripe intensity is observed, which is interpreted as stripes forming inside magnetic flux lines. The behavior of concomitant charge order under high magnetic fields is much less clear. We report on a high energy x-ray study that focused on magnetic field effects of the static charge stripe order in $La_{2-x}Sr_xCuO_4$ for a doping concentrations close to x=1/8. The results support 2-dimensional electronic models and demonstrate the competition of charge stripe order with superconductivity.

key words: charge stripe order, x-ray diffraction, high magnetic field

Pseudogap ground state and its doping evolutionof the high-Tc cuprates $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$:NMR study under high magnetic-fields up to 44 T

Guo-qing Zheng
Okayama University, Department of Physics, Japan
zheng@science.okayama-u.ac.jp

We study the zero-temperature-limit pseudogap state and the doping evolution of the hole-doped cuprate superconductor $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ under high magnetic fields up to 44 T. We have obtained a complete phase diagram that spans from an antiferromagnetic insulating state, to a pseudo-gapped superconducting state, and into a conventional metallic state for the single-layered $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$.

Over a wide doping range of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, a pseudogap shows up before a superconducting state sets in. We find that there remains substantial density of states at the Fermi level when the superconductivity is removed by applying a very strong magnetic field [1], which suggests that the ground state of the pseudogap is a “Fermi-patch ” metal. This is in contrast to the electron-doped counterpart in which the zero-temperature normal state is a correlated Laudau Fermi liquid [2]. We will also present results on the doping evolution of the Fermi surface remnant, and discuss the implications [3].

This work was done in collaboration with S. Kawasaki (Okayama U), A.P. Reyes, P.L. Kuhns (NHMFL), and C.T. Lin (MPI-Stuttgart).

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Striped Organization of Hole Excitations and Oxygen Interstitials in Oxygen-Doped Cuprates

A. V. Mitin

P. L. Kapitza Institute for Physical Problems, Kosygin Str., 2, 119334, Moscow, Russian Federation

mitin@kapitza.ras,ru

There is increasing evidence that the conundrum of cuprate underlying physics has to bear in mind the local lowering of crystal symmetry. In light of the approaches developed, the bound states of dopant ions and hole orbitals in lightly doped cuprates can be treated as a kind of inverse pseudoatoms, which tend to arrange into chains. As a result, the superconducting correlations of charge and spin degrees of freedom should be accompanied by convolution of one axis belonging to the coordinate sector of phase space. The kinetics of paired holes in CuO_2 layers, hence, has to be confined within extended quantum protectorates – bosonic stripes (BS). Modeling this situation for $YBa_2Cu_3O_{6+\delta}$ showed that the formation of frustrated network composed of the narrowest BS with a minimal width $w_n = 2a$ could be displayed as maxima in transport properties at $T \leq 1200$ K, where a is the mean Cu-O interval in CuO_2 layers. This prediction was confirmed experimentally. When δ is increased, the width w_n of dominating BS tends to expand, while their thermostability drops. According to this scenario, the significant difference in superconducting properties of optimally doped $YBa_2Cu_3O_{6+\delta}$ and $La_2CuO_{4+\delta}$ has to be caused by peculiarities of hole organization into BS with $w_n = 6a$ and $12a$, respectively. The simulated parameters for $HgBa_2Ca_2Cu_3O_{8+\delta}$, $YBa_2Cu_3O_{6+\delta}$ and $La_2CuO_{4+\delta}$ are consistent with experimental data. It is shown that the concept of BS hierarchy may help to reveal the puzzling nature of superconducting state in cuprates and its interrelation with pseudogap regime, where the nanochannels from BS would survive well above room temperature.

Key words: cuprates, hole segregation, stripes, electronic properties, superconductivity

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Phonon anomaly and spectral kinks in cuprates: Interplay between charge-lattice interaction and strong electron correlations

R. Citro*[1], G. De Filippis[2] , V. Cataudella[2] , C.A. Perroni[2], A. S. Mishchenko[3,4], N. Nagaosa[3,5]

[1] SPIN-CNR and Dipartimento di Fisica "E. R. Caianiello", Università di Salerno - I-84100 Salerno, Italy, EU, [2] SPIN-CNR and Dipartimento di Scienze Fisiche, Universit`a di Napoli Federico II - I-80126 Napoli, Italy, EU. [3] Cross-Correlated Materials Research Group (CMRG), ASI, RIKEN - Wako 351-0198, Japan, [4] RRC "Kurchatov Institute" - 123182 Moscow, Russia, [5] Department of Applied Physics, The University of Tokyo - 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

R. Citro

***c**itro@sa.infn.it; Tel: 089 969187*

We investigate the interplay between strong electron correlations and charge-lattice interaction in cuprates. The coupling between half-breathing bond-stretching phonons and doped holes in the t-t'-J model is studied by the limited phonon basis exact diagonalization method. Nonadiabatic electron-phonon interaction leads to the splitting of the phonon spectral function at half-way to the zone boundary at a critical wavevector qs = {(±π/2, 0), (0,±π/2)} and to low-energy kink feature in the electron dispersion[1], in agreement with experimental observations. Another kink due to strong electron correlation effects is observed at higher energy, depending on the strength of the charge-lattice coupling. A possible interpretation of the origin of phonon anomaly in terms of the interaction with the charge mode observed in the mid-infrared in the optical conductivity experiments[2] is also discussed.

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XXV

A. Yaresko
V. B. Zabolotnyy
T. Mertelej
M. Tortello
A. Iadecola
A. Ricci
L. Stojchevska

On the nature of an energy barrier between (π,0) and (0,π) magnetic orders in Fe pnictides

A. Yaresko*, L. Boeri, O. K. Andersen
Max Planck Institute for Solid State Research, Stuttgart, Germany

A. Yaresko
* *a.yaresko@fkf.mpg.de*

As temperature is lowered most of undoped Fe arsenides, parent compounds for recently discovered Fe based superconductors, undergo a transition into a collinear state with stripe-like magnetic order in which anti-ferromagnetic (AFM) Fe chains order ferromagnetically along the direction perpendicular to the chains. Two such collinear magnetic structures, characterized by ordering vectors (π,0) or (0,π), are connected by infinite number of non-collinear states with two AFM sublattices of second Fe neighbors rotated by an arbitrary angle with respect to each other. In a classical Heisenberg model all these states are degenerate. Band structure calculations show, however, that the degeneracy is lifted already at the mean field LSDA level and that in Fe arsenides (π,0) and (0,π) magnetic orders are separated by an energy barrier comparable to the energy difference between Neel and stripe AFM orders. We discuss a microscopic origin of the energy barrier and demonstrate that it is closely related to orbital degrees of freedom. The results for arsenides are compared to KFe_2Se_2 for which we found that a non-collinear 90-degree spin arrangement is more favorable than collinear ones. A doping dependence of the barrier is also discussed.

Keywords: electronic structure; superconductivity; exchange interactions

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Fermiology of LiFeAs and related iron pnictides as seen by ARPES

V. B. Zabolotnyy[*1], D. V. Evtushinsky[1], T. K. Kim[1], I. V. Morozov[1,2], A. N. Yaresko[3], A. A. Kordyuk[1], S. Aswartham1, G. Behr[1], S. Wurmehl[1], A. Vasiliev[2], R. Follath4, and B. Büchner[1], S. V. Borisenko[1]
[1]*Leibniz-Institute for Solid State Research, IFW-Dresden, D-01171 Dresden, Germany*
[2]*Moscow State University, Moscow 119991, Russia*
[3]*Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany*
[4]*Helmholtz-Zentrum Berlin, BESSY, D-12489 Berlin, Germany*

V. B. Zabolotnyy
v.zabolotnyy@ifw-dresden.de

We study LiFeAs family of single crystals, for wich LDA calculations predict absence of surface states. The measurements provide a direct access to the information on the low energy electronic structure, which includes the detailed knowledge of the Fermi surface, band renormalization, electronic self-energy and symmetry of the superconducting order parameter. Along with pristine compounds, the Co substituted samples were studied. The bottom of electron-like bands was found to sink by about 17 meV upon 5% Co doping, which indicates that the chemical substitution indeed results in charge doping.

key words: LiFeAs, Fermi surface, ARPES

Time resolved femtosecond optical spectroscopy of electron doped 1111 and 122 iron-pnictide superconductors

T. Mertelj[1], L. Stojchevska[1], P. Kusar[1], C. Gadermaier[1], V. V. Kabanov[1], and D. Mihailovic[1] Jiun-Haw Chu[2] and Ian R. Fisher[2], N. D. Zhigadlo[3], S. Katrych[3], Z. Bukowski[3], S. Weyeneth[4] and J. Karpinski[3]

[1]*Complex Matter Department, Jozef Stefan Institute, Jamova 39, Ljubljana, SI-1000 Ljubljana, Slovenia*

[2]*Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, California 94305, USA*

[3]*Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Switzerland*

[4]*Physik-Institut der Universität Zürich, 8057 Zürich, Switzerland*

T. Mertelj

e-mail: tomaz.mertelj@ijs.si

We present a systematic study of carrier relaxation dynamics on doping in F and Co doped Sm-1111[1,2] and Co doped Ba-122 iron pnictide superconductors.

In undoped and weakly doped samples a single relaxation process with a divergent relaxation time at the spin density wave (SDW) transition is observed. From the relaxation time at the room temperature the second moment of the Eliashaberg function is determined, which indicates a rather weak electron-phonon coupling.[3,4] Below T_{SDW} the temperature dependence of the relaxation indicates appearance of a bottleneck due to the opening of a charge gap in the SDW state with a BCS-like temperature dependence.

In the superconducting dome region multiple relaxation processes are present with distinct superconducting state quasiparticle recombination dynamics exhibiting a temperature dependent superconducting gap consistent with the BCS temperature dependence and a pseudogap-like response, similar to the pseudogap response in the cuprates, with onset around 200K. The polarization anisotropy of the pseudogap-like response links it to the presence of nematic fluctuations at temperatures up to 200K.

Key words: iron-pnictide superconductors, optical femtosecond spectroscopy, spin-density wave systems, carrier relaxation dynamics

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Point-contact Andreev-reflection spectroscopy in Fe-based superconductors: Multi-gap superconductivity and strong electron-boson interaction

M. Tortello,[1] D. Daghero,[1] G.A. Ummarino,[1] V.A. Stepanov,[2] N. D. Zhigadlo,[3] and J. Karpinski,3 J. Jiang,4 J.D. Weiss,4 E.E. Hellstrom,4 and R.S. Gonnelli1
1Dipartimento di Fisica, Politecnico di Torino, 10129 Torino, Italy. 2P. N. Lebedev Physical Institute, Russian Academy of Sciences, 119991 Moscow, Russia. 3Laboratory for Solid State Physics, ETHZ, CH-8093 Zurich, Switzerland 4Applied Superconductivity Center, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA

M. Tortello
mauro.tortello@polito.it

Point-contact Andreev-reflection spectroscopy measurements have been performed in Ba(Fe1-xCox)2As2 single crystals (x=0.1, Tc = 24.5 K) and SmFeAsO1-xFx polycrystals (x=0.09, Tc = 42 K and 0.2, Tc = 52 K) . Results obtained in the Co-doped Ba-122 compound indicate the presence of two superconducting gaps with no line nodes on the Fermi surface. The point-contact Andreev-reflection spectra also feature additional structures related to the electron-boson interaction (EBI), from which the characteristic boson energy nb(T) is obtained, very similar to the spin-resonance energy observed in neutron-scattering experiments. Both the gaps and the additional structures can be reproduced within a three-band s± Eliashberg model by using an electron-boson spectral function peaked at n0 = 12 meV = nb(0). Results on Sm-1111 compounds give reproducible evidence for multi-gap, nodeless superconductivity. EBI features have also been observed whose temperature dependence is not compatible with a phononic origin. Gaps and most of the EBI features can be reproduced within a three-band s± Eliashberg model by assuming n0 = 20 meV as given by the relation n0 = 4.65kBTc, inferred from neutron-scattering results on other Fe-based superconductors. The strong electron-boson coupling may also explain some anomalies in the PCAR conductance curves, namely the excess conductance at high energy, which greatly complicates the normalization of the conductance curves and sometimes prevents a good fit of the curves with models based on constant, BCS-like OPs.

key words: Point-contact Andreev-reflection spectroscopy, symmetry of the order parameter, strong-coupling superconductivity

Local atomic correlations in $FeSe_{1-x}Te_x$ iron-chalcogenides by EXAFS

A. Iadecola[1], B. Joseph[2] and N.L. Saini[1]
[1]*Dipartimento di Fisica, Università degli studi di Roma "Sapienza", Roma, Italy*
A. Iadecola
antonella.iadecola@gmail.com

S ocal structure of the $FeSe_{1-x}Te_x$ has been studied by extended absorption fine structure (EXAFS) measurements as a function of temperature. Temperature dependent Se K-edge polarized EXAFS measurements are made on the $FeSe_{0.25}Te_{0.75}$ single crystal, while both Se K-edge and Fe K-edge EXAFS are performed on polycrystalline $FeSe_{1-x}Te_x$. The Se-Fe bond length is found to be significantly shorter than the average crystallographic Fe-Se/Te distance, and almost equal to the one for the system without Te. This suggests that the Se and Te occupy distinct sites, indicating breaking of the average crystal symmetry with locally inhomogeneous atomic distribution. The mean square relative displacements (MSRD) of the Se-Fe bonds in the two crystallographic directions reveal different temperature dependence suggesting anisotropic atomic displacements. The results provide a clear evidence of local inhomogeneities and possible role of coexisting electronic components characterized by local structural configurations in the $FeSe_{1-x}Te_x$ superconductors.
Keywords: EXAFS, Local structure, Fe-based superconductors
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Direct evidence of nanoscale phase separation in the iron chalcogenide superconductor $K_{0.8}Fe_{1.6}Se_2$ from scanning nanofocused x-ray diffraction

A. Ricci[1], N. Poccia[1], B. Joseph[2]
[1]*Department of Physics, Sapienza University of Rome, P. le A. Moro 2, 00185 Rome, Italy*
[2]*National Institute of Material Science,1-2-3 Sengen, Tsukuba, 3050047 Japan.*
A. Ricci
alessandro.ricci@uniroma1.it

It is well known that phase separation is a common feature of high temperature superconductors. It has been proposed that the quantum macroscopic phase able to resist to the de-coherence attacks of high temperature takes advantage from material complexity such as frustrated phase separation. The technical advance in focusing the synchrotron radiation x-rays down to a beam size of 300 nm has been used to directly visualize the frustrated nanoscale phase separation in K0.8Fe1.6Se2 single crystal using scanning nano-focus x-ray diffraction. The mapping shows the spatial distribution of two phases : i) the magnetic expanded phase with superlattice modulation and ii) the superconducting compressed phase. The results provide a direct evidence for nano phase homogenous domains smaller than 300 nm and different micron size regions with percolating magnetic or superconducting domains forming a multiscale complex network of the two phases.

This work has been done in collaboration with G. Campi, G. Arrighetti, L. Barba, M. Reynolds, M. Burghammer, H. Takeya, Y. Mizuguchi, Y. Takano, M. Colapietro, N. L. Saini, A. Bianconi

Study of quasiparticle relaxation dynamics in $SrFe_2As_2$ spin-density wave iron-pnictide single crystals

L. Stojchevska[1], P. Kusar[1], T. Mertelj[1], V. V. Kabanov[1], X. Lin[2], G. H. Cao[2], Z. A. Xu[2] and D. Mihailovic[1]

[1] *Complex Matter Department, Jozef Stefan Institute, Jamova 39, Ljubljana, SI-1000 Ljubljana, Slovenia*

[2] *Department of Physics, Zhejiang University, Hangzhou 310027, People`s Republic of China*

L. Stojchevska

e-mail: ljupka.stojchevska@ijs.si

We present a study of quasiparticle relaxation dynamics and low-energy electronic structure in undoped $SrFe_2As_2$ in the normal and SDW state using optical pump-probe femtosecond spectroscopy. Below T_{SDW} the transients are dominated by a single exponential relaxation process across the SDW induced charge gap. At T_{SDW}=200 K we observe a remarkable critical slowing down in the quasiparticle relaxation dynamics presented in the form of a long-lived relaxation tail. Above T_{SDW} the amplitude of the initial subpicosecond relaxation strongly drops. From temperature dependence of the transient reflectivity amplitude we determine the SDW-state charge gap magnitude, $2\Delta_{SDW}/k_BT_{SDW}$=7.2±1. Moreover, we estimate the second moment of the Eliashberg function $\lambda<(\hbar\omega^2)>$=110±10 meV^2 from the relaxation time above T_{SDW}. We compare the results with our recent data in SmFeAsO and find that they are similar both in the normal and SDW state indicating a moderate electron phonon coupling.

Key words: optical pump-probe femtosecond spectroscopy, iron-pnictide superconductors, spin-density wave systems, carrier relaxation dynamics.

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XXVI

V. Dobrosavljevic
S. Feng
S.I. Mukhin
F. Giustino
T.M. Mendonça

Electronic Griffiths Phases and Quantum Criticality at Disordered Mott Transitions

Vladimir Dobrosavljevic
Department of Physic and National High Magnetic Field Laboratory Florida State University, Tallahassee, FL 32310, USA
Email: vlad@magnet.fsu.edu

The effects of disorder are investigated in strongly correlated electronic systems near the Mott metal-insulator transition. We find that correlation effects lead to strong disorder screening, a mechanism restricted to low-lying electronic states, very similar to what is observed in underdoped cuprates. Our results suggest, however, that this effect is not specific to disordered d-wave superconductors, but is a generic feature of all disordered Mott systems. In addition, we show that the resulting spatial inhomogeneity rapidly increases as the Mott insulator is approached at fixed disorder strength. This behavior, which can be described as an *Electronic Griffiths Phase*, displays all the features expected for disorder-dominated *Infinite-Randomness Fixed Point* scenario of quantum criticality.

Key words: disorder, Mott transitions, quantum criticality

Magnetic field induced reduction of the low-temperature superfluid density in cuprate superconductors

Shiping Feng**,** Zheyu Huang, and Huaisong Zhao
*Department of Physics, Beijing Normal University**,** Beijing, 100875, China*
Shiping Feng
E-mail: spfeng@bnu.edu.cn

Within the framework of the kinetic energy driven superconducting mechanism [1,2], the weak magnetic field induced reduction of the low-temperature superfluid density in cuprate superconductors is studied in the linear response approach [3,4]. The electromagnetic response kernel is evaluated by considering both couplings of the electron charge and electron magnetic momentum with a weak magnetic field [4] and employed to calculate the superfluid density based on the specular reflection model [5], then the main features of the weak magnetic field induced reduction of the low-temperature superfluid density [6] are well reproduced. The theory [4] also shows that the striking behavior of the weak magnetic field induced reduction of the low-temperature superfluid density is intriguingly related to both depairing due to the Pauli spin polarization and nonlocal response in the vicinity of the d-wave gap nodes on the Fermi surface to a weak magnetic field.

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Lax-pair and Hamiltonian Equations for Macroscopic Quantum Order of Correlated Electron System: Analytic Solution

S.I. Mukhin

Department of Theoretical physics and quantum technologies, Moscow Institute for Steel and Alloys, Moscow, Russia

**sergeimoscow@online.ru*

It is demonstrated by Lax-pair method for inverse scattering problem that there exists an exact quasi-classical solution of the Hubbard model that describes the quantum ordered state (QOS) of a correlated fermionic system. The QOS is represented by a classical macroscopic field i.e. the "quantum order parameter", QOP, that minimizes the Euclidian action of the fermionic system and breaks spontaneously the Matsubara's time invariance (Mukhin, 2010). The effective Euclidian action for the QOP is now derived exactly and it is shown that QOP dynamics along the Matsubara's "time" maps onto a completely integrable infinite dimensional system of degrees of freedom. The Green's function of the QOP has only second order poles in the complex plane of frequences. Hence, QOP does not scatter anything in Minkowski world and might be a candidate for a "hidden order" in high-Tc cuprates. The QOP as well may describe the "dark matter" state in our Universe. The fermionic system in the QOS is predicted to possess the fingerprints of the QOP that include the "light-mass fermions", the pseudo-gap in the fermionic spectrum, the suppressed linear specific heat of fermions at low temperatures, the peculiarities measurable by e.g. the ARPES experiments. An impact of QOS on the temperature of the Cooper-pairing and superconducting transition is also discussed.

Key words: quantum order, integrable infinite-dimensional system, dark mass, hidden order parameter, light-mass fermions.

Electron-phonon interaction and superconductivity in carbon materials

Feliciano Giustino
Department of Materials, University of Oxford, United Kingdom
Feliciano.Giustino@materials.ox.ac.uk

Carbon is wonder element which underpins life on our planet, represents currently the vast majority of our energy sources, and is arguably the building block of nanotechnology. Remarkably many allotropes of carbon have been reported to be superconductors, from zero-dimensional fullerenes to three-dimensional diamond. In this talk I will describe our theoretical and computational efforts to understand the interactions between electrons and phonons as well as the atomistic mechanism of superconductivity in bulk and nanostructured carbon materials. We have recently shown that the electron-phonon interaction is exceptionally strong in diamond, and leads to an unusually large zero-point renormalization of the electronic band structure [1]. This property is closely related to the superconductivity and the Kohn anomaly of boron-doped diamond. For B-doped diamond we investigated the atomistic origin of superconductivity and the Kohn anomaly, and in particular we elucidated the role of the boron dopants [2]. Superconductivity has also been demonstrated in two-dimensional carbon materials such as graphite intercalation compounds. Along this direction we investigated the strength of the electron-phonon interaction in graphitic nanomaterials such as single- and multi-layer graphene, and compared our calculations with angle-resolved photoemission measurements [3]. Finally we studied the electron-phonon interaction in the recently discovered graphane, the fully hydrogenated version of graphene [4]. For hole-doped graphane we computed an exceptionally large electron-phonon interaction, leading to a giant Kohn anomaly in the phonon dispersions and possibly to high-temperature superconductivity. I will conclude this talk by discussing the intriguing potential of sp3-bonded carbon nanostructures for superconductivity.

This work has been performed in collaboration with C.-H. Park, S. G. Louie, J. Noffsinger, M. L. Cohen, G. Savini, A. C. Ferrari.

Keywords: electron-phonon interaction, superconductivity, Kohn anomaly, diamond, graphene

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The complexity of oxygen inhomogeneities in Hg-based superconductors: a view with the magnifying glass of local probe techniques

T.M. Mendonça,[1,2,*] J.G. Correia[3], H. Haas[3], J.N. Gonçalves[4], P. Odier[2], C. Darie[2], J.P. Araújo[1]

[1] *IFIMUP and IN – Instituto de Nanociências e Nanotecnologias, Departamento de Física da Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal*
[2] *Institut Néel, CNRS, Av. des Martyrs 25, F-38042 Grenoble CEDEX 9, France*
[3] *Instituto Tecnológico e Nuclear, E.N. 10, 2686-953 Sacavém, Portugal*
[4] *Departamento de Física and CICECO, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*

T.M. Mendonça
** taniamel@mail.cern.ch*

We present a study of lattice sites and collective ordering of oxygen atoms in $HgBa_2CaCu_2O_{6+\delta}$ (Hg-1212) and $HgBa_2Ca_2Cu_3O_{8+\delta}$ (Hg-1223) using the Perturbed Angular Correlation (PAC) technique at ISOLDE/CERN. The charge distribution at the Hg neighborhood determines the electric field gradients (EFG) at ^{199m}Hg nuclei, which act as fingerprints for different oxygen doping configurations at the Hg planes. The experimental data was interpreted and assigned to multiple O_δ configurations, which were obtained with *ab-initio* simulation methods of the experimental observables.
A complementary effort was done to produce unit cell energies and density of states for different oxygen doping configurations including single O_δ atoms, $O_{2\delta}$ dumbbells and atomistic relaxations. The obtained results have been also used to produce *n*-diffraction patterns and compared with data obtained from conventional diffraction techniques, thus confirming the importance of local techniques to disentangle configurations and local inhomogeneities which cannot be resolved otherwise.

Keywords: cuprates, oxygen ordering, local probe techniques

XXVII

A. S. Alexandrov
E. V. L. De Mello
J. Ashkenazi
S. Wilson

Strong-coupling theory of high-temperature superconductivity

A. S. Alexandrov
Department of Physics, Loughborough University, United Kingdom
a.s.alexandrov@lboro.ac.uk

In the last two decades there have been tremendous attempts to built an adequate theory of high-temperature superconductivity. Most studies (including our efforts) used some model Hamiltonians with input parameters not directly related to the material. The dielectric response function of electrons in strongly correlated high-temperature superconductors is apriori unknown. Hence one has to start with the generic Hamiltonian including unscreened Coulomb and Froehlich electron-phonon interactions operating on the same scale since any ad-hoc assumption on their range and relative magnitude might fail. Using such a generic Hamiltonian I have built the analytical theory of high-temperature superconductivity in doped polar insulators predicting the critical temperature in excess of a hundred Kelvin without any adjustable parameters. The many-particle electron system is described by an analytically solvable polaronic "t-Jp" Hamiltonian with reduced hopping integral, large phonon-induced antiferromagnetic exchange, and a high-temperature superconducting state of small superlight bipolarons protected from clustering. The theory is fully compatible with the key experiments [1-7].

Key words: cuprates, theory, bipolarons

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The Disordered Induced Interaction of Cuprates

E. V. L. de Mello & R. B. Kasal
Instituto de Física, Universidade Federal Fluminense, Niterói, RJ 24210-340, Brazil
E. V. L. de Mello
evandro@if.uff.br

There are processes in nature that resemble a true force but arise due to the minimization of the local energy. The most well-known case is the exchange interaction that leads to magnetic order in some materials. We discovered a new similar process occurring in connection with an electronic phase separation transition that leads to charge inhomogeneity in cuprate superconductors. The minimization of the local free energy drives the charges into regions of low and high densities. This motion leads to an effective potential with two-fold effect: creation of tiny isolated regions or micro-grains, and two-body attraction, which promotes local or intra-grain superconducting pairing. Consequently, as in granular superconductors, the superconducting transition appears in two steps. First, with local intra-grain superconducting amplitudes and then, at lower temperature, the superconducting phase is attained by intergrain Josephson coupling. We show here that this approach reproduces the cuprates phase diagram, provides an interpretation to the pseudogap phase and yields the position dependent local density of states measured by tunneling experiments.

The "ABC" Theory for Layered High-T_C Superconductors, SC Fluctuations, and Fractal Structure

Josef Ashkenazi, Neil F. Johnson, and Zhenyuan Zhao
Department of Physics, University of Miami, P.O. Box 248046, Coral Gables, FL 33124, USA
Josef Ashkenazi
jashkenazi@miami.edu

The study of strongly correlated layered superconductors (such as the cuprates and the Fe-based SCs) requires a large-U approach, where carriers are *not* based on independent electrons but on combinations of atomic-like *configurations*. Applying such an approach [1], a combination state of degenerate auxiliary Bose condensates (ABC) is obtained, which is characterized by fluctuating striped structures, and quantum criticality. This theory describes correctly many anomalous features of the cuprates [1], including their non-Fermi-liquid behavior, phase diagram, and high-T_C SC. Their quasi-2D character results in the existence of a temperature range $\{T_{fluc}\}$, above T_C, where SC fluctuations exist but the global phase coherence of the Cooper pairs (CPs) is incomplete. This regime does *not* coincide with the pseudogap state, and can be modeled as a dynamical competition between: (1) the entropy-driven tendency of a coherent SC state to break up into smaller clusters of CPs, where the intra-cluster phase coherence is strong but inter-cluster coherence is weak; and (2) the tendency of the SC mechanism to synchronize the phases within two clusters, forming one larger coherent cluster. The solution of this model [2] yields an expression for the distribution of phase-coherent cluster sizes which is in exact agreement with the fractal expression obtained for the size-distribution of ordered oxygen interstitial (i-Os), observed [3] in La_2CuO_{4+y}. Consequently the fractal spaces of the clusters of CPs and of ordered i-Os could exactly fit with each other, resulting [2] in the raise of T_C into the $\{T_{fluc}\}$ regime, in agreement with the observation of Fratini *et al.* [3]. The success of this model introduces a dynamical equivalence between SC fluctuations in layered SCs, and a variety of phenomena in social science [2].

Key words: superconductivity, fluctuations, inhomogeneity, cuprates, fractal, complexity.

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Structural and magnetic phase transitions in iron pnictides

Stephen Wilson
Boston College, Department of Physics, Higgins Hall Room 330E140, Chestnut Hill, MA 02467 USA
stephen.wilson@bc.edu

The details of the coupling between the structural and magnetic phase transitions in the parent iron pnictides are important to understanding the normal state interactions out of which high temperature superconducting phase arises; yet research elucidating this coupling remains an ongoing challenge. In this talk, we will present a review and recent analysis of the static, antiferromagnetic, order and structural distortions in the parent and lightly doped iron pnictides. Particular focus will be given to the phase behavior within the bilayer parent $BaFe_2As_2$ system where the phase transitions are to a greater degree continuous or weakly first order. Potential universalities in the magnetic and structural phase behavior in the iron pnictides will also be discussed.

XXVIII

T- Tohyama
C. Panagopoulos
N. L. Wang
N. D. Zhigadlo
B. Joseph

Theory of Inelastic X-Ray Resonance Scattering in Iron Arsenides

Takami Tohyama[1,2], Eiji Kaneshita[3], Kenji Tsutsui[4]
[1]*Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*
[2]*JST, Transformative Research-Project on Iron Pnictides (TRIP), Chiyoda, Tokyo 102-0075, Japan*
[3]*Sendai National College of Technology, Sendai 989-8502, Japan*
[4]*Synchrotron Radiation Research Center, Japan Atomic Energy Agency, Hyogo 679-5148, Japan*
Takami Tohyama
tohyama@yukawa.kyoto-u.ac.jp

After intensive study of iron-based superconductors, it has been recognized that both spin and orbital degrees of freedom are the key to understanding the physics of iron arsenides. Theoretical calculations within the random-phase approximation (RPA) for a five-orbital Hubbard model have nicely explained spin excitations observed by inelastic neutron scattering experiments for antiferromagnetic (AFM) phase [1]. For charge dynamics, the in-plane anisotropy of optical conductivity has been explained by taking into account orbital characters of interband excitations [2]. Now, it is desired to detect both the excitations at the same time in the energy and momentum spaces. For this purpose, we propose resonant inelastic x-ray scattering (RIXS) tuned for Fe L_3 edge [3]. Our calculations of Fe L_3-edge RIXS are performed for a five-band Hubbard model by using the RPA and a fast-collision approximation. In the AFM phase, we find that the magnon excitations predominantly composed of single orbital component appear with a weak intensity as compared with orbital excitations lying just above the magnon excitations in contrast with the case of cuprates. The dominant orbital excitations are found to be accompanied by the spin-flip process, producing composite excitations of the coupled orbital-spin degrees of freedom. We also predict the polarization and momentum dependence of the Fe L_3-edge RIXS prior to forthcoming experiments.

Key words: Iron Arsenids, Antiferromagnetic phase, RIXS

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Spin and charge dynamics in the parent $CaFe_2As_2$

Christos Panagopoulos[*1,2]
[1]*Division of Physics and Applied Physics, Nanyang Technological University, Singapore*
[2]*Department of Physics and FORTH, University of Crete, Greece*
[*] *chpanagopoulos@gmail.com*

Transport, spectroscopic and magnetization measurements were performed on $CaFe_2As_2$ single crystals, a parent material of the iron-based superconductor family. We report systematic studies on the temperature and field dependence of spin and charge correlations resembling signatures associated with the emergence of filamentary superconductivity at temperatures nearer 10K in this parent compound.

Key words: magnetoresistance, spin and charge dynamics

Optical spectroscopy study on Fe-pnictides/chalcogenides

Nan Lin Wang
Institute of Physics, Chinese Academy of Sciences, Beijing, China
nlwang@aphy.iphy.ac.cn

I present our optical spectroscopic measurements on different Fe-based superconducting systems. We find that, for all FeAs-based compounds, the optical conductivity spectra contain, in addition to the free carrier response at low frequency, a temperature-dependent gap-like suppression at rather high energy scale near 0.6 eV. This suppression evolves with the As-Fe-As bond angle induced by electron- or hole-doping. Furthermore, the feature becomes much weaker in the Fe-chalcogenide compounds. We elaborate that the feature is caused by the strong Hund's rule coupling effect between the itinerant electrons and localized electron moment arising from the multiple Fe 3d orbitals. Our experiments unambiguously demonstrate the coexistence of itinerant and localized electrons in iron-based compounds, which would then lead to a more comprehensive picture about the metallic magnetism in the materials.

Key words: optical spectroscopy, iron-based superconductors

Work done with Z. G. Chen, R. H. Yuan, W. Z. Hu, G. Li, B. Cheng, J. Dong, T. Dong, P. Zheng, G. F. Chen, J. L. Luo, Z. Fang, X. Dai, C. L. Zhang and P. Dai

Recent progress in crystal growth of oxypnictide superconductors

N.D. Zhigadlo, S. Katrych, Z. Bukowski, J. Karpinski, and B. Batlogg
Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland
N.D. Zhigadlo
e-mail: zhigadlo@phys.ethz.ch

Further progress to understand the nature of superconductivity in the Fe-based compounds depends crucially on their availability as sufficiently large single crystals of high-quality. Till now, crystal growth of *R*FeAsO (*R*-1111 with *R*=rare earth) oxypnictides has proven to be a difficult task. With the aim of producing large crystals of $RFeAsO_{1-x}F_x$, suitable for various physical measurements, we adopted high pressure method and carried out a systematic investigation of the parameters controlling the growth of crystals, including the thermodynamic variables (T, P), reagent composition and the kinetic factors, such as reaction time and cooling rate. By varying each parameter while maintaining constant the others, we found the thermodynamic conditions under which an optimum equilibrium is reached. Under these conditions, we further optimized the growth protocol, by establishing the most appropriate growth duration, reagent type (precursor) and composition. NaCl/KCl, KAs, and NaAs fluxes were used to grow $RFeAsO_{1-x}F_x$ crystals at a pressure of 30 kbar. In the case of NaCl/KCl flux crystals having up to 300 μm in linear sizes were reproducibly obtained and the reaction time was one of the parameters that appeared to have influence on the crystal size. Application of KAs or NaAs fluxes let to mm sizes of superconducting Nd-1111 and Sm-1111 single crystals. In this case heat treatment at 1350-1450 ºC lasted for 2 h was followed by slow cooling (~70 h) under a natural temperature gradient. Larger size of *R*FeAsO crystals suggests that liquid KAs or NaAs has reasonable solubility and diffusivity of oxygen at high temperatures. Besides F substitution for O superconductivity in *R*FeAsO single crystals has been induced by partial substitution of Sm by Th, Fe by Co, and As by P. Investigation of the crystal structure confirmed high structural perfection and show modification due to substitutions, which is linked to superconducting properties. The magnetic and transport properties obtained for *R*FeAsO single crystals are compared with other Fe-based pnictides.

Key words: *R*FeAsO; high pressure; single crystals

Local atomic correlations in RFeAsO (R=La, Pr, Nd, Sm) oxypnictides by EXAFS

Boby Joseph[1]
[1]*Dipartimento di Fisica, Università di Roma "La Sapienza" - P. le Aldo Moro 2, 00185 Roma, Italy*
**Joseph.Boby@roma1.infn.it*

Local structure of RFeAsO (R=La, Pr, Nd, Sm) system has been studied as a function of chemical pressure varied due to different rare-earth size using Fe K-edge extended X-ray absorption fine structure (EXAFS) measurements [1]. Results indicate that the Fe-As bond length and the corresponding MSRD hardly show any change, suggesting the strongly covalent nature of this bond, while the Fe-Fe and Fe-Re bond lengths decrease with decreasing rare-earth size. Temperature dependent Fe–As bond dynamics of $NdFeAsO_{1-x}F_x$ (x = 0.0 and 0.18) is studied using arsenic K-edge EXAFS measurements [2]. The Fe–As bond length shows only a weak temperature dependence, consistent with the strong covalent nature of this bond. The temperature dependence of the mean square relative displacements of the Fe–As bond length are well described by the correlated Einstein model for all the samples, but with different Einstein temperatures for the superconducting and non-superconducting samples. The results indicate distinct local Fe–As lattice dynamics in the superconducting and non-superconducting iron-pnictide systems

Keywords: EXAFS, Local structure, Fe-based superconductors

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XXIX

D. Manske
F. Marsiglio
Y. Takada
L. Vidmar
G. De Filippis

Consequences of broken time-reversal symmetry in triplet Josephson junctions

Dirk Manske[1], Philip Brydon[2], Manfred Sigrist[3]
[1]*Max Planck Institute for Solid State Research, D-70569 Stuttgart Germany*
[2]*Institute for Theoretical Physics, TU Dresden, D-01062 Dresden, Germany*
[3]*Institute for Theoretical Physics, ETH Zürich, CH-8093 Zürich, Switzerland*

Dirk Manske
d.manske@fkf.mpg.de

There has been recently great theoretical interest in the behavior of Josephson junctions involving triplet superconductors [1,2]. In this talk, I discuss the novel Josephson effect between two triplet superconductors that are separated by a thin ferromagnetic layer (so-called TFT junction); in such a case the time reversal-symmetry can be broken due to the misalignment of the two **d**-vectors. We find that this allows the appearance of an additional spontaneous magnetization of the tunneling barrier, which radically alters the behavior of the junction [3]. In particular, we find that the junction can be stabilized in a fractional state, i.e. the free energy lies at a phase difference intermediate between zero and π (so-called ϕ-junction). Due to the increased transparency through one spin channel, there occurs also a pronounced enhancement of the critical current that should be observable in experiment [4]. Furthermore, we also demonstrate that the **d**-vector misalignment results in the appearance of a Josephson spin current, even when the equilibrium (conventional Josephson) charge current is vanishing.

Key words: Sr_2RuO_4, unconventional superconductivity, triplet-ferromagnet-triplet Josephson junction, spin current, fractional flux quanta, nanoscale device

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Suspicions about the conventional (Eliashberg) electron-phonon mechanism of superconductivity

Frank Marsiglio
Dept. of Physics, University of Alberta
fm3@ualberta.ca

As more and more classes of superconducting materials are being discovered, each with its own explanation of `glue' or mechanism for the pairing, a growing suspicion is that perhaps some key ingredient has been missed all along. In Superstripes 10 a possibility for this `key ingredient' was proposed. In this talk, we note that an additional wrinkle is the propensity for electrons, when interacting with phonons, to form small polarons, even when the coupling strength is not so strong. This phenomenon, now well established by exact results, is not compatible with the Eliashberg description of so-called strong coupling (conventional) superconductors. We discuss recent progress in our understanding of the polaron problem, particularly when the electron interactions are with acoustic phonons.

Superconductivity in a Correlated Jahn-Teller System

Chishin Hori, Hideaki Maebashi, and Yasutami Takada
Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan.
Yasutami Takada
*takada@issp.u-tokyo.ac.jp

Recent discoveries of superconductivity in cobalt oxides and iron pnictides have ignited intensive studies, both experimentally and theoretically, on the superconducting mechanism in a multi-orbital system. Due to the intrinsic complexity, a wide variety of relevant issues have been addressed in relation to this system, but we confine ourselves to discussing the character of superconductivity emerging in a two-dimensional square lattice with each site composed of doubly degenerate orbitals like the e_g orbitals in the d bands. More specifically, we consider an $E_x e$ Jahn-Teller crystal in which both electron-electron (*e-e*) and electron-phonon (*e-ph*) interactions play important roles. The pairing interaction is calculated in the RPA for all possible kinds of Cooper pairs in this system and it is substituted into the integral kernel of the gap equation in the Eliashberg theory to evaluate the transition temperature Tc. The character of superconductivity is governed by the pairing state with highest T_c.
According to our numerical calculations as well as analytical ones based on the Landau's theory of phase transitions, the character depends critically on the connectivity of neighboring *E e* centers. If electrons hop between sites without breaking the nature of the orbitals (or keeping the orbital symmetry), we have revealed that a novel chiral p-wave pairing state, which is very specific to the degenerate multi-orbital system and proposed here for the first time, is obtained by use of the cooperative effects of orbital and spin fluctuations that are enhanced by the e-ph and *e-e* interactions, respectively. This chiral p-wave state is not very robust to the breaking of the orbital symmetry and yields another kind of the spin-singlet pairing state induced by the simultaneous enhancement of orbital and spin fluctuations.

key words: superconductivity, Jahn-Teller effect, electron correlation, chiral p-wave pairing

Bipolaron in the *t-J* Model Coupled to Longitudinal and Transverse Quantum Lattice Vibrations

L. Vidmar[1] and J. Bonča[1,2]
[1]*J. Stefan Institute, 1000 Ljubljana, Slovenia*
[2]*Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana, Slovenia*

L. Vidmar
**lev.vidmar@ijs.si*

We explore the influence of two different polarizations of quantum oxygen vibrations on the spacial symmetry of the bound magnetic bipolaron in the context of the *t-J* model by using exact diagonalization within a limited functional space. Linear as well as quadratic electron-phonon coupling to transverse polarization stabilize *d*-wave symmetry, however, the existence of a magnetic background is essential for the formation of a *d*-wave bipolaron state. On the other hand, with increasing linear electron-phonon coupling to longitudinal polarization the symmetry of a *d*-wave bipolaron state changes to a *p* wave, and bipolaron develops a large anisotropic effective mass.
In the second part of my talk, the idea of the kinetic energy gain of bipolarons based on electron-phonon coupling will be presented. I will focus on magnetic bipolaron linearly coupled to transverse polarization of oxygen vibrations, as described within the *t-J*-Holstein model. With increasing electron-phonon coupling, bipolaron kinetic energy is lowered in comparison with that of the polaron. This effect is accompanied with "undressing" of bipolaron from lattice degrees of freedom. Consequently, the effective bipolaron mass becomes smaller than the polaron mass.

Key words: electron-phonon coupling, strong correlations, bipolaron formation

Relevance of Charge-Lattice Interaction in Cuprates

G. De Filippis and V. Cataudella
SPIN-CNR and Dip. di Scienze Fisiche, Università di Napoli Federico II, I-80126
G. De Filippis
E-mail:giuliode@na.infn.it

We provide evidence in favor of the relevance of charge-lattice coupling in the under-doped phase of cuprates. We show that a number of experimental observations (the anomaly of the half breathing bond stretching phonon occuring at half-way to the Brillouin zone boundary in the [100]-direction[1], the kinks observed in Angle Resolved Photoemission Spectra (ARPES)[1], the multi-peak structure of the optical conductivity in the infrared region[2,3], the anomalous temperature dependence of the ARPES in undoped cuprates[4] and, finally, the strong anisotropy between nodal and antinodal directions[5]) are explained by the cooperative interplay of coupling of holes to magnetic and lattice fluctuations. This scenario is supported by the analysis of the ground and excited state properties of one hole in the t-t'-t''-J model, including the charge-lattice interaction with local and breathing modes, through exact diagonalization techniques, diagrammatic Quantum Monte Carlo approaches and self-consistent methods.

Key words: cuprates, electron-phonon interaction, strong electron correlations

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XXX

Y. Soh
A- T. Boothroyd
W. Prellier
J. N. Goncalves
Y. Wakisaka

Similarity in the magnetotransport of chromium and the normal state of high T_c and heavy fermion superconductors

Yeong-Ah Soh
Imperial College, Department of Materials, London SW7 2AZ, UK
ya.soh@imperial.ac.uk

In this talk, I will present magnetotransport measurements performed on an epitaxial chromium film. Four key discoveries were made: a) an enhancement of the orbital magnetoresistance, which becomes enormously anisotropic below the Neel temperature, b) an anomalous negative magnetoresistance cusp at T_N, c) violation of Kohler's rule both above and below T_N - by quantifying the deviation from Kohler's rule, we are able to extract changes in the carrier density of the material through magnetoresistance, d) and unusual temperature dependence of the Hall coefficient, Hall and magneto-conductivities, which suggests the existence of two different scattering lifetimes associated with transport due to electric and magnetic fields. The unusual temperature scaling of the transport coefficients we observe in chromium is similar to the normal state magnetotransport behaviour in optimally doped high T_C superconductors and heavy fermion superconductors. Our observations show that two dimensionality or Kondo physics are not prerequisites for non-Fermi liquid transport behaviour observed in this regime of high T_C superconductors and heavy fermion superconductors.

Hour-glass magnetic spectrum in stripe-ordered $La_{2-x}Sr_xCoO_4$

A.T. Boothroyd[1], P. Babkevich[1,2], D. Prabhakaran[1], P.G. Freeman[3†]
[1] *Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, OX1 3PU, U.K.*
[2] *Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
[3] *Institut Laue–Langevin, BP 156, 38042 Grenoble Cedex 9, France*
[†] *Present address: Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn–Meitner Platz 1, D-14109 Berlin, Germany*

A.T. Boothroyd[1]
a.boothroyd@physics.ox.ac.uk

The momentum-resolved magnetic spectrum of many hole-doped copper oxides, including both superconductors and non-superconductors, exhibits a characteristic hour-glass shape. The origin of this feature has been debated for over a decade. We have recently observed the same hour-glass spectrum in neutron scattering measurements of the hole-doped antiferromagnet $La_{2-x}Sr_xCoO_4$, which has stripe correlations and is an insulator [A. T. Boothroyd *et al.*, Nature **471**, 341 (2011)]. The hour-glass spectrum of $La_{2-x}Sr_xCoO_4$ bears a remarkable similarity with that of the hole-doped superconductors. The results provide strong evidence that slowly fluctuating stripes cause the hour-glass spectrum in the copper oxide superconductors

Keywords: hour-glass spectrum; stripes; $La_{2-x}Sr_xCoO_4$

Recent advances in metastable oxide films and artificial heterostructures grown by laser ablation

W. Prellier
Laboratoire CRISMAT, CNRS UMR 6508, ENSICAEN6 Bd Maréchal Juin, F-14050 Caen Cedex, France
(prellier@ensicaen.fr)

Thin films and artificial heterostructures offer excellent opportunities to manipulate the strain and chemical heterogeneity in order to exhibit completely new or enhance the properties, which were absent in the parent compounds. It is for example possible to overcome the natural preference for disorder or low-dimensional ordering in certain materials by controlling the location of cations. Consequently, there has been recently growing interest in tailoring materials in thin films forms, having original properties that can not be obtained in the form of bulk materials, using the process of the *pulsed laser deposition* technique.
In this talk, I will illustrate the above approach by presenting the growth and characterizations of technologically important novel oxides. In particular, I will show our latest results on the synthesis and characterization of metastable phases [1] as well as the physical properties and structural characterization of complex superlattices made from perovskites.[2,3]

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Ferroelectricty and Electric Field Gradients: an ab-initio study

J. N. Gonçalves[1], A. Stroppa[2], V. S. Amaral[1], J. G. Correia[3], T. Butz[4], S. Picozzi[2]
1. Departmento de Física and CICECO, Universidade de Aveiro, P-3810-193 Aveiro, Portugal
2. CNR-SPIN L'Aquila, Italy
3. Instituto Tecnológico e Nuclear, UFA, P-2686-953 Sacavém, Portugal
4. Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany

J. N. Gonçalves
joaonsg@gmail.com

Keywords: ferroelectric; hyperfine; ab-initio

The hyperfine interaction between the quadrupole moment of an atomic nuclei and the electric field gradient (EFG) provides information on the electronic distribution, at a given site. In ferroelectric materials, the main property is the macroscopic polarization, which also depends on the electronic distribution. Since early studies of ferroelectricity a clear relation between the EFG and the polarization was observed in some materials.

There is great interest in ferroelectric/multiferroic materials nowadays, and the calculation of EFGs and ferroelectric polarization is now possible by first-principles but a study which considers the correlation between them is still lacking. This would be useful for the analysis of EFG results in materials using hyperfine interactions techniques (Mössbauer, NMR, PAC, NQR) which provide atomic scale information of the electronic charge density which is not obtained with conventional polarization measurements.

We present an analysis of the two quantities from density functional theory for a series of multiferroic and ferroelectric compounds. The EFG tensor and its properties, including orientation and correlation between components, are analysed in detail and its correlation with electric polarization is considered, providing

Temperature-dependent angle-resolved photoemission spectroscopy of Ta_2NiSe_5

Y. Wakisaka[1], T. Sudayama[1], T. Mizokawa[1, 2], N. L. Saini[3, 1], M. Arita[2], H. Namatame[2], M. Taniguchi[2, 4], N. Katayama[5], M. Nohara[5], H. Takagi[5]
[1]Department of Physics & Department of Complex Science and Engineering, University of Tokyo, Chiba, Japan
[2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima, Japan
[3]Department of Physics, University of Rome, Rome, Italy
[4]Graduate School of Science, Hiroshima University, Hiroshima, Japan[5]Department of Advanced Materials, University of Tokyo, Chiba, Japan

Y. Wakisaka
wakisaka@sces.k.u-tokyo.ac.jp

Ta_2NiSe_5 has a layered structure where each layer is loosely stacked by van der Waals interaction [1]. Each layer consists of nickel single chains and tantalum double chains running in parallel forming a quasi-one-dimensional structure. Its resistivity generally shows a semiconductive behavior with an anomaly in the logarithmic derivative around 330 K, which is attributed to a structural phase transition though no long range order related to charge- or spin-density-waves is observed. In a previous angle-resolved photoemission spectroscopy (ARPES) [2], a characteristic flat band feature near the valence band top was observed below the structural transition, which was related to an excitonic insulator state in analogy with *1T*-$TiSe_2$ [3]. In order to further investigate the nature of the phase transition, temperature-dependent ARPES experiment was performed including the temperatures above the phase transition. In the figure, second derivative intensity plots taken at 40 K, 180 K, and 340 K are shown. The solid curves represent parabolic fits to experimentally determined peak positions. It is seen that the valence band approaches Fermi level with weakening of its flatness behavior as the temperature increases.

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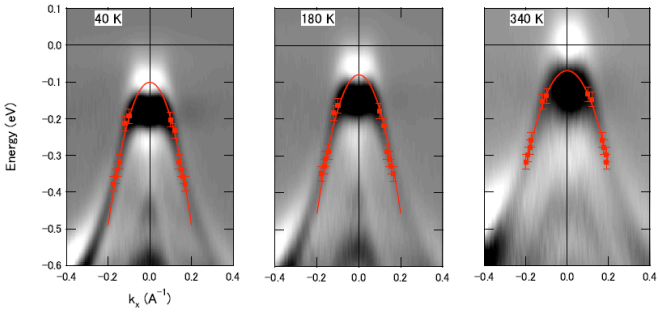

XXXI

D. M. Eagles
D. Pavuna
B. Deveaud-Pledran
A. Bianconi
K. A. Müller

XXXI

Three small systems showing probable room-temperature superconductivity

D.M. Eagles
19 Holt Road, Harold Hill, Romford, Essex RM3 8PN, England
d.eagles@ic.ac.uk

Keywords:Room-temperaturesuperconductivity,bipolarons,polymer films,carbonnanotubes, CdF_2 sandwich structures.

Of various claims of room-temperature superconductivity, three which I think are probably valid are: 1. Superconductivity for T well above 300 K in narrow channels through thin films of oxidised atacticpolypropylene(OAPP) and otherpolymers, claimed mainlybyL.N. Grigorov and coworkers, dating from 1988; 2. Superconductivity at temperatures up to at least 700 K in some carbon nanotubes, discussed by G.-M. Zhao and coworkers from 2001, following suggestions of possible room-temperature superconductivity in nanotubes by Tsebro and coworkersin1999;3. Superconductivityabove300Kin sandwich structuresbased onCdF_2 , reportedbyN.T.Bagraev and coworkers since2009. Abriefdiscussion willbegiven of the work mentionedin2. and3. above,but most of my talk will concentrateonthework mentionedin1. Firstthemostimportantexperimental resultson filmsofOAPP and someothernon-conjugated polymers will be summarised, together with a theory of Grigorov and coworkers for why there are conducting channels in polar elastomers such as atactic polypropylene. Then I will show workIpublishedinJ.Supercond15,243(2002),interpretingdetails oflargediamagnetism as a function of magnetic field in two films of OAPP in terms of a model involving induced currents inloops of superconductor based on a theory ofShoenberg. After thatI shallgivedetails of my latest version of a model for the superconductivity in OAPP films involving Bose condensation of biopolarons in arrays of nanofilaments. This model differs in several ways from a version I published in Phil Mag. 85, 1931 (2005).

XXXI

Doping, Strains and Electric Field Effects on Superconductivity in Thin $La_{2-x}Sr_xCuO_4$ Films

D. Pavuna[1], G. Dubuis[1,2], A. T. Bollinger[2], I. Božović[2]

[1]EPFL, Station3, CH-1015 Lausanne, Switzerland [2]BNL, NY11973-5000, USA

D. Pavuna

First we briefly review main results of systematic experiments on strained thin films of LSCO grown by laser ablation [1-3]. We then discuss method to smoothly tune the carrier concentration of MBE grown LSCO films by means of an applied electric field [4,5]. Thin film devices were made in an electrical double layer transistor configuration utilizing an ionic liquid as gate electrolyte. Very large fields and induced changes in surface carrier density enable shifts in T_c by up to 30K. As reported elsewhere in detail [4], numerous R(T) and carrier density curves were recorded and have shown to collapse onto a single function as predicted for a 2D S-I transition. The observed critical resistance is precisely the quantum resistance for pairs, $R_Q = h/(2e)^2 = 6.45$ kΩ, suggestive of a phase transition driven by quantum phase fluctuations, and Cooper pair (de)localization. The implications of these results and further ongoing work will be discussed [5].

Keywords: Superconductivity, Field Effect, Films

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2. C. Cancellieri et al., Phys. Rev. B76, 174520 (2007)
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Vortices in exciton-polariton condensates

Benoit Deveaud-Plédran,
EPFL Lausanne Switzerland
benoit.deveaud-pledran@epfl.ch

The idea of a possible Bose Einstein condensation in the solid state has been explored since the beginning of the sixties with the hope to get transition temperatures much more accessible than the temperatures needed for the condensation of atomic vapors (less than 1μK for Rubidium). The advantage in solids is that people are trying to condense excitons (an electron-hole pair in a semiconductor) with a mass similar to that of an electron, i.e. four orders of magnitude less than a rubidium atom. The price to pay is the disorder inherent to any real solid-state system as well as the limited lifetime of the quasi-particles.
We are studying exciton polaritons, quasi-particles made one half for excitons and one half from a confined photon. Polaritons are bosons with a mass five orders of magnitude lighter than an electron. Then, condensation at temperatures of the order of 300 K has been observed. The price to pay is the incredibly short lifetime of the polaritons : one picosecond.
During this talk, I will detail our studies on the physical properties of polariton condensates. In particular, I will focus on the evidence for superfluidity through the observation of quantized vortices. I will show their time resolved behavior, and show the first direct evidence for half quantized vortices, a specialty of spinor condensates. I will also show how the superfluid properties are modified by an obstacle and how dark solitons and vortex pairs are created in the wake of the obstacle.

Poster session

P. Babkevic
T. Charikova
L. Fanfarillo
O. Ivanenko
Y. Liang
T. Machida
K.V. Mitsen
H. Nakamura
K. Veende

Magnetic spin resonance in $FeSe_xTe_{1-x}$ probed by inelastic neutron scattering

Peter Babkevich
Oxford University
p.babkevich1@physics.ox.ac.uk

A common feature in many high-Tc superconductors is the emergence of a sharply peaked mode below Tc localised in momentum and energy space. The precise origin of this mode is still a subject of debate but the existence of a superconductivity-induced spin resonance has been shown to relate to the superconducting state and gap symmetry. In iron-based superconductors the existence of a spin resonance at the antiferromagnetic ordering wavevector Q0 = (0.5, 0.5, 0) is consistent with a pairing state with either s± or p-wave symmetry. In our work we have used inelastic neutron scattering to probe the magnetic spin dynamics of optimally doped sample of $FeSe_{0.5}Te_{0.5}$ and magnetic but non-superconducting $Fe_{1.1}$ $Se_{0.25}$ $Te_{0.75}$. By this method, we demonstrate that the resonance is intimately connected to the superconducting state and using polarised neutrons ascertained the symmetry of the gap function.

Doping and Disorder Dependencies of ihe Anomalous Hall Effect Behavior In Electron-Doped Cuprates

T. Charikova[1], N. Shelushinina[1], G. Harus[1], V. Neverov[1],D. Petukhov[1], A. Ivanov[2]
[1]*Institute of Meta l Physics RAS, S.Kovalevskaya str.,18, Ekaterinburg, 620990, Russia,*
[2]*Moscow Engineering Physics Institute, Kashirskoye highway, 31, Moscow, 115409, Russia*
T. Charikova
charikova@imp.uran.ru

Transport properties of $Nd_{2-x}Ce_xCuO_{4+\delta}$ (x=0.14; 0.15; 0.17 and 0.18) single crystal films (*B* || *c*, *J* || *ab*) with different degree of nonstoichiometric disorder δ are investigated in magnetic fields up to 9T at T=(0.4 - 4.2)K. An analysis of normal state (at $B>B_{c2}$) Hall coefficient R_H^n dependence on Ce doping takes us to a conclusion about the coexistence of electrons and holes in this nominally electron-doped cuprate system. Due to ARPES results [1] the two types of carriers may originate from electron like and hole like parts of the Fermi surface in cuprates.

In accordance with $R_H^n(x)$ analysis an anomalous sign reversal of Hall effect R_H^f observed in the mixed state at $B<B_{c2}$ may be ascribed to a flux-flow regime of Bardeen and Stephen for two types of carriers with opposite charges and rather different superconductivity gaps.

We have found also that for optimally doped (x=0.15) samples annealing in vacuum leads to an essential increase of the normal-state Hall coefficient (decrease of $|R_H^n|$) due to removing of the interstitial apical oxygen and delocalization of the charge carriers. As for the mixed state we have seen that the amplitude of anomalous Hall peak quickly dropped with the increase of the degree of disorder (from optimally to non optimally reduced film) and for the most disordered film no sign reversal of the Hall effect in the mixed state have been observed.

[1] N.P. Armitage et al., Rev. of Modern Physics, **82** (2010) 2421.

Electron-doped cuprates, disorder, Hall effect

Current Landau interaction contribution to superconducting-fluctuation: diamagnetism and conductivity

L.Fanfarillo[1], L. Benfatto[2,1], C. Castellani[1]
[1]*Department of Physics, Sapienza University of Rome, P.le A. Moro 2, Rome, Italy.*
[2]*Institute for Complex Systems (ISC), CNR, U.O.S. Sapienza , P.le A. Moro 2, Rome, Italy.*

L. Fanfarillo
Laura.Fanfarillo@roma1.infn.it

It is generally believed that, owing to their low superfluid densities and short correlation lengths, superconducting fluctuations in underdoped cuprates should be significant for transport and thermodynamic properties. Although there has been ample experimental evidence for such correlations, prompted mainly by measurements of a large Nerst effect [1], there is still disagreement about the range of temperatures in which they are relevant, their magnitude and their role in the phenomenology of the pseudogap [1,2]. Recently Bilbro et al. [3] presented a detailed THz time-domain spectroscopy study of the fluctuation superconductivity in LSCO. They showed that not only the fluctuation conductivity persists up to temperatures lower than Nerst signal, but more specifically it is about two orders of magnitude smaller than the fluctuating diamagnetism in the same system. Using a t-J model in the slave boson formulation we succeed in reconciling the apparent disagreement of the different experimental measurements. We derive the effective action for superconducting-fluctuations by taking into account the corrections to the physical observables due to the current Landau interactions. By explicitly computing the superconducting-fluctuation contribution to diamagnetism and conductivity above T_c we demonstrate that their different magnitude is a direct outcome of the proximity to the Mott-insulator in the presence of current Landau interactions. This result is independent on the exact functional form of the superconducting-fluctuations, which can have both Ginzburg-Landau and Kosterlitz-Thouless character.

Key words:Superconducting-fluctuations, Landau interaction, diamagnetism, paraconductivity.
[1] L.Li *et al.,* Phys. Rev. B 81, 17 (2010).
[2] L.S Bilbro *et al.,* Nature Physics, nphys1912, 10.1038 (2011)
[3] L.S Bilbro *et al.,* arxiv 1103.2402 (2011)

The possible mechanism of Fermi arcs and pseudogap formation in cuprates HTSC

O.M. Ivanenko, K.V. Mitsen
Lebedev Physical Institute, 119991 Moscow, Russia

O.M. Ivanenko
ivanenko@lebedev.ru

In the framework of the model for the electron structure of HTSC cuprates supposed by us earlier, Fermi arcs observed in ARPES appear over the parts of *d*-gaped Fermi surface (FS) where pair breaking due to pair hybridization (the value of $\Gamma \propto T$) of band states with negative-U centers (NUC) takes place. The transition from the superconducting to the normal state is related to the disappearance of phase coherence, and the pseudogap, which persists in the vicinity of antinodal directions, is of superconductive nature (at optimal doping). At the same time, as the doping is reduced, an insulating gap opens in the FS region from points $(\pm\pi,0; 0,\pm\pi)$ towards the nodal directions. Other consequences of pair hybridization between the band states and NUCs are nondegenerate distribution of mobile holes and importance of the processes of hole–hole scattering trough the intermediate states at NUCs, which emerge as the dominant mechanism of carrier relaxation.
key words: pseudogap, Fermi arcs, negative-U center

Magnetic response and superconductivity in electron-doped cobaltates

Ying Liang *[1], Bin Liu [2] , Shiping Feng[1] .
[1]*Department of Physics, Beijing Normal University, Beijing, 100875, China.*
[2] *Department of Physics, Beijing Jiaotong University, Beijing 100044,China.*

Ying Liang
e_mail of the presenting author : liang@bnu.edu.cn

Based on the charge-spin separation fermion-spin theory, the mechanism of superconductivity in $Na_xCoO_{2-y}H_2O$ is studied. It is shown that dressed fermions interact occurring directly through the kinetic energy by exchanging magnetic excitations. This interaction leads to a net attractive force between dressed fermions (then the electron Cooper pairs), and their condensation reveals the superconducting ground state. Within this framework, we study the doping and energy evolution of the magnetic excitations in the superconducting state by calculating the dynamical spin structure factor. It is shown that there is a broad commensurate scattering peak at low energy, then the resonance energy is located among this low energy commensurate scattering range. This low energy commensurate scattering disperses outward into a continuous ring-like incommensurate scattering at high energy, which is similar to the case in electron-doped cuprates, and could be measured by the inelastic neutron and could be measured by the inelastic neutron scattering experiment.
key words : triangular lattice; superconducting state; commensurate

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One-dimensional electronic order in $Fe_{1.07}Te$ probed by scanning tunneling spectorscopy

T. Machida (presenting author)[*1,2] , K. Kogure[1], T. Kato[1], H. Nakamura[1], H. Takeya[2], T. Mochiku[2], S. Ooi[2], Y. Mizuguchi[2], Y. Takano[2], H. Sakata[1], and K. Hirata[2]
[1]*Department of Physics, Tokyo University of Science, Tokyo, Japan.*
[2]*Superconducting Materials Center, National Institute for Materials Science, Ibaraki, Japan.*

T. Machida
Machida.Tadashi@nims.go.jp

We use scanning tunneling microscopy and spectroscopy to explore the electronic structure of $Fe_{1.07}Te$ that is the parent compound of the iron-chalcogenide superconductors (SCs). Tunneling spectroscopy reveals the particle-hole asymmetry characterized by the greater electron extraction probabilities than those for injection and two gap-like structures with the gap edges at approximately 130 and 50 meV. Within the larger gap, a unidirectional electronic order with a period of a_0 (a_0 inter-chalcogen distance) is observed. From the one-dimensionality of the electronic order, it is conceivable that the structural or antiferromagnetic transition is closely related to the formation of this electronic order. These findings give us important insights into further understanding of the parent state of iron-chalcogenide SCs.

Model for the electron structure of HTSC

K.V. Mitsen, O.M. Ivanenko
Lebedev Physical Institute, 119991 Moscow, Russia
K.V. Mitsen
mitsen@lebedev.ru

We suggest a model for the electron structure of HTSC cuprates that makes it possible to trace the evolution of their electronic structure with the doping and temperature and provides a new explanation for a number of features typical of HTSCs, including the pseudogap and the Fermi arcs. According to this model, unusual properties of these compounds result from their unique electronic structure, favorable for the formation of two-atomic negative-U centers (NUCs) and realization of a peculiar mechanism of the electron–electron interaction. One of the basic statements of the model is that charges introduced upon doping remain localized in the vicinity of the dopant ions. The key role of doping is related to the local modification of the electron structure of CuO_2 planes adjacent to the dopants (such a plane being originally a charge-transfer insulator) that results in the activation of NUCs. In turn, free hole carriers appear as a result of the transitions of electron pairs to NUCs.

Keywords: electron structure; negative-U centers; localization

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Impurity resonance states in $Bi_2Sr_{1.6}La_{0.4}CuO_{6+\delta}$

H.Nakamura(presenting[1], T.Machida[1,2], T.Kato[1], M.Fujimoto[1],H.Funahashi[1], M.Iguchi[1], K.kogure[1], T.Yamasaki[1], S.Ooi[2], T.Mochiku[2], S.Nakao[3],K.Hirata[2],T.Hasegawa[3], and H.Sakata[1]
[1]*Department of Physics, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan*
[2]*Superconducting Materials Center, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*
[3]*Department of Chemistry, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*
H. Nakamura
e-mail: giraffes14o01@yahoo.co.jp

Using scanning tunneling spectroscopy (STS), we observed impurity resonance in single crystals of Zn (nominal concentration ~ 0.6%) doped $Bi_2Sr_{1.6}La_{0.4}CuO_{6+\delta}$ (T_C=28K) (Bi2201). Many impurity resonances characterized by the peak structure near E_F were observed. The number of the resonances was less than that of the doped impurities (0.45% determined by inductively coupled plasma optical emission spectrometry). This impurity resonance was not observed in large-gap region. This result indicates that the impurity resonance appeared in only small-gap region less than Δ_{cut}~26meV. Almost the same result was observed in Bi2212 [1]. Both the average gap size (Δ_{avg}) and the Δ_{cut} in Bi2201 is about half as large as that in Bi2212. The disappearance of the impurity resonance in large-gap region is the universalistic phenomenon in Bi based high -temperature superconductors.

[1] T.Machida and et al, Phys. Rev. B **82** 180507(R)

Interband Superconductivity in spin-polarized subbands

N.Kristoffel[1], K.Veende[2] .
[1]*Institute of Physics, University of Tartu, 142 Riia Street, 51014 Tartu, Estonia.*
[2] *Institute of Physics, University of Tartu, 4 Tähe Street, 51010 Tartu, Estonia*

K.Veende
Kadri.Veende@ut.ee

Singlet superconductivity in spin-polarized band components dependent on pairing conditions is investigated and illustrated. Two subbands of a common origin, shifted on the energy scale (by magnetic action, impurities, other structural elements of the sample, etc.), are proposed to be coupled by an interband pairing interaction. The two-time Green's functions method has been used in the calculation of various superconducting characteristics. In the presence of the appropriate attractive coupling leading to the formation of pairs of interband constitution the singlet superconductivity (under obvious conditions) becomes possible. This conclusion holds also for the absence of the spin polarization. This general result exposes the origin of the used Suhl-type interaction to be important. On the calculated route of the system from the normal to the superconducting state with improved pairing conditions the inclination of metastable orderings of opposite type against the residing ordering becomes possible with expected first order phase transitions.

Keywords: interband pairing, spin polarization, phase diagram

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