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***45th Course* INTERNATIONAL SCHOOL OF SOLID-STATE PHYSICS**

# *Quantum Phenomena in Complex Matter*

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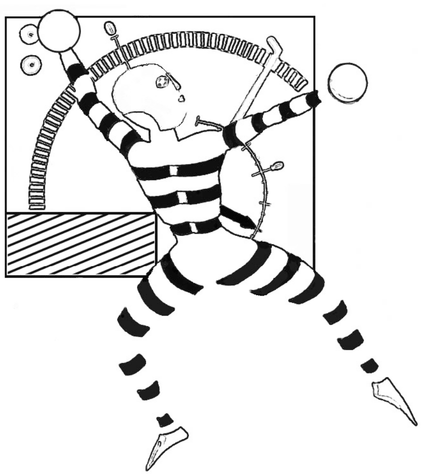
# STRIPES08

# Book of abstracts



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# PREFACE

Stripes2008 continues the successful series of international conferences held in Rome on (1996) (1998) (2000), (2004) and (2006)on nanoscale striped phases in cuprate superconductors and related phenomena, following the high degree of interest of the community in this field focusing on:

- Striped phases in highly correlated electronic systems
- Phase separation
- Striped phases in complex materials
- Anisotropic superconductors
- Competion between CDW and superconductivity
- Quantum condensates in ultracold fermion gases
- Feshbach shape resonances in superlattices
- Photoinduced phase transitions
- Quantum size effects and quantum coherence
- Polaron liquids
- Pairing mechanisms.
- Quantum phase transitions
- Manganites
- Intercalated graphite and graphene
- Complex materials
- Doped quaternary iron arsenide rare earth oxides, AOFeAs (A=rare earth), dopedLaFeAsO, NdOFeAs

Antonio Bianconi

# 27 July Sunday 8:30-10:30

## Session 1

- **S. Uchida**
- **J. M. Tranquada**
- **C. Di Castro**
- **S. Brazowski**

# Role of Apical Oxygen Atoms in High-$T_c$ Superconductivity

S. Uchida

*Department of Physics, University of Tokyo, Hongo 7-3-1,*
*Bunkyo-ku, Tokyo 113-0033, Japan*

uchida@phys.s.u-tokyo.ac.jp,

Although a major playing field of the high-$T_c$ superconductivity in copper oxides is the $CuO_2$ plane, an indispensable role of the out-of-plane atoms, in particular, the apical oxygen atoms, has progressively been anticipated. In earlier days, Muller and Kamimura pointed out a possible role of apical-O. Now it is well known that the distance of the apical-O from the $CuO_2$ plane determines the curvature of Fermi surface via long-range hopping terms, t' and t'', and is correlated with the magnitude of optimal $T_c$ in each material. Recent findings are: i) The pairing amplitude ($\Delta_0$) is locally modulated in accordance with the modulation of the apical-O distance. ii) Disorder at the apical-O sites and nearby atomic sites appreciably influences bulk $T_c$ and is a source of nanoscale gap inhomogeneity.
More recently, it has been revealed that the apical-O distance controls the competition between superconducting and “pseudogap” phases, and also does the (Josephson) coupling strength between neiboring $CuO_2$ planes. These facts indicate that the apical-O might be a key to understand the mysterious properties of high-$T_c$ cuprates, and give a hint to find a way toward higher $T_c$ in cuprates.

# Stripe Order and Superconductivity in $La_{2-x}Ba_xCuO_4$

J. M. Tranquada,* G. D. Gu, C. C. Homes, M. Hücker, Q. Li, and G. Y. Xu

*Condensed Matter Physics & Materials Science Department,*
*Brookhaven National Laboratory, Upton, NY 11973-5000, USA*

*jtran@bnl.gov

It is well known that bulk superconductivity is strongly depressed in $La_{2-x}Ba_xCuO_4$ at x=1/8, and it has been established that this dip in the transition temperature, $T_c$, correlates with the appearance of charge and spin stripe order.[1] We have recently reported evidence from transport, susceptibility, and optical conductivity experiments[2,3] for the onset of two-dimensional superconducting fluctuations at ~ 40 K, followed by a Kosterlitz-Thouless transition to 2D superconducting order at 16 K. Photoemission and tunneling measurements[4] indicate the presence of a d-wave-like gap, similar to that in other superconducting cuprates. To explain this unusual state, it has been proposed that the superconducting wave function within a $CuO_2$ plane oscillates sinusoidally so as to minimize the overlap with the spin-ordered regions.[5] A consequence of this modulated superconductivity is frustration of the Josephson coupling between the planes. Efforts to study the crossover to more conventional behavior as x deviates from 1/8 will also be discussed.

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Keywords: stripe order, superconductivity, $La_{2-x}Ba_xCuO_4$

# Universality classes for Coulomb-frustrated phase separation

Carlo Di Castro

*Università degli studi di Roma "La Sapienza"*

* email@: Carlo.DiCastro@Roma1.infn.it

Strongly correlated electronic systems often display a strong tendency towards phase separation with negative short-range electronic compressibility or a cusp singularity in the free energy density due to the crossing of the free energies of two phases as the density is varied. Both situations are frustrated by the long range Coulomb interaction. We will discuss universal aspects of the phase diagram in both cases [1] for two- and three-dimensional systems subject to the three-dimensional long-range Coulomb interaction. Within the first case the transition from the homogeneous phase to the inhomogeneous phase is first order in isotropic three-dimensional systems except for a critical point at a given value of frustration above which no inhomogeneous state can exist. Close to the critical point, inhomogeneities are predicted to form a BCC lattice with subsequent transitions to a triangular lattice of rods and a layered structure. Inclusion of a strong anisotropy allows for second and first-order transition lines joined by a tricritical point. The latter behavior remains unchanged when considering two-dimensional systems. On the contrary, the second case points to a major role covered by the system dimensionality. For two-dimensional systems there is always a range of densities where phase separation exists, no matter how strong is the frustration [3,4] whereas in three dimensional systems one recovers a maximum frustration above which only uniform phases are allowed due to the importance of screening effects [4,5]. In all cases, one finds that inhomogeneities can not have all linear dimensions larger than the three dimensional screening length [6] except exponentially close to phase boundaries.

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# Solitons in strongly correlated electronic systems from experience of quasi-1D conductors

S. Brazovskii *[1,2]

[1] *CNRS, UMR 8626, Univ. Paris-Sud, Orsay, France*
[2] *L.D. Landau Institute, Moscow, Russia*

*brazov@lptms.u-psud.fr

Correlated electronic systems show a symmetry breaking, which gives rise to topological defects – from macroscopic stripes as solitonic lattices to microscopic solitons as anomalous quasi-particles. The effect is well established in quasi-1D systems, where solitons emerge as elementary excitations, and instantons appear as transient processes, originating the pseudogap. These states accumulate electrons or holes embedded by doping, tunnelling, photoemission, optics, junctions. In general systems: from nearly antiferromagnetic oxides to high gap superconductors, the solitons become the combined topological excitations. With onset of 2D or 3D long range order, the topologically nontrivial solitons experience a confinement resulting in a spin-charge recombination. It originates the symmetry broken spin- or charge- roton configurations with charge- or spin- kinks localized in the core, correspondingly for cases of repulsion and attraction. These complex excitations can be viewed as nucleuses of the melted stripe phase, which appears in doped AFM insulators or is expected as the FFLO state in spin-polarized superconductors. These particles would determine the observable properties, usually ascribed to conventional electrons. Thus, the associated mid-gap states will give rise to growing arcs of Fermi surfaces. Individual solitons may be accessed when they are trapped by dopant; that might be responsible for local rods observed by STM in cuprates, and for the whole issue of their strong inhomogeneity. This picture suggests that the stripes are present even when we cannot visualize them, e.g. in cuprates away from the magic concentration x=1/8. They are still around, being dispersed as an ensemble of their nucleuses.

Keywords: : soliton, superlattice, topological defect

# 27 July Sunday 11:00-12:40

## Session 2

- **S. Alexandrov**
- **A. Bussman-Holder**
- **V. Cataudella**
- **A.V. Balatsky**
- **H. Keller**

# Unconventional pairing by conventional phonons in cuprate superconductors

Sasha Alexandrov

*Physics Department, Loughborough University, United Kingdom*

A.S.Alexandrov@lboro.ac.uk

A great number of observations point to the unconventional pairing symmetry in cuprate and some other superconductors. It has been thought for a long while that Cooper pairs in the Bardeen-Cooper-Schrieffer (BCS) theory with the electron-phonon interaction (EPI) are singlets and their wave function is isotropic (s-wave). This wisdom led some authors to a conclusion that EPI cannot explain high-temperature superconductivity. Here I show that an inevitable anisotropy of sound velocity in crystals makes the conventional (acoustic) phonon-mediated attraction of electrons non-local in space providing unconventional Cooper pairs with a nonzero orbital momentum. As a result of this anisotropy quasi-two dimensional charge carriers weakly coupled with acoustic phonons undergo a quantum phase transition from a conventional s-wave to an unconventional d-wave superconducting state with less carriers per unit cell. In the opposite strong-coupling regime rotational symmetry breaking appears as a result of a reduced Coulomb repulsion between unconventional bipolarons dismissing thereby some constraints on unconventional pairing in the Bose-Einstein condensation (BEC) limit. The conventional acoustic phonons, and not superexchange, are shown to be responsible for the unconventional symmetry of cuprate superconductors, where the on-site Coulomb repulsion is large. Nowadays compelling evidence for a strong EPI has arrived from isotope effects, angle resolved photoemission spectroscopies and a number of optical, neutron-scattering and tunnelling measurements in cuprates. While the coupling with particular phonon modes is quite different EPI with conventional acoustic phonons and the substantial sound-speed anisotropy explain alone the unconventional symmetry of cuprate superconductors.

Keywords: pairing symmetry, acoustic phonons, cuprates

# Multi-Component Superconductivity and Novel Isotope Effects Stemming from Unconventional Electron-Lattice Coupling

Annette Bussmann-Holder[1], Hugo Keller[2], K. Alex Müller[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*

a.bussmann-holder@fkf.mpg.de

Hole doping the insulating parent compounds of cuprate superconductors leads to an immediate suppression of antiferromagnetism together with the appearance of a bad metal state. Since doping causes a mismatch in charge, lattice and electronic energy levels, a release of this energy imbalance can be achieved by forming bound electron-lattice states in terms of extended variable range polarons. A further energy gain is achieved if these polaronic regions self-organize dynamically into patterns. This pattern formation has the advantage that pseudo-antiferromagnetic correlations persist and form an embedding matrix for the polaronic regimes. The polaron formation has the important consequence of a renormalization of the electronic energy bands whereby a level shift and an exponential band width reduction take place. While the former effect does not carry an isotope effect, the latter is sensitive to isotopic substitutions. It is shown that many unconventional isotope effects as observed experimentally are a consequence of this modeling. Also, very specific predictions for further isotope effects are made and compared to available data. From these isotope effects it can be concluded which lattice distortions are the most relevant ones to superconductivity in cuprates.

# Electron-phonon effects in undoped cuprates

V. Cataudella[1*], G. De Filippis[1], A. Mishchenko[2], N. Nagaosa[3]

[1]*Coherentia-CNR-INFM and Dip. Scienze Fisiche - Università di Napoli Federico II - I-80126 Napoli, Italy*
[2]*CREST, Japan Science and Technology Agency (JST), AIST, 1-1-1, Higashi, Tsukuba 305-8562, Japan and RRC "Kurchatov Institute", 123182, Moscow, Russia*
[3]*CREST, Department of Applied Physics, The University of Tokyo, 7- 3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan*

*vittorio.cataudella@na.infn.it

The recent advances in angle resolved photoemission spectroscopy (ARPES) made possible an accurate analysis of the low energy excitations of cuprates suggesting a possible significant role played by electron-phonon interactions in these materials[1]. We address this controversial point by presenting very accurate calculations of the spectral function of a t-J model including the electron-phonon interaction (Holstein Model) at any electron-phonon coupling strength for the undoped case. The obtained temperature dependence compares well with the experimental findings at a semi-quantitative level.[2] We also clarify that a strong electron-phonon coupling is not incompatible with the destruction of the anti-ferromagnetic phase observed in cuprates at very low doping if a non local electron-phonon coupling is taken into account.[3] Finally, a possible scenario at increasing doping (nodal-antinodal dichotomy) is suggested.

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# Collective Modes and Isotope Effect in Inhomogeneous Superconductors

A.V. Balatsky[1*], J. C. Davis [2], H. Eisaki [3], K. Fujita [2], I. Grigorenko [1], K. McElroy[4], J.A. Slezak[2], M. Wang [2], J.X. Zhu [1], S. Uchida [5].

[1]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA.*
[2]*Department of Physics, Cornell University, Ithaca, NY 14853, USA.*
[3]*AIST, 1-1-1 Central 2, Umezono, Tsukuba, Ibaraki, 305-8568 Japan.*
[4]*Department of Physics, University of Colorado, Boulder, CO 80309, USA.*
[5]*Department of Physics, University of Tokyo, Tokyo, 113-8656, Japan.*

* avb@lanl.gov

Experimental evidence suggests that nanoscale electronic inhomogeneity plays an important role in a large classes of materials. Local tunneling data indicate strong nanoscale inhomogeneity of superconducting gap in high temperature superconductors. Strong local nanoscale inhomogeneity in the bosonic scattering mode has also been observed in the same samples [1,2]. We argue that these two inhomogeneities are directly related to each other in the overdoped samples. In order to address local boson scattering effects, we would need to develop a local strong coupling model of pairing in a coarse-grained superconducting state. We used Local Inelastic Tunneling Spectroscoy and Fourier Transform Inelastic Tunneling Spectroscopy to address the role of bosonic modes. One implication of this locality is that $O^{16}$ ->$O^{18}$ isotope substitution effect needs to be considered within this local approximation. We will present a simple model that yields features that are broadly consistent with the doping and isotope substitution trends observed experimentally. We also will discuss isotope effect in a striped phase [3]. To illustrate universality of these questions, we will also discuss possible extensions of similar ideas to observed electronic defects and inhomogeneities in graphene that also exhibits Dirac excitation spectrum [4].

Keywords: inhomogeneity, inelastic tunneling spectroscopy, isotope effect, bosonic modes.

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# Unconventional Isotope effects and Multi-Component Superconductivity in Cuprates

Hugo Keller*

*Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*

*keller@physik.unizh.ch

In the first part a brief review of unconventional oxygen-isotope ($^{16}O/^{18}O$) effects (OIE's) in cuprate high-temperature superconductors (HTS's) is presented. Since the discovery of the HTS's OIE's on various quantities have been observed, including the superconducting transition temperature $T_c$, the superconducting gap$\Delta_0$, the in-plane penetration depth $\lambda_{ab}(0)$, the pseudogap temperature T*, the charge-ordering temperature $T_{co}$, the antiferromagnetic transition temperature $T_N$, and the spin-glass freezing temperature $T_g$,. The doping dependence of some of these unusual OIE's are discussed in more detail. The various OIE's observed in HTS's appear to be generic for different families of HTS's at all doping levels. In conclusion, lattice effects which in most theoretical models are neglected play an essential role in the basic physics of cuprates and are the origin of these unusual OIE's.
In the second part detailed investigations of the temperature dependence of the London magnetic penetration depth $\lambda$ along the three principal crystallographic directions (a, b, and c) in single-crystal La214, Y123, and Y124 are presented. Both in-plane components ($\lambda_a$ and $\lambda_b$) show an inflection point in their temperature dependence which is absent in the component along the c-direction ($\lambda_c$). The experiments provide convincing evidence that the in-plane superconducting order parameter is a mixture of s+d-wave symmetry, whereas it is mainly s-wave along the c-direction with a negligibly small d-wave contribution. These results strongly suggest that coupled s+d-wave order parameters are universal and intrinsic to HTS's.

Keywords: isotope effect, lattice effects, polarons, superconducting gap, pairing symmetry

# 27 July Sunday 15:00-17:00

## Session 3

- **D. Mihailovic**
- **T. Mizokawa**
- **D. Reznik**
- **H.-J. Grafe**
- **S. D. Conradson**
- **C. Panagopoulos**

# Investigation of the pairing boson in cuprate superconductors: Analysis of the non-equilibrium relaxation pathways by ultrafast optical spectroscopy.

Dragan Mihailovic[1]

[1] *Jozef Stefan Institute and International Postgraduate School, Jamova 39, SI-1000 Ljubljana, Slovenia*

* dragan.mihailovic@ijs.si

In a superconductor near equilibrium, the QP energy fluctuation spectrum can be related to the energy dissipation spectrum by the fluctuation-dissipation theorem (FDT). An equivalent statement can be made about the time-dynamics of QP relaxation (the Fourier transform of the FDT), so measurement of the time-dynamics of the QP density relaxation under near-equilibrium conditions can in principle be directly related to the virtual excitations involved in pairing of QPs in the superconducting state. Under non-equilibrium conditions, the statement is modified by non-equilibrium population factors, but the detailed analysis of the density relaxation pathways can give us new direct and detailed information on which excitations are involved in the energy relaxation processes, and more precisely, the QP recombination and pairing. We will discuss the results of recent non-equilibriums state experiments in a number of cuprates with the aim of determining the dominant processes involved in superconducting pairing and discuss the results from the point of view of our current theoretical understanding of superconductivity in these materials.

Keywords: pairing boson, QP relaxation, utrafast spectroscopy

# Local lattice distortion and photo-induced phase transition in transition-metal compounds with orbital degeneracy

T. Mizokawa[1], K. Takubo[1], T. Sudayama[1], Y. Wakisaka[1], N. Takubo[2], K. Miyano[2], N. Matsumoto[3], S. Nagata[3], T. Katayama[4], M. Nohara[4], H. Takagi[4], M. Ikeda[5], N. Kojima[5], M. Arita[6], H. Namatame[6], M. Taniguchi[6]

[1]*Department of Complexity Science and Engineering & Department of Physics, University of Tokyo, 5-1-5 Kashiwanoha, Chiba 277-8581, Japan*
[2]*Research Center for Advanced Science and Technology (RCAST), University of Tokyo, Tokyo 153-8904, Japan*
[3]*Department of Materials Science and Engineering, Muroran Institute of Technology, 27-1 Mizumoto-cho, Muroran, Hokkaido, 050-8585 Japan*
[4]*Research Center for Advanced Science and Technology (RCAST), University of Tokyo, Tokyo 153-8904, Japan*
[5]*Research Center for Advanced Science and Technology (RCAST), University of Tokyo, Tokyo 153-8904, Japan*
[6]*Research Center for Advanced Science and Technology (RCAST), University of Tokyo, Tokyo 153-8904, Japan*

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

Transition-metal compounds with spin, charge, and orbital degrees of freedom tend to have frustrated electronic states coupled with local lattice distortions and to show drastic response against external stimuli such as optical excitation. By means of photoemission spectroscopy, we have studied the electronic states of transition-metal compounds with corner-sharing and edge-sharing $MX_6$ octahedra (M=transition metal, X=O,S,Se,Br) such as prerovskite-type $Pr_{0.55}(Ca_{1-y}Sr_y)_{0.45}MnO_3$ and $Cs_2Au_2Br_6$, spinel-type $CuIr_2S_4$, and quasi-one-dimensional $Ta_2NiSe_5$. In the perovskite compounds with corner-sharing octahedra, the charge-orbital states are stabilized by Jahn-Teller or Breathing-type lattice distortions and can be destroyed by optical excitations. On the other hand, the charge-orbital states in the edge-sharing systems are stabilized by dimer formation and tend to be robust against optical excitations. Based on the photoemission results, we will discuss effects of local lattice distortions on the excitonic states obtained by optical excitations as well as those in ground states.

Keywords: photoemission, photo-induced phase transition, phase competition

# Signatures of dynamic stripes reflected in bond-stretching and buckling phonon anomalies in YBCO

D. Reznik

*Forschungszentrum Karlsruhe, IFP Postfach 3640, D-76021 Karlsruhe, Germany.*

* Reznik@llb.saclay.cea.fr

We report results of a detailed inelastic neutron scattering study of renormalization of the bond stretching and bond-buckling phonons in optimally doped YBCO. This renormalization is strongest half way to the zone boundary in the (010)-direction approximately half-way to the zone boundary. It manifests itself as a transfer of phonon spectral weight to low energies. We explain this effect as a softening of the stretching and buckling vibrations, which modifies phonon eigenvectors near branch anticrossings. In contrast with the LaSrCuO system, where a similar phonon anomaly occurs, the anomalous renormalization of the bond-stretching mode extends in the transverse direction, which is consistent with a quasi-1D behavior. Effects of $T_c$ on the phonons will be discussed. The results will be compared with predictions of LDA calculations.

# Nuclear Magnetic Resonance evidence for correlations between antiferromagnetism and pseudogap effects in Zn- and Ni-doped $(Eu,Nd)Ba_2Cu_3O_{6+y}$ single crystals

H.-J. Grafe*[1], F. Hammerath [1], D. Paar[1], G. Urbanik[1], V. Kataev[1], Th. Wolf[2], G. Khaliullin[3], B. Büchner[1]

*[1]IFW Dresden, Institut für Festkörperforschung, Helmholtzstrasse 20, D-01069 Dresden, Germany.*
*[2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany. [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany.*

* h.grafe@ifw-dresden.de

We present $^{63,65}$Cu Nuclear Quadrupole Resonance (NQR) and $^{17}$O Nulcear Magnetic Resonance (NMR) measurements on $(Eu,Nd)Ba_2(Cu,Ni,Zn)_3O_{6+y}$ single crystals heavily doped with magnetic (Ni) and non-magnetic (Zn) impurities. Owing to the impurity doping only traces of superconductivity are found at low temperatures for both, Ni and Zn doping. Nevertheless, the effect of Ni on the magnetic correlations is completely different from that of the non-magnetic Zn doping. The Ni enhances magnetic correlations and induces a wipeout of both, the copper NQR [1] and oxygen NMR signal comparable to that found in stripe ordered lanthanum cuprates. In contrast, the magnetism is suppressed in the Zn doped samples where no wipeout effect is observed and the nuclear spin lattice relaxation rate of the Cu shows a pseudogap like decrease at low temperatures. Our findings are in a striking correspondence with the different impact of Ni and Zn impurities on the charge pseudogap evidenced by recent optical data [2], uncovering thereby a close relationship between the magnetic correlations and pseudogap phenomena.

Keywords: high temperature superconductivity, impurity doping, pseudogap, nuclear magnetic resonance and relaxation, Y-based cuprates, stripe order

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## Consequences of Phase Separation – Stripes et al. in Cuprates

S. D. Conradson,[1] A. D. Andersson,[1] and J. S. Lezama-Pacheco[1,2]

[1]*Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2]*Department of Physics, CINVESTAV-Mérida, Mérida Yucatán México, 97310*

*conradson@lanl.gov

Phase separation within the $CuO_2$ planes of cuprates, whether as periodic "stripes" as seen in scattering in some materials or as the patchwork texture on the surface found by STM in others, is assumed to be sufficiently ubiquitous that it is part of the generic phase diagram. Substantial effort has therefore gone into the possible roles of stripes in the superconductivity and other properties. One consequence of phase separation that has, however, been neglected, is the interfaces that must occur between the two structures. In our work on other systems that exhibit nanoscale heterogeneity we have discovered that the interfaces are focal points for the epitaxial stress that, most importantly, interact strongly with defects. For example, in Pu alloys, we have found that the heterogeneity is associated with the local self-irradiation damage, indicating that the interfaces impede recombination. In our work on magnetic materials we have observed that interfaces locally modify bonding and thus the electronic structure; elastic and electronic strain are correlated. We have now extended these ideas to stripes. Calculations have been performed on $La_{2-x}D_xCuO_4$ containing Bianconi-Oyanagi-Saini LTT-LTO-type stripes to obtain the energy landscapes for polarons. Interaction energies between the polarons and the interfaces are typically of the order of one hundred meV, which causes the polarons to organize geometrically identically with the stripe. O-based polarons are most stable at the interface, forming a coincident charge stripe. This model has also been used to evaluate dynamical properties, paralleling the previous work of Horovitz, Barsch, and Krumhansl.

# Charge dynamics in underdoped "spin-glass" cuprates

Christos Panagopoulos[1,,2]

*[1] Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom*
*[2] Department of Physics, University of Crete and FORTH, P.O. Box 2208, 71003, Heraklion, Greece*

*cp200@cam.c.uk

We have investigated the charge dynamics of La2CuO4 lightly doped with Li and Sr. Our experiments were extended to dilution fridge temperatures and reveal evidence for dynamic rather than static charge heterogeneities. These properties are found to be sensitive to carrier concentration and dopant substitution.

Keywords: Spin, charge, dynamics, cuprates

# 27 July Sunday 17:30-19:30

## Session 4

- **J. Ashkenazi**
- **O. V. Dolgov**
- **N. Kristoffel**
- **Rakhmanov**
- **I. Martin**
- **S. Feng**

# The Lagrange Field Behind the Emergence of Inhomogeneity and High-$T_C$ Superconductivity in the Cuprates

J. Ashkenazi*

*Department of Physics, University of Miami, Coral Gables, FL 33124, USA*

* jashkenazi@miami.edu

The electrons at the vicinity of $E_F$ in the high $T_C$ cuprates correspond to large-U orbitals, and could be approached through the "slave-fermion" method. Within this method an electron creation operator is expressed in terms of the operators of two auxiliary particles, one of which is a spin-carrying boson ("svivon"), and the other is a charge-carrying fermion ("quasi-electron" or "QE"). This approach requires the fulfillment of a constraint within each lattice site which could be imposed in terms of a Lagrange Bose field (consisting of "lagrons") coupling between svivons, and between QE's. Consequently, these auxiliary particles (rather than electrons) play the role of quasiparticles in the cuprates (except for the normal state in the heavily overdoped regime).

Bose condensation of svivons and lagrons results in the formation of static or dynamical stripe-like inhomogeneities. Pairing of QE's corresponding to antinodal electrons through lagrons results in a pseudogap state where Fermi arcs remain around the nodal points. High-$T_C$ superconductivity occurs when QE's corresponding to the Fermi arcs become paired as well due to their coupling to the antinodal QE's via svivons. The gap structure around the antinodal points is characterized by a heterogeneous peak-dip-hump structure, and it becomes more homogeneous around the nodal points. The resulting electron spectral functions are characterized by a low-energy kink, and a high-energy waterfall-like feature in agreement with experiment. A crossover to a Fermi-liquid normal state (characterized by electron quasiparticles) occurs upon overdoping.

Keywords: superconductivity, inhomogeneity, cuprates, auxiliary particles, Lagrange.

# Superconducting glue: are there limits on $T_c$?

O.V. Dolgov* [1]

[1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70506 Stuttgart, Germany

* o.dolgov@fkf.mpg.de

Possible mechanisms of high-temperature superconductivity are briefly discussed. In the literature up to now a number of incorrect and unfounded statements exists. One of these - that the static dielectric function cannot be negative - is discussed in detail, as well as its consequence, a strong coupling limit on the transition temperature $T_c$. Proofs are given that the static dielectric function not only can but indeed must be negative in many stable systems, including most of the conventional metals. Various types of electron - electron interaction in superconducting cuprates are discussed. The role of the electron - phonon interaction in cuprates is highlighted.

Keywords: high-temperature superconductivity, static dielectric function, electron - phonon interaction

# Interband model scenario of cuprate superconductivity

N. Kristoffel, P. Rubin, T. Örd

*Institute of Physics, University of Tartu, Estonia*

kolja@fi.tartu.ee

A multiband approach to hole and electron doped cuprate superconductivity is developed. Bare model nonrigid electron spectrum includes nodal and antinodal defect subbands created by doping. Progressive doping quenches bare gaps between itinerant and defect subsystem states. The leading pairing channel is supposed to be the pair transfer connecting itinerant and defect bands. Band overlap conditions determine the phase diagram special points and drive the Fermi surface reconstruction. The supercarrier density varies with the disposition of the chemical potential and bands. The pairing strength and the phase coherence develop simultaneously. The interband pairing scheme creates comparable behaviour of superconducting characteristics for both types of doping despite the realization on different sublattices. Illustrative calculations have given self-consistent rersults and reproduce qualitatively (without quantitative contradictions) doping dependences of $T_c$, superconducting gaps and “extrinsic” pseudogaps, supercarrier density and effective mass, coherence length and penetration depth, critical magnetic fields and some other properties. The isotope effect on supercarrier density in multiband superconductors is predicted. Interband pairing scenario is suggested by these results to be an essential aspect of cuprate superconductivity.

Keywords: multiband cuprates, interband pairing, doping

# Phase Separation in a Model of Strongly Correlated Electron System with Two Types of Charge Carriers

A.L. Rakhmanov*, K.I. Kugel, and A.O. Sboychakov

*Institute for Theoretical and Applied Electrodynamics, Russian Academy of Sciences, Izhorskaya str. 13, Moscow, 125412 Russia*

* alrakhmanov@mail.ru

We used the two-band Hubbard model to analyze a possibility of a phase separation in a strongly correlated electron system with two types of charge carriers [1-4]. It was demonstrated that in the limit of strong on-site Coulomb repulsion, such a system has a tendency to phase separation even in the absence of magnetic or any other ordering and nearest-neighbor Coulomb repulsion [3]. This tendency turned out to be specially pronounced, if the ratio of the bandwidths is large enough. The characteristic size of inhomogeneities was estimated accounting for the surface energy and the electrostatic energy related to the charge imbalance. The number of itinerant charge carriers can be significantly lower than that implied by the doping. The model is used to study the phase separation in doped manganites and related magnetic oxides [1,2]. The system exhibits magnetic ordered (antiferromagnetic, ferromagnetic, or canted) states as well the paramagnetic states with zero and nonzero density of the itinerant electrons. A similar approach was used to describe characteristic features of band structure and phase separation in multiband superconductors, especially in cuprates [4]. We predicted a peak in the density of states at the Fermi level in the case of optimum doping corresponding to the minimum energy difference between the centers of two bands.

Keywords: phase separation, Hubbard model, manganites, cuprates

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# Inhomogeneous phases in high-temperature superconductors and heavy-fermion systems

Ivar Martin, J.X. Zhu, and A. R. Bishop

*Los Alamos National Laboratory, Los Alamos, NM 87545*

i-martin@lanl.gov

Interplay between strong correlations and electronic kinetic energy naturally leads to intrinsically inhomogeneous phases. In the cuprates, many experimental probes, including elastic and inelastic neutron scattering, STM, and NMR, provide strong evidence for existence of stripe phases, in which the weakly doped antiferromagnetic regions alternate with highly-doped metallic or superconducting regions. Theoretically, such phases appear naturally in the Hubbard model treated at the unrestricted mean field level [Int J of Mod Phys, v. 14, pp. 3567-3577 (2000), Europhys. Lett., v. 56, 849 (2001)]. In the present work we demonstrate that similar phases also generically occur in heavy fermion (HF) materials. The physics of HF materials is defined by the interplay between the localized band of f-electrons and conduction band of d-electrons. In the Kondo screened phase, the two bands effectively merge to form a single band of heavy electrons. Based on the Kondo-Heisnberg and Anderson-Hstroeisenberg lattice models, we demonstrate that the remnants of the antiferromagnetic correlations in the Kondo screened phase can lead to formation of the inhomogeneous phase with alternating regions of well-screened and poorly screened f-electron moments. Our findings suggest universality of the frustrated phase separation physics in strongly correlated systems and may help to understand some of the surprising results indicating electronic inhomogeneity of some stoichiometric HF systems.

Keywords: Heavy fermions, spin liquids, intrinsic inhomogeneity

# Doping and energy dependent spin response in the hole-doped and electron-doped cuprate superconductors

Shiping Feng*, Li Cheng, and Jingge Zhang

*Department of Physics, Beijing Normal University, Beijing 100875, China*

* E-mail: spfeng@bnu.edu.cn

Within the kinetic energy driven superconducting mechanism [1,2], we calculate the dynamical spin structure factor of the hole-doped and electron-doped cuprate superconductors in terms of the collective mode in the dressed charge carrier particle-particle channel, and reproduce all main features found in inelastic neutron scattering measurements [3], including the energy dependence of the incommensurate magnetic scattering at both low and high energies and commensurate resonance at intermediate energy for the hole-doped cuprate superconductors [2], and the energy dependence of the commensurate magnetic scattering and resonance at low energy and incommensurate magnetic scattering at high energy for the electron-doped cuprate superconductors [4]. Although there are some differences of the low energy dynamical spin response, both hole-doped and electron-doped cuprate superconductors have a dome shaped doping dependent magnetic resonance energy [2,4]. The theory also show that the differences of the low energy dynamical spin response between the hole-doped and electron-doped cuprate superconductors is mainly caused by the superconducting gap function in the electron-doped case deviated from the monotonic d-wave function.

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# 28 July Monday 8:30-10:30

## Session 5

- **Z. X. Shen**
- **T. Hanagouri**
- **A. Fujimori**
- **M. Oda**
- **D. Pavuna**

# Angle-Resolved Photoemission Study of High-Tc Superconductors

Zhi-xun Shen

*Department of Physics, Applied Physics and SLAC Photon Science, Stanford University, Stanford, CA 94305*

zxshen@stanford.edu

In this talk, we will report our recent angle-resolved photoemission data from the high temperature superconductors. The focus of the talk will be on the following subjects: i) temperature and doping dependent data on the relationship between pseudogap and superconducting gap; ii) new insights on the intricate electron-phonon interaction in cuprates; iii) the Fermi surface dependent pairing and many-body interactions in self-doped multilayer cuprates; iii) electronic structure and electron-phonon interaction in layered manganties. If time permits, I will also show new time resolved photoemission data from charge density wave systems.

# Superconducting Gap and Coherence Effect of a High-$T_c$ Cuprate $Ca_{2-x}Na_xCuO_2Cl_2$ Probed by Quasi-particle Interference

T. Hanaguri[*1,2], Y. Kohsaka[1,2], M. Ono[1,2], M. Maltseva[3], P. Coleman[3], J. C. Davis[4], C. Lupien[5], I. Yamada[6], M. Azuma[6], M. Takano[6], K. Ohishi[7], and H. Takagi[1,8]

[1] *Magnetic Materials Laboratory, RIKEN, Wako 351-0198, Japan.*
[2] *CREST, Japan Science and Technology Agency, Kawaguchi 332-0012, Japan.*
[3] *Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA.*
[4] *LASSP, Department of Physics, Cornell University, Ithaca NY 14853 USA*
[5] *Département de Physique, Université de Sherbrooke, Sherbrooke, QC J1K 2R1 Canada*
[6] *Institute for Chemical Research, Kyoto University, Uji 601-0011, Japan*
[7] *Advanced Science Research Center, Japan Atomic Energy Agency, Ibaraki 319-1195, Japan*
[8] *Department of Advanced Materials, University of Tokyo, Kashiwa 277-8561, Japan*

* hanaguri@riken.jp

Momentum-space electronic states of nearly-optimally-doped $Ca_{2-x}Na_xCuO_2Cl_2$ (Na-CCOC, $T_c$ ~ 28 K) have been studied through the Fourier analysis of the quasi-particle interference (QPI) patterns imaged by spectroscopic-imaging scanning tunneling microscopy. Analyses based on the octet model of QPI provide us with the information on the superconducting-gap, as well as the part of the Fermi surface where Bogoliubov quasi-particles are coherent. The d-wave superconducting-gap dispersion of nearly-optimally-doped Na-CCOC is found to be almost identical to that of optimally-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) with $T_c$ ~ 86 K. By contrast, the length of the "Fermi arc" in Na-CCOC, on which QPI is identified, is much shorter than that in Bi2212.This may explain the drastic difference in $T_c$ between Na-CCOC and Bi2212.
Magnetic-field effects on QPI have also been investigated. If the phase of the d-wave superconducting order parameter is preserved during the quasi-particle scattering process of interference, the amplitudes of QPI modulations are enhanced by magnetic fields, while they are suppressed if the phase is reversed. The observed phase-sensitive scattering clearly indicates the importance of the coherence effect which is a direct consequence of the d-wave pairing and opens a new approach to investigate the nature of Bogoliubov quasi-particles in anisotropic superconductors.

Keywords: quasi-particle interference, scanning tunneling microscopy, superconducting gap

# Unusual High-Temperature Behaviors of Charge Carries in High-$T_c$ Cuprates from Photoemission Spectroscopy

A. Fujimori*

*Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo, Japan.*

* fujimori@phys.s.u-tokyo.ac.jp

The most striking and intriguing aspect of the high-$T_c$ cuprates is the pseudogap opening and the concomitant Fermi "arc" formation in the underdoped region [1]. Two energy scales [2] and a finite arc length are necessary to describe the gap in the normal state for consistency with thermodynamic properties. In this talk, first, the two gap energy/temperature scales ($\Delta^*/T^*$ and $\Delta_0/T_c$) in $La_{2-x}Sr_xCuO_4$ are demonstrated and are compared with those of other cuprate families to identify universal versus material-dependent behaviors of the cuprates. Then, another temperature scale, the "coherence temperature" $T_{coh}$, is introduced to describe crossover from arc metal to polaron hopping with increasing temperature. $T_{coh}$ increases with hole doping, in contrast to the pseudogap temperature T*, reminiscent of small hole pockets. The temperature dependence of the chemical potential reflects the doping and temperature dependent crossover from hole-like to electron-like Fermi surfaces, but the shift is much stronger than what would be expected for any uncorrelated and correlated electron models [3], implying that charge carriers have extra entropy due to dressing phonons.

This work has been done in collaboration with T. Yoshida, M. Hashimoto, W. Malaeb, K. Tanaka, W.-S. Lee, X.J. Zhou, Z. Hussain, Z.-X. Shen, M. Kubota, K. Ono, Seiki Komiya, Yoichi Ando, T. Kakeshita, H. Eisaki, Y. Fujimaki, T. Kurahashi and S. Uchida

Keywords: (ARPES, Fermi arc, psudogap, polaron)

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# On the Relations among the Pseudogap, Electronic Charge Order and Fermi-arc Superconductivity in High-$T_c$ Cuprates

M. Oda[*1], Y. H. Liu[1], K. Takeyama[1], T. Kurosawa[1], N. Momono[2] and M. Ido[1]

[1]*Department of Physics, Hokkaido University, Sapporo, Japan*
[2]*Department of Materials Science and Engineering, Muroran Institute of Technology, Muroran 050-8585, Japan*

*moda@sci.hokudai.ac.jp

We report scanning tunneling microscopy and spectroscopy (STM/STS) studies on the electronic charge order and the energy gap inhomogeneity in the superconducting and pseudogap states of underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$. It has been demonstrated that the static charge order with a period of 4ax4a (a: the lattice constant along the Cu-O bond directions) develops markedly in the inhomogeneous pseudogap state, whereas it is very weak in the homogeneous pseudogap state. The static charge order can be understood in terms of a pinning picture in which the dynamically fluctuating charge order, which seems to be intrinsic in the homogeneous pseudogap state, is pinned down by scattering centers, leading to the energy gap inhomogeneity. We suggest that the electronic charge order will be associated with incoherent quasiparticle or pair states on antinodal parts of the Fermi surface near the zone boundary, which is responsible for the pseudogap; the static charge order will remain below $T_c$, together with the inhomogeneous gap structure around the antinodal region, and coexist with the superconductivity caused by the pairing of coherent quasiparticles on the Fermi-arc around the node point of the d-wave gap near ($\pi/2$, $\pi/2$) or the so-called “Fermi-arc superconductivity.”

# Direct Angle Resolved Photoelectron Spectroscopy (DARPES) on Oxide Films: Doping, Strains, Fermi Surface Topology and High-$T_c$ Superconductivity

Davor Pavuna

*Institute of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

davor.pavuna@epfl.ch

Since 1997 we systematically perform Direct ARPES (=DARPES) on in-situ grown, non-cleaved, ultra-thin (<25nm) cuprate films. Specifically, we probe low energy electronic structure and properties of high-$T_c$ films under different degree of epitaxial (compressive vs tensile) strain [1-4]. In overdoped in-plane compressed $La_{2-x}Sr_xCuO_4$ (LSCO) thin films we double $T_c$ from 20K to 40K, yet the Fermi surface (FS) remains essentially 2-dimensional (2D) [1]. In contrast, tensile strained films show 3-dimensional (3D) dispersion, while $T_c$ is drastically reduced. It seems that the in-plane compressive strain tends to push the apical oxygen far away from the $CuO_2$ plane, enhances the 2D character of the dispersion and increases $T_C$, while the tensile strain seems to act exactly in the opposite direction and the resulting dispersion is 3D [2]. We have the FS topology for both cases. As the actual lattice of cuprates is 'Napoleon-cake'-like i.e. rigid $CuO_2$ planes alternate with softer 'reservoir' (that strains distort differently) our results tend to rule out 2D rigid lattice mean field models [2]. We have recently determined the FS topology from the observed wavevector quantization by DARPES in cuprate films thinner than 18 units cells (<24nm) [3,4].

Keywords : Superconductivity, Eelctronic Properties, Films

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# 28 July Monday 11:00-12:40

## Session 6

- **A. Bianconi**
- **S. V. Borisenko**
- **A. Ino**
- **T. Yoshida**
- **A. Bansil**

# Feshbach shape resonances in nanoscale superlattices: cuprates, biborides and FeAs superconductors

Antonio Bianconi

*Department of Physics, University of Rome La Sapienza, Roma, Italy*

antonio.bianconi@roma1.infn.it

We discuss the key role of the nanoscale architecture in controlling Feshbach shape resonance in the exchange-like interband pairing term as the possible mechanism for high Tc that occurs in multiband superconductivity as a resonance in the configuration interaction between different pairing channels in different subbands (1-3). In the superlattices the different spatial location and disparity of the wavefunction symmetry of the two components make possible the interband exchange pairing. We discuss the shape resonance that occurs at the 2D to 3D electronic topological transition in the electronic spectrum in the superlattice of quantum wells and we discuss how the $T_c$ amplification can be manipulated by controlling the architecture of the superlattice of quantum wells. The competition between the high $T_c$ superconductivity order and the charge order is a key term for evading de-coherence effects at high temperature. We discuss the case of cuprates (4,5), diborides and of the new FeAs superconductors (6).

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# A struggle for the Fermi surface: density waves vs. superconductivity

S. V. Borisenko*[1]

[1]*Institute for Solid State Research, IFW-Dresden, Dresden, Germany*

* S.Borisenko@ifw-dresden.de

We characterize the pseudogap in HTSC cuprates and in CDW-bearing transition metal dichalcogenides by means of very high resolution ARPES. The size, the degree of momentum anisotropy, the character of the spectral weight depletion and the temperature evolution clearly point to a possible common origin of the two pseudogaps.

Keywords: ARPES, HTSC cuprates, CDW, pseudogap

# Quasiparticle Fine Structures in Single-Layer and Bilayer Cuprates Studied by Low-Energy ARPES

A. Ino[*1], T. Yamasaki[1], T. Kamo[1], H. Anzai[1],
T. Fujita[1], Y. Nakashima[1], M. Arita[2],
H. Namatame[2], M. Taniguchi[1,2], A. Fujimori[3], Z.-X. Shen[4], M. Ishikado[3], K. Fujita[3],
S. Uchida[3]

[1]*Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
[2]*HSRC, Hiroshima University, Higashi-Hiroshima 739-0046, Japan*
[3]*Department of Physics, University of Tokyo, Tokyo 113-0033, Japan*
[4]*Department of Physics, Applied Physics and SSRL Synchrotron Radiation Laboratory, Stanford University, Stanford, California 94305, USA*

*ino@hiroshima-u.ac.jp

Angle-resolved photoemission spectroscopy (ARPES* is a powerful tool to map out quasiparticle excitations in energy-momentum space. It enables us to resolve band-dependent and energy-dependent quasiparticle properties responsible to macroscopic transport properties. However, due to the effect of transition matrix-element, the ARPES spectral intensity is strongly dependent on the energy of excitation photon. We performed high-resolution ARPES study of single-layer and bilayer cuprates using low-energy synchrotron radiation (hν = 6-10 eV*. We report on nodal scattering rates, fine structures in quasiparticle dispersion, and directional-dependence of the gap magnitude, obtained by using optimum excitation-photon energy.

Keywords: ARPES, quasiparticle structure, and gap anisotropy

# Observation of the Multiband Electronic Structure in the Trilayer High-$T_c$ Cuprates $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$

T. Yoshida*[1], S. Ideta[1], K. Takashima[1], M. Hashimoto[1], K. M. Kojima[1], A. Fujimori[1], S. Uchida[1], H. Anzai[2], T. Fujita[2], Y. Nakashima[2], A. Ino[2], M. Arita[3], H. Namatame[3], M. Taniguchi[2,3] , D. H. Lu[4], Z.-X. Shen[4]

*[1]Department of Physics, University of Tokyo, Tokyo 113-0033, Japan*
*[2]Graduate School of Science and Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*
*[4]Department of Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA94305, USA*

* yoshida@wyvern.phys.s.u-tokyo.ac.jp

It has been empirically known that the $T_c$ of optimally doped high-$T_c$ cuprates increases with the number of neighboring $CuO_2$ layers (n* from single-layer (n=1* to trilayer (n=3*. However, the microscopic origin of the correlation between the n and the superconductivity is still unclear so far. Since the optimally doped trilayer system $Bi_2Sr_2Ca_2Cu_3O_{10+\_}$ (Bi2223* has the highest $T_c$ (~110 K* among the Bi-based high-$T_c$ cuprates, the electronic structure of this system would give an insight into the crucial factor for higher $T_c$. However, because of the difficulty in growing high-quality single crystals, the studies of the electronic structure by angle resolved photoemission spectroscopy (ARPES* on Bi2223 have been far behind of those on other single-layer and bilayer cuprates. Previous ARPES studies on Bi2223 reported a large superconducting gap compared to those of Bi2212 reflecting the large value of $T_c$. However, the observed quasi-particle bands were not resolved into the multibands corresponding to the three neighboring $CuO_2$ layers [1, 2].

In the present study, by using improved quality of the single crystals, we have observed the multiband electronic structure of the trilayer system Bi2223 by ARPES for the first time. Corresponding to the inner and outer $CuO_2$ planes, two distinct Fermi surface sheets were observed and the inner-plane band has a larger superconducting gap than that of the outer-plane band. The observed Fermi surface area, gap and spectral line shape indicate that the outer-plane band is overdoped, similar to the result of the four layer system $Ba_2Ca_3Cu_4O_8F_2$ (F0234* [3], while the inner-plane band is underdoped.

Keywords: ARPES, high- $T_c$ superconductor, Bi2223

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# Recent Progress in Modeling Highly Resolved Spectroscopies in Complex Materials

A. Bansil

*Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA*

bansil@neu.edu

Spectroscopies resolved highly in momentum, energy or spatial dimensions are playing a key role in unraveling the nature of the ground state and excitation properties in wide classes of novel materials. However, spectroscopies do not provide a direct map of the electronic spectrum, but act as a very complex 'filter' or 'mapping' of the energy levels, Fermi surfaces (FSs* and excitation spectra of interest. With this motivation, we have been pursuing techniques for formulating and implementing methodologies for making a direct connection between the electronic spectrum and what is measured in various highly resolved spectroscopies. In this talk, I will highlight some of our recent work aimed at understanding scanning tunneling microscopy/spectroscopy (STM* and angle-resolved photoemission (ARPES* spectra from the cuprate high-temperature superconductors. With regard to STM, we have developed a framework for a material-specific modeling of the spectrum in the normal as well as the superconducting state where effects of multiple orbitals in the semi-infinite solid and are properly taken into account. Our results on Bi2212 show that the matrix element strongly modifies the tunneling current and reveal new insights into how different tunneling channels contribute and how the spectrum develops a striking asymmetry between the processes of electron extraction vs injection. In connection with ARPES, we discuss recently reported high-energy kinks or 'waterfall effects' above 200 meV. Our analysis indicates that bosonic coupling to collective modes in the spin channel can induce waterfall-like effects in the electronic dispersion with electron as well as hole doping. Interplay between the self-energy and matrix element effects yields interesting insights into the nature of the resulting ARPES spectrum. Work supported by the Office of Science, Basic Energy Sciences, U.S.D.O.E.

# 28 July Monday 15:00-17:00

## Session 7A

- **J. D. Dow**
- **J. Roehler**
- **S. Sanna**
- **Y. Dagan**
- **A. N. Lavrov**
- **T. B. Charikova**

# High-temperature superconductivity

John D. Dow*[1], Dale R. Harshman[1,2,3], and Anthony R. Fiory[4]

*[1]Physics Department, Arizona State University, Tempe, AZ 85287 U.S.A.*
*[2]Physics Department, University of Notre Dame, Notre Dame, IN 46556 U.S.A.*
*[3]Physikon Researh Corporation, Lynden, WA 98264 U.S.A.*
*[4]Newark College of Engineering, Newark, NJ 07102 U.S.A.*

*catsc@cox.net

A theory of high-$T_C$ superconductivity is presented which (i* explains the cuprates (with cuprate-planes*; (ii* describes the superconducting ruthenates (without cuprate-planes*: doped $Ba_2YRuO_6$ and $Sr_2YRuO_6$; (iii* treats the superconductivity of $GdSr_2Cu_2RuO_8$ and $Gd_{2-z}Ce_zSr_2$-$Cu_2RuO_{10}$ (rutheno-cuprates whose cuprate-planes do not superconduct*, and (iv* expounds an organic compound whose superconductivity is due to the element S rather than O, κ- $[BEDT$-$TTF]_2Cu[NCS]_2$ [1].
In $YBa_2Cu_3O_7$, the theory is consistent with the observation that no Cu-containing plane superconducts, and hence only the BaO plane superconducts. The superconductivity is s-wave in character (not d-wave* [2], provided fluxon de-pinning has been properly accounted for. The superconducting layers (i.e., BaO* are p-type and adjacent to the n-type cuprate-planes. The hole-pairing is not phononic, but Coulombic. Many experiments can be explained by this theory, which contradicts the theories with d-wave superconductivity in the cuprate planes.

Keywords: superconductivity in BaO; s-wave pairing; Coulomb pairing.

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# La doping and phase separation in the solid solution $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$

J. Röhler*[1], C. Trabant[1], A. Krapf [2], V. Martovitsky[3], L. Dudy[2]

[1]*Fachgruppe Physik, Universität zu Köln, 50937 Köln, Germany*
[2]*Institut für Physik, Humboldt-Universität Berlin, 12489 Berlin, Germany*
[2]*P.N. Lebedev Physical Institute, 119991 Moscow, Russia*

*juergen.roehler@uni-koeln.de

The solid solution $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ (BSLCO* is one of the few hole doped superconducting cuprates which is chemically controlled by only one variable (0 < x < 1 *. But there is some ambiguity in the homogeneity of the doped phases. BLSCO single crystals were studied using Cu-K and La-K EXAFS, x-ray diffraction, O-K and Cu-$L_{III}$ XAS. We found phase separation in both, the underdoped (0.35 < x < 1*, and the overdoped (0 < x < 0.35* regimes, on a nanoscale in the former, and on a macroscopic scale in the latter. Electronic homogeneity, as evidenced by the doping dependence of the supercell symmetries, is constrained to the insulating (fully monoclinic, x > 0.8*, and the optimum doped (fully orthorhombic, x ~ 0.35* regimes. Underdoped crystals consist of metastable sequences (along the c-axis* of monoclinic lamellas alternating with orthorhombic lamellas, each about 50-80 Å thick. Overdoped (La-poor* crystals appear macroscopically segregated into orthorhombic optimum doped, and strongly overdoped blocks, possibly La-free overdoped $Bi_{2-x}Sr_{2+x}CuO_{6+\delta}$. This macroscopic decomposition is also indicated by O-K XAS measurements, which yield in the overdoped regime a saturated hole count around the optimum, $n_h = 0.16$. La is always found to substitute Sr, not Bi. Hence the La dopants control the injection of holes into the $CuO_2$ planes via the interstitial oxygens $\delta$ and their order / disorder. The implications for the universal phase diagram of the cuprate superconductors are discussed, and comparison is made with the phase separation phenomenology in the $La_2CuO_{4+\delta}$/$La_{2-x}Sr_xCuO_4$, and $YBa_2Cu_3O_x$ systems.

Keywords: phase separation, nanoscale inhomogeneities, superconducting cuprates

# What drives the $T_c^{max}$ of cuprates?

S.Sanna[a,] S.Agrestini[b], K.Zheng[a], A.Bianconi[c], N.Saini[c]

[a] *CNISM and Physics Department, University of Parma*
[b] *Laboratoire CRISMAT of Caen, France*
[c] *Physics Department and CNISM, University of Roma "La Sapienza"*

*Samuele.Sanna@fis.unipr.it

For perovskite high temperature superconductive (HT$_c$S* cuprates the superconducting temperature $T_c$ is dependent upon hole density h characteristically in a dome shape, with a maximum $T_c$ ($T_c^{max}$* at optimal doping $h^{opt} \approx 0.16$ holes per $CuO_2$ in copper plane. $T_c^{max}$ varies strongly across different HT$_c$S families from a few tens of Kelvin to 130 K, which suggests that structure modification at constant doping plays a strategic role. Generally, it is difficult to experimentally distinguish the specific role of doping from that of structure modifications, since their changes usually take place simultaneously.
Here we show that the $(Ca_xLa_{1-x}$*$(Ba_{1.75-x}La_{0.25+x}$*$Cu_3O_y$ compound [1] permit to greatly vary the $T_c$ at constant doping by acting only on the structure by a globally isoelectronic substitution of $Ca^{II}$_$La^{III}$_$Ba^{II}$. A systematic XANES study is performed on oxygen optimally doped samples ($0 \le x < 0.5$, $y \approx 7.12$* which shows that in spite of the drastic increase of $T_c$ from 40 K (x = 0* to 80 K (x = 0.4*, the hole doping is constant throughout the range of $0 \le x < 0.5$ from the O K-edge and Cu $L_3$-edge XANES results. Conversely, high resolution x-ray diffraction patterns reveal that the $T_c$ variation is related to the lattice modifications induced by the cationic size difference.
This work shows that the chemical mismatch pressure [2] on the $CuO_2$ plane is a driving parameter in defining the superconducting critical temperature.

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# Do electrons superconduct in the electron-doped cuprate superconductors?

Y. Dagan [1*], R. L. Greene [2].

*[1] School of Physics and Astronomy, Tel Aviv University, Tel Aviv, Israel.*
*[2] Center for Nanophysics and Advanced Materials, University of Maryland, College Park, Maryland, USA.*

* yodagan@post.tau.ac.il

A striking property of the high $T_c$ cuprate superconductors is the extreme sensitivity of many of their electronic properties to the number of charge carriers put into the copper-oxygen planes (doping*. From a chemical point of view these charge carriers can be either holes or electrons. Whether these two types of cuprates share similar physical properties and a common mechanism for superconductivity is still an open question.
Our transport studies on the electron-doped cuprate $Pr_{2-x}Ce_xCuO_4$ reveille a special normal state governed by a quantum critical point slightly above optimum doping. While at high temperatures both holes and electrons play a role in the normal state properties, at low temperatures and away from the critical point only one type of carriers seems to dominate. Moreover, the analysis of the temperature and doping dependences of the resistivity and the Hall angle lead us to a remarkable conclusion, namely, that in electron doped cuprates holes are responsible for the superconductivity.
The superconducting state was studied by planar tunnelling spectroscopy. It is characterized by an order parameter having a nonmonotonic d wave symmetry for the whole doping range studied, with a BCS like temperature dependence.

Keywords: Electron-doped cuprates, transport, tunneling, quantum criticality.

# Magnetic-field induced superconductor-antiferromagnet transition in lightly doped $RBa_2Cu_3O_{6+x}$ (R = Y, Lu* crystals

A. N. Lavrov[1], L. P. Kozeeva[1], M. R. Trunin[2], V. N. Zverev[2]

[1]*Institute of Inorganic Chemistry, Novosibirsk, Russia.*
[2]*Institute of Solid State Physics, Chernogolovka, Russia.*

E-mail: lavrov@che.nsk.su

In high-$T_c$ cuprates, the superconductivity emerges when charge carriers are doped into the parent antiferromagnetic (AF* insulator. Despite decades of intensive research, the role of AF correlations in $CuO_2$ planes in establishing the superconducting state still remains far from being clear. In a prototype compound $La_{2-x}Sr_xCuO_4$, the long-range AF order is destroyed by doped holes way before the superconductivity (SC* sets in, which has led to a general belief that the spin frustration is a prerequisite for metallic conduction and superconductivity. Spin excitations, on the other hand, are often suggested to provide glue for SC pairing. The destructive impact of static spin order–in contrast to dynamic one–on superconductivity was further supported by the observation of the SC suppression at peculiar 1/8 doping in $La_{2-x}Ba_xCuO_4$. However, the incompatibility of static AF order and SC may be not a general feature of cuprates. Our study of lightly doped $RBa_2Cu_3O_{6+x}$ (R = Y, Lu* crystals has demonstrated that the destruction of static AF order is required neither for metallic hole conduction in $CuO_2$ planes nor for superconductivity; in a certain doping range the static spin order and superconductivity are found to coexist. Detailed magnetoresistance measurements of lightly doped $RBa_2Cu_3O_{6+x}$ crystals with $T_c$<15-20 K gave a clear picture of the magnetic-field induced superconductivity suppression and recovery of the long-range AF state. What remains still unanswered is whether the AF order and SC in lightly doped $RBa_2Cu_3O_{6+x}$ reside in nanoscopically separated phases or coexist on an atomic scale.

Keywords: phase diagrams, hole segregation, magnetoresistance.

# Effect of nonstoichiometric disorder on the upper critical field in $Nd_{2-x}Ce_xCuO_{4+\delta}$ single crystals.

T.B. Charikova*[1], N.G. Shelushinina[1], G.I.Harus[1], A.A. Ivanov[2]

[1]*Institute of Metal Physics Ural Division RAS, Ekaterinburg, Russia*
[2]*Moscow Engineering Physics Institute, Moscow, Russia*

* charikova@imp.uran.ru

The results of an investigation of the in-plane $\rho_{ab}$(T* resistivities (0.4K ≤ T ≤ 40K* in magnetic fields up to H=9T (H || c, J || ab* for electron doped superconductors $Nd_{2-x}Ce_xCuO_{4+\delta}$ (x= 0.15; 0.18; 0.20* with different oxygen content δ will be presented. We have determined experimentally that single crystals of $Nd_{2-x}Ce_xCuO_{4+\delta}$ with different cerium content and different nonstoichiometric disorder are in the range of BCS-coupling. The slope of the upper critical field decreases with increase of the disorder parameter in experiment for $Nd_{2-x}Ce_xCuO_{4+\delta}$ single crystals with different nonstoichiometric disorder as it should be for superconductors with dwave pairing. The critical temperature also decreases with increase of the disorder in quantitative accordance with theory for d-wave superconductors with anisotropic scattering. This work was done within RAS Program (project N 01.2.006 13395*, with partial support by the RFBR (grant N 07-02-00396*.

Keywords: Electron doped superconductors, upper critical field, d-wave paring with anisotropic scattering

# 28 July Monday 15:00-17:00

## Session 7B

- **T. Tohyama**
- **S. I. Mukhin**
- **M. Capone**
- **V. Hinkov**
- **E. Taylor**
- **T. Jarlborg**

# Origin of Spatial Variation of Pairing Gap in Bi-Based High-$T_c$ Cuprates

M. Mori,[1] G. Khaliullin,[2] T. Tohyama,[*3] S. Maekawa[1]

[1]*Institute for Materials Research, Tohoku University, Sendai, Japan*
[2] *Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany*
[3]*Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto Japan*

* tohyama@yukawa.kyoto-u.ac.jp

In hole-doped high-$T_c$ cuprates, a correlation between the maximum $T_c$ and the energy-level separation of in-plane oxygens and apical ones has been noticed in the early nineties. Hence, a role of apical oxygen on $T_c$ is of considerable interest. In $Bi_2Sr_2CaCu_2O_8$ (Bi-2212*, a mismatch between the rock-salt $BiO_2$ layers and the $CuO_2$ planes causes an extra modulation of the crystal structure. In such a "supermodulated" lattice, the distance d from the $CuO_2$ layer to the apical oxygen is periodically varied. Given that bonds within the $CuO_2$ plane itself are much less affected by the supermodulation, Bi-2212 material provides a unique opportunity to study the impact of apical oxygen on superconductivity, by monitoring local electronic properties as a function of d that varies spatially within a supermodulation period. Very recently, scanning tunneling microscopy on Bi-2212 cuprate superconductor has revealed a spatial variation of the energy gap that is directly correlated with a modulation of the apical oxygen position. We identify two mechanisms by which out-of-plane oxygens can modulate the pairing interaction within the $CuO_2$ layer: a covalency between the $x^2$-$y^2$ band and apical p-orbital, and a screening of correlation U by apical oxygen polarization. Both effects strongly depend on the apical oxygen position and their cooperative action explains the experiment.

Keywords: Bi-2212, lattice distortion, Madelung potential, STM

# Ingap sidebands: possible scenario for PG state of high-Tc cuprates with coupled fluctuating competing orders

S.I. Mukhin*

*Theoretical Physics Department, Moscow Institute for Steel and Alloys, Moscow, Russia*

* sergeimoscow@online.ru

A density of states "bunching" mechanism is proposed. It is shown that resonant fluctuations of the order competing with the one that has condensed, may form ingap high-density electronic "sideband" with quartic dispersion near its edges: $\varepsilon(k) = \pm\sqrt{m^4/\Delta^2 + (v_F k)^4/\Omega^2}$ , here Δ is amplitude of the condensed order, **m**(<< Δ* and Ω are amplitude and frequency of the resonant fluctuating mode of competing order; $v_F$ and **k** are Fermi-velocity and deviation of electron momentum from the Fermi-momentum respectively. It is proposed that Ω is bosonic mode frequency involved in the peak-dip-hump structure of the photoemission spectra in the antinodal region of the Brillouin zone in high-Tc cuprates, while Δ and **m** are the major ingredients forming the pseudogap (PG* picture observed in the ARPES measurements.

Keywords: fluctuating competing orders**,** Floquet indices, nesting

# Tendency toward phase separation and the correlation strenght of the cuprates

M. Capone[1*]

[1]Statistical Mechanics and Complexity Center, CNR-INFM, and University of Rome "La Sapienza", Piazzale A. Moro 2, 00185, Rome, Itay

* massimo.capone@roma1.infn.it

The properties of lightly doped models for the cuprates are discussed using Dynamical Mean-Field Theory and cluster extensions. We will review some analyses of the Hubbard model that confirm the relevance of electron-electron correlation in determining the general trends of the phase diagram [1]. Yet, comparison with experimental data of optical conductivity suggests that the correlation strength is not significantly larger than the bandwidth, so that the parent compounds can not be considered as pure Mott insulators, and antiferromagnetic correlations are crucial in determining their behavior [2].
The role of antiferromagnetic correlations in underdoped cuprates is indeed crucial to understand the peculiar effect of electron-phonon interaction in this regime [3], and the tendency towards phase separation [4]. We discuss the two issues within the Hubbard-Holstein model, in which the correlated electrons are coupled with local lattice distortions.

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# Exotic phases in underdoped cuprates – competition and spontaneous symmetry breaking

V. Hinkov*[1], D. Haug[1], B. Fauqué[2], P. Bourges[2], Y. Sidis[2], A. Ivanov[3], C. Bernhard[4], C. T. Lin[1], B. Keimer[1]

[1]*Max-Planck-Institut, FKF, Stuttgart, Germany*
[2]*Laboratoire Léon Brillouin, CEA-CNRS, Gif-sur-Yvette, France*
[3]*Institut Laue-Langevin, Grenoble, Europe*
[4]*Department of Physics, University of Fribourg, Fribourg, Switzerland*

*V.Hinkov@fkf.mpg.de

The phase diagram of the cuprate high-$T_c$ superconductors is characterized by the competition between different strongly correlated electronic states. While at the lowest doping levels antiferromagnetism prevails, at medium hole-doping levels below $p_{h,opt}$ (optimal doping* different exotic phases have been invoked. Some of them break time-reversal symmetry like the "orbital currents" reported by Fauqué et al., Phys. Rev. Lett. **96**, 197001 (2006*, while others break symmetries of the crystal lattice, e.g. the rotational (C4* and translational symmetry like the static "stripe"-phases in the $La_{2-x}Sr_xCuO_4$ family reported by Tranquada et al., Nature **375**, 561 (1995*.
$YBa_2Cu_3O_{6+x}$ is suited for the investigation of phases breaking the C4 symmetry, since the 1D CuO-chains stabilize an orthorhombic structure which thus determines a preferential orientation and serves as a weak aligning field. Here we will report a systematic, doping-dependent investigation of the spin-excitation spectrum and show evidence for the occurrence of states which break the C4 symmetry, while keeping the translational symmetry of the lattice preserved, see V. Hinkov et al., Nature Physics **3**, 780 (2007* and Science **319**, 597 (2008*. Such states of matter have been previously postulated by Kivelson et al., Nature **393**, 550 (1998*, who termed them electronic liquid crystals, alluding to their symmetry properties analogous to conventional liquid crystals.
Finally, we will discuss how our findings can be interpreted within the framework of quantum phase transitions and argue that there is a quantum critical point around an oxygen content of $x \sim 0.5$, where nematic order disappears and a gap opens up in the spin fluctuation spectrum.

Keywords: Spontaneous symmetry breaking, Stripe phases, electronic liquid crystal

# Spin-polarized Fermi superfluids as Bose-Fermi mixtures

E. Taylor[*,1], A. Griffin[2], and Y. Ohashi[3]

[1] *CNR-INFM BEC Center, Dipartimento di Fisica, Universita di Trento, Povo, Italy*
[2] *Department of Physics, University of Toronto, Toronto, Canada*
[3] *Faculty of Science and Technology, Keio University, Hiyoshi, Yokohama 223, Japan*

* etaylor@science.unitn.it

In the strong-coupling Bose-Einstein condensation (BEC* region where a Feshbach resonance gives rise to tightly bound dimer molecules, we show that a spin-polarized Fermi superfluid reduces to a simple Bose-Fermi mixture of Bose-condensed dimers and the leftover unpaired fermions. Using a many-body functional integral formalism, the Gaussian fluctuations give rise to an induced dimer-dimer interaction mediated by the unpaired fermions, with the dimer-fermion vertex being given by the (mean-field* Born approximation. Treating the pairing fluctuations to quartic order, we show how the action for a spin-polarized Fermi superfluid reduces to one for a Bose-Fermi mixture. This Bose-Fermi action includes an expression for the effective dimer-unpaired fermion interaction in a spin-polarized Fermi superfluid beyond the Born approximation, in the BEC limit. In the low-density limit, we show how this dimer-fermion interaction gives the s-wave scattering length $a_{BF}=1.18a_F$ ($a_F$ is the s-wave fermion scattering length*, a result first derived by Skorniakov and Ter-Martirosian in 1957 for three interacting fermions.

Keywords: Fermi gas condensates, spin-polarized, Bose-Fermi mixtures

# Properties of high-$T_c$ copper oxides from band models of spin-phonon coupling.

T. Jarlborg

*DPMC, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland*

e-mail: thomas.jarlborg@physics.unige.ch

All high-$T_C$ cuprates contain 2-dimensional (2D* layers of CuO planes. Undoped systems
are often antiferromagnetic insulators, but small hole doping makes them metallic. The Cu-d and O-p electrons in the layers lead to a cylindrical Fermi surface (FS* with very small band dispersion in the perpendicular $\vec{z}$ -direction. In this work I will show that the electronic structure is very sensitive to potential modulations (phonons and/or spin waves* within these planes. Ab-initio LMTO band calculations, for long (1D along $\vec{x}$ * unit cells of La- or Hg-based copper oxides with phonon distortions and spin waves, show that the modulations will create partial gaps near $E_F$ . The energy position of the gap is a function of the wave length of the potential modulations, which leads to a correlation between wave length and doping. Spin-phonon coupling (SPC* is inherent, which means stronger spin waves when they coexist with phonons and large $\lambda_{sf}$ for spin fluctuations. A 2D extension of potential modulations along $\vec{x}$ and $\vec{y}$ is made through a nearly free-electron band model with parameters from the LMTO results. Many typical properties of high-$T_C$ cuprates, such as pseudogaps, stripe-like modulations, FS-arcs, phonon softening, loss of magnetic modulations at high T, and correlation between doping and q-dependent excitations are some of the consequencies of SPC. The pseudogap is a normal state property in this scenario and it competes with superconductivity. These and other aspects of SPC within the 2D band will be discussed, as well as possible corrections of the spin-polarized part of density functional.

Keywords: Band structure, spin-phonon coupling, cuprates.

# 28 July Monday 15:00-17:00

## Session 8A

- **M. Doria**
- **M. Fratini**
- **P. G. Freeman**
- **T. Adachi**
- **C. Janowitz**
- **M. R. Trunin**
- **J. Miranda Mena**

## The confined vortex phase and phase segregation

M. M. Doria [*1,4], Antonio R. de C. Romaguera [2,4], A. Ludu [3,4], F. M. Peeters [4]

[1] *Universidade Federal do Rio de Janeiro, Rio de Janeiro 21941-972 RJ, Brazil*
[2] *Universidade Federal Rural de Pernambuco, Recife 52171-900 PE, Brazil*
[3] *Louisiana State University, Baton Rouge, LA 70803, USA*
[4] *Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium*

* mmd@if.ufrj.br

Competing orders can lead to phase segregation, a phenomena at the heart of many compounds with new magnetic and transport features not found in homogeneous systems. For instance, stripes result from the coexistence of different phases in the cuprate and manganite compounds. Here we assume intrinsic mesoscopic segregation as a consequence of the coexistence of superconductivity and magnetism and study the resulting vortex patterns. A scenario for the spontaneous vortex phase is proposed as the regime where vortices interconnect nearest neighbor magnetic domains inside the superconductor. We also claim the existence of a new regime where vortices are confined inside the compound and cannot be externally observed because of the Meissner shielding. Thus a vortex state is possible even without the presence of an external applied field and is generally characterized by these confined vortex loops added of broken loops that spring to the surface. These two types of curved vortex lines in space are truly three-dimensional spatial structures, obtained in our treatment of the Ginzburg-Landau theory [1], numerically solved in three-dimensions. We show the remarkable effects of the Lorentz force that serve as a basis for the observation of confined loops. We propose ways to experimentally detect them through a current bias and find distinct segregated phases similar to stripes. We also study the onset of the confined phase in nearly type I superconductors ($\kappa \approx 1/\sqrt{2}$* where vortex attraction and not repulsion determines the interaction.

Keywords: vortex, magnetism, superconductivity

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# Critical opalescence in superoxygenated $La_2CuO_{4+y}$

M. Fratini*, N. Poccia, Alessandra Vittoriani Orgeas and A. Bianconi

*Università degli Studi di Roma "La Sapienza", Dipartimento di Fisica, Piazzale Aldo Moro 2, 00185 Roma, Italy*

* michela.fratini@roma1.infn.it

How quantum coherence could show up at room temperature, evading the temperature decoherence effects can be understood by studying the lamellar High Tc Superconductors $Mg_{1-x}A_x$ [$B_2$] , $ReO_{1-x}F_x$ [FeAs] and ABO [$CuO_2$]. These materials share a common heterostructure at atomic limit (or nanoscale architecture* made of a superlattice of thin metallic layers with a spacing between the layers ranging between 0.35 to 1 nm. The Fermi liquid in the metallic layers appears to have the common characteristic of a quantum criticality in the phase diagram (which is not present in the standard macroscopic quantum coherent systems like the low temperature BCS superconductors.

The super-oxygenated $La_2CuO_{4+y}$ (LCO* system provides the simplest case between cuprates families because of i* its simple lattice structure, ii* the mobility of dopants, interstitial oxygen ions (iO* and iii* the proximity of the internal chemical pressure $\eta_c$ to the critical value for the formation of a "commensurate stripes" crystalline phase that competes with the superconducting order. This system shows i* long range 3D ordering of iO at T1=330 K, ii* short range ordering of local lattice distortions at T2=180K, iii* onset of superconducting phase at Tc=41K co-existing with iv* long range magnetic ordering below $T_M$=41K. At room temperature the system shows mesoscopic bubbles of short range local lattice fluctuations above T2 (called Q3* and microsopic bubbles of long range 3D ordering of iO. (called Q2*.

In this work we use advannced X-ray micro-diffraction, which allows us to detect the coexistence of Q2 and Q3 phase in the same single crystal. The mapping of the domain size of the Q2 and Q3 phase shows a power law behaviour (with a cut-off*. This result is assigned to the criticality of the system being close to the tricritical point identified in the phase diagram ($T_c$, doping and chemical pressure*. This conclusion is supported by the photoinduced phase transition near the critical point .

Moreover the investigation of the order to disorder transition of iO shows a hysteretic loop between 240 K and 360K, cleary indicating that it is to be considered a continuous marginal first order phase transition with a small discontinuity at 330K. Each thermal cycle has been recorded with a different photon flux. We observe that the width of the hysteretic loop decreases with the increasing of the incident photon flux; this means that the photon flux increases the velocity of ordering dynamics. These results give us the intriguing possibility to manipulate and control structural inhomogeneities on the atomic scale length in such systems, using X-ray rays.

# Asymmetry in the Magnetic Excitation Spectrum of Charge Stripe Ordered La(2-x*Sr(x*NiO(4+delta*.

P.G. Freeman[1] , A. T. Boothroyd[2], S. R. Giblin[3], S. M. Hayden[4], D. Prabhakaran[2], M. Enderle[1], K Hadril[5] and R. Mole[6].

*[1]Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France.*
*[2]Department of Physics, Oxford University, Oxford, OX1 3PU, United Kingdom.*
*[3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom.*
*[4]Department of Physics, University of Bristol, Bristol, BS8 1TL, United Kingdom.*
*[5]Institut für Physikalische Chemie, Universität Göttingen, Tammanstrasse 6, 37077 Göttingen, Germany.*
*[6]FRM II, Lichtenbergstrasse, 1 85747 Garching, Germany.*

e-mail: freeman@ill.fr

We have studied the model charge ordered system La(2-x*Sr(x*NiO(4+delta* extensively at the commensurate x = 1/3 doping[1]. Symmetric spin wave dispersion is observed at x = 1/3 and is relatively well understood in terms of simple linear spin wave theory. In our current research we show that away from the x = 1/3 doping, the magnetic excitation spectrum of charge stripe-ordered La(2-x*Sr(x*NiO(4+delta* displays strong asymmetry in the magnetic excitation spectrum. There are strong similarities observed in our work on the spin excitation spectrum of La(2-x*Sr(x*NiO(4+delta* away from x = 1/3 and the hourglass spin excitation spectrum of the hole doped cuprate superconductors[2]. We use a recent theoretical prediction of the asymmetry in the excitation spectrum of La(2-x*Sr(x*NiO(4+delta* to elucidate features of the magnetic excitation spectrum, and show the limitations of this model[3].

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# Inhomogeneity of superconductivity and stripe correlations in single-layer high-$T_c$ cuprates

T. Adachi*[1], Y. Tanabe[1], Y. Fukunaga[1],
K. Omori[1], H. Sato[1], T. Noji[1], K. Kudo[2], T. Nishizaki[2], T. Sasaki[2], N. Kobayashi[2],
Y. Koike[1]

[1]*Department of Applied Physics, Tohoku Univ., 6-6-05 Aoba, Aramaki, Sendai 980-8579, Japan*
[2]*Institute for Materials Research, Tohoku Univ., 2-1-1 Katahira, Sendai 980-8577, Japan*

*E-mail: adachi@teion.apph.tohoku.ac.jp

Our recent works on the inhomogeneity of superconductivity and the magnetic-field effects on the charge-spin stripe correlations in La-214 and Bi-2201 high-$T_c$ cuprates are reviewed.
The possible inhomogeneity of superconductivity has been investigated by means of bulk probes reflecting the bulk properties of a sample, that is, the magnetic susceptibility and specific heat in $La_{2-x}Sr_xCuO_4$ [1-4] and (Bi,Pb*$_2Sr_2CuO_{6+\delta}$ single crystals from the underdoped to overdoped regime. It has been found that both the Meissner volume fraction, regarded as corresponding to the superconducting (SC* volume fraction in a sample, and the Sommerfeld constant at zero temperature, reflecting the density of states in the ground state, exhibit significant dependence on the hole concentration. These results strongly suggest that a phase separation into SC and normal-state regions takes place in both the underodped and overdoped regimes of $La_{2-x}Sr_xCuO_4$ and (Bi,Pb*$_2Sr_2CuO_{6+\delta}$ irrespective of ways of doping, i.e., the cation substitution and introduction of excess oxygen.
The in-plane electrical resistivity, $\rho_{ab}$, has been measured in various magnetic fields for single-crystalline $La_{2-x}Ba_xCuO_4$ with x = 0.08 – 0.125 [5,6]. An anomalous increase in $\rho_{ab}$ has been found in the less-stabilized stripe-ordered state of x = 0.10, while almost no enhancement of $\rho_{ab}$ has been observed in the stabilized stripe-ordered state of x = 0.11 and 0.125. In conclusion, when the charge-spin stripe order is not fully stable in zero field, magnetic field operates to stabilize the charge-spin stripe order.
These results arrow us to conclude that an inhomogeneous SC state tends to be realized in both the underdoped and overdoped regimes in high-$T_c$ cuprates and that non-SC regions may be related to the stripes.

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Keywords: Inhomogeneous superconductivity, Stripe correlations, Bulk-probe measurements

# Structural, superstructure and charge order in Bi-cuprates

C. Janowitz*, L. Dudy, B. Müller, O. Lübben, A. A. Kamal, B. Ziegler, A. Krapf, H. Dwelk, and R. Manzke

*Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr.15, D-12489 Berlin, Germany*

* christoph.janowitz@physik.hu-berlin.de

Inhomogeneities in any form play an essential role for the unusual properties of the cuprates. Most interesting is the microscopic phase separation in form of checkerboard or static stripe order for certain magic doping fractions. Preferentially in the LSCO system it has been detected unequivocally by inelastic neutron scattering, by scanning tunnelling- microscopy and –spectroscopy and by transport measurements. Bi-cuprates, favoured for photoemission studies, are unfortunately prone to structural inhomogeneity and superstructure modulations. We have therefore performed combined STM and high resolution photoemission studies on (Pb*Bi-2201 for different compositions and identified the contributions due to superstructures beyond the well known 1x5 reconstruction. Since the inclusion of the related scattering vectors gives a nearly perfect image of the experimental Fermi surface[1*], it can be speculated how far such modelling is necessary to understand other features such as the pseudogap, polarization effects and generally the spectral lineshape. A careful analysis of transport data reveals depressions of the superconductivity for certain doping fractions also in the Bicuprates. The electronic structure from the antiferromagnetic to the superconducting regime[2*], the boson-fermion interaction[3*] and possible signatures of the reduced dimensionality of the electronic system[4*] will be discussed.

Keywords: ARPES, charge inhomogeneity, STM

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# Peculiarities of the microwave conductivity of superconducting single crystals with different doping levels

M.R. Trunin*

*Institute of Solid State Physics RAS*
*142432 Chernogolovka, Moscow district, Russia*

*trunin@issp.ac.ru

Results of recent investigations of the temperature dependences of the surface impedance Z(T*=R(T*+iX(T* and microwave conductivity σ(T*= σ'(T*-iσ'' (T* in $YBa_2Cu_3O_{7-x}$, $Ba_{1-x}K_xBiO_3$, and $V_3Si_{1-x}$ single crystals are discussed.

In the superconducting state of $YBa_2Cu_3O_{7-x}$ with x>0.35 the behavior of the superfluid density $n_s$(T,x*∝ σ'' $_{ab}$(T,x* can be treated in the framework of d-density wave scenario of pseudogap in underdoped HTSC. The observed peculiarities of the imaginary part σ''$_{\_c}$(T,x* of the c-axis conductivity at $T<<T_c$ are determined by a strong decrease of the interlayer coupling integral with an increase of x [1].

Measurements of the surface impedance Z(T* in $Ba_{1-x}K_xBiO_3$ crystals with $T_c$=11K (x ≈ 0.5* and $T_c$=30K (x ≈ 0.4* allow one to establish that the former is a BCS-superconductor (Z(T* saturates exponentially with lowering temperature at $T<<T_c$* and the latter is not (Z(T* is linear at $T<<T_c$*. In addition, it is found that the temperature dependences of the upper critical field $H_{c2}$(T* of the crystals with $T_c$>20K are similar to those in HTSCs, both exhibiting strong positive curvature. On the contrary, $H_{c2}$(T* curves of the crystals with $T_c$<15K are in complete agreement with the BCS theory [2].

The temperature dependences of the microwave complex conductivity of $V_3Si_{1-x}$ single crystals with different stoichiometry allowed us to observe a number of peculiarities of two-band superconductors, namely, a nonlinear metallic behavior of resistivity at $T>T_c$, a positive curvature of σ'' (T* curves close to $T_c$, and a coherence peak in σ' (T* centered at $T \approx T_c/2$ [3].

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## Stripes formation induced by temperature and doping.

Joaquin Miranda Mena and Viktor Kabanov.

*Jozef Stefan Institute, Jamova 39, Ljubljana,SI 1001, Slovenia*

e-mail: joaquin.miranda.ijs.si

Formation of charged clusters in 2D systems, are studied by means of Landau theory of phase transitions. We analyzed shapes and sizes of clusters when the coupling between the order parameter and the charge density is introduced in two different ways. In the first type of models the charge density is coupled to the order parameter linearly as suggested by Spivak et al [1]. In the second type of models the charge is coupled to the square of the order parameter as we have proposed in ref. [2]. However, in both cases the long-range Coulomb potential is present and we prove that it is the key factor for the patterns obtained. In particular we show that a stripe phase exists in the wide range of the parameters.

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[2] Joaquin Miranda and Viktor Kabanov, Physica C., Vol.468, Pages 358-361 (2008*

Keywords: Phase transition. Stripes. Cuprates. Manganites

# 28 July Monday 15:00-17:00

## Session 8B

- **M. Kenzelmann**
- **M. V. Krasinkova**
- **I. Eremin**
- **M. Grilli**
- **G. Litak**
- **D. Orgad**
- **R. Movshovic**

# Unconventional magnetism in a heavy-fermion superconductor

M. Kenzelmann[1,2,*]

[1]*Laboratory for Developments and Methods, Paul Scherrer Institute, Switzerland*
[2]*Laboratory for Solid State Physics, ETH Zurich, Switzerland*

* kenzelmann@phys.ethz.ch

I will talk about the magnetic properties of the heavy-fermion singlet superconductor $CeCoIn_5$ close to the quantum phase transition where superconductivity is suppressed by magnetic fields. Our experiments provide experimental evidence for a novel vortex structure that is not described by the Abrikosov-Ginzburg-Landau paradigm. Because superconducvitiy in $CeCoIn_5$ is Pauli-limited, high magnetic fields break up Cooper pair singlets inside the vortex cores, leading to the presence of magnetic moments in the vortex cores. Further, I will comment on the possibility of a Fulde, Ferrell, Larkin and Ovchinnikov (FFLO* vortex phase in $CeCoIn_5$, and provide evidence that the superconducting gap function is directly coupled to the magnetism.

Keywords: superconductivity, heavy fermions, vortices

# On the role of oxygen ion polarization in phase transitions, stripe structure, and highly correlated electron state in transition metal oxides

M.V.Krasinkova

*Ioffe Physico-Technical Institute, Russian Academy of Sciences, St.Petersburg, Russia*

e-mail: marinak@mail.ioffe.ru

Using cuprate superconductors and manganites as examples, it is shown that taking into account polarization of anions by cations in transition metal oxides leads to new ideas on chemical bonds in these materials and on the state and behavior of valence electrons in them.

Polarization of anions by cations can give rise to σ- and π-type covalent components of the interionic bond. Therefore, valence electrons are divided into the σ and π electrons that have different states and behaviors and, hence, lead to different material properties. Formation of one-electron σ bonds between ions and their ordering in definite directions cause phase transitions with symmetry lowering.

Formation of covalent bonds means the appearance of exchange interaction between valence electrons that results in their highly correlated state. The correlated state of σ electrons manifests itself in their spatial and spin ordering accompanied by formation of polarization-localized Wigner lattices resulting from the exchange interaction between electrons rather than the Coulomb interaction. Such a state of σ electrons is responsible for dielectric and magnetic properties of transition metal oxides.

The role of doping in these materials consists in a further strengthening of the covalent component of interionic bonds, which is accompanied by further symmetry lowering, to the appearance of quasi-one-dimensional chains of covalently bonded ions along which π orbitals with different π-electron delocalization degrees can be formed. The exchange and Coulomb interactions between π electrons lead to formation of quasi-one-dimensional Wigner crystals responsible for transport properties of these materials, including superconductivity.

# Magnetic excitation, electron-phonon interaction, and stripes in lamellar cobaltates

Ilya Eremin[1,2*], Maxim Korshunov[1,3], and Alexander Donkov[1]

*[1] Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany*
*[2]Institut für Theoretische Physik, TU Braunschweig, 38106 Braunschweig, Germany.*
*[3]L.V. Kirensky Institute of Physics, Siberian Branch of RAS, Krasnoyarsk, Russia.*

* ieremin@pks.mpg.de

The recent discovery of the superconductivity in hydrated lamellar cobaltate $Na_xCoO_2$•$yH_2O$ has raised tremendous interest in the nature and symmetry of the superconductive pairing in these materials. The phase diagram of this compound with geometrically frustrated triangular lattice, with varying electron doping concentration x and water intercalation y, is rich and complicated; in addition to superconductivity, it exhibits magnetic and charge orders, and some other structural transitions.
Here we present a study of the relation between the fermionic and the bosonic degrees of freedom in the lamellar cobaltate with triangular lattice of Co, $Na_xCoO_2$. We have derived the single-electron energies and the effective tight-binding description for the $t_{2g}$ bands crossing the Fermi level[1] on the bases of the ab-initio band structure for $Na_xCoO_2$. The Fermi surface topology changes with doping that is reflected in the behavior of the magnetic susceptibility. It shows two different regimes, with the tendency towards the antiferromagnetic (AFM* and the ferromagnetic (FM* fluctuations, divided by the critical concentration $x_m$. We further analyze the influence of the electronic correlations in this system and possible symmetry of the superconducting gap in the superconducting $Na_xCoO_2$•$yH_2O$[2]. Finally I will discuss the strength of the electron-phonon interaction in lamellar cobaltates and compare the results with the recent Raman data[3] and discuss the origin of magnetic and charge ordered phase at Na concentration of x=0.5.

Keywords: triangular lattice, electron-phonon interaction, magnetic excitations, density wave transition

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# Spectroscopic evidences of quantum critical fluctuations in cuprates.

S. Caprara, C. Di Castro, T. Ens, and M. Grilli

*SMC - Istituto Nazionale di Fisica della Materia,*
*Dipartimento di Fisica, Università "La Sapienza", Roma, Italy*

e-mail: marco.grilli@roma1.infn.it

We discuss the relevant role of bosonic excitations as mediators of a retarded interaction between the electrons in the cuprates. These bosonic excitations, should have a nearly quantum-critical behavior to account for the specific temperature dependence of optical and Raman spectra [1]. Within the stripe quantum critical point theory for high Tc superconductors, we point out that charge and spin collective fluctuations are good candidates to account for the doping and temperature dependence of both the optical and Raman spectra.
In the case of Raman we find that the charge and spin collective modes contribute in a complementary way to the scattering in the $B_{1g}$ and $B_{2g}$ channels [2]. In particular we find that, for symmetry reasons, only charge modes can contribute at very low energies in the $B_{1g}$ channel thereby providing a direct confirmation that the order associated to the quantum critical point near optimal doping of cuprates occurs at finite wavevectors, which precisely corresponds to those of stripe fluctuations [3].
For the optical conductivity we find that momentum conservation possibly introduces non-universal frequency scales that may (partially* mask the quantum-critical effects of the collective modes in the finite-frequency absorption. Therefore the lack of specific peak features and scaling cannot be invoked against the role of collective critical charge fluctuations in optical spectra [4].

Keywords: Stripe quantum critical point, Raman spectroscopy, optical conductivity.

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[4] S. Caprara, M. Grilli, C. Di Castro, and T. Enss, Phys. Rev. B **75**, 140505 (2007*.

# Charge Order Versus Superconductivity in Inhomogeneous Systems

Grzegorz Litak*

*Department of Mechanic, Technical University of Lublin, Nadbystrzycka 36,
PL-20-618 Lublin, POLAND*

* g.litak@pollub.pl

We examine the disordered system with defined centers of carries attraction. By changing concentration of such centers we can model different phases including superconductivity and charge order. To study electron correlations and to describe disorder effects, the Negative U Hubbard model and the Coherent Potential Approximation (CPA* have been applied [1]. The charge and superconduction orders have been defined on the bipartite lattices. In this paper we also discuss the corresponding phase diagram defined for the concentration of negative centers.

Keywords: CDW, superconductity, CPA

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# Effects of geometrical fluctuations on the transition temperature of disordered quasi-one-dimensional superconductors

Dror Orgad[*1]

[1]*Racah Institute of Physics, The Hebrew University, Jerusalem, 91904, Israel*

[*]orgad@phys.huji.ac.il

We study the superconducting transition temperature, $T_c$, of an array of fluctuating, maximally gapped interacting ladders, embedded in a disordered plane. Renormalization group analysis indicates that geometrical fluctuations mitigate the suppression of the intra-ladder pairing correlations by the disorder. In addition, the fluctuations enhance the Josephson tunneling between the ladders. Both effects lead to an increase of $T_c$ in the Josephson coupled array. These findings may be relevant to the understanding of the 1/8 anomaly in the lanthanum based high-temperature superconductors.

Keywords: Stripe fluctuations, Disorder effects, Lanthanum based cuprates

# Possible Fulde Ferrel Larkin Ovchinnikov inhomogeneous Superconducting state in $CeCoIn_5$

R. Movshovich[1*], Y. Tokiwa[1], F. Ronning[1], E. D. Bauer[1], P. Papin[1], A. Bianchi[2], Z. Fisk[3]

[1] *Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA.*
[2] *Departement de physique Montreal, Universite de Montreal, QC, H3C 3J7 Canada*
[3] *University of California, Davis, California 95616, USA*

* roman@lanl.gov

$CeCoIn_5$ undergoes a phase transition within a superconducting (SC* state. A new superconducting state occupies a high field - low temperature (HFLT* part of the SC state. Several properties of the SC state in $CeCoIn_5$ make it the strongest candidate so far for realization of the spatially inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO* superconducting state predicted theoretically in 1960's. $CeCoIn_5$ is a very pure compound, with electronic mean free path reaching several microns within superconducting state. In spite of the superficial simplicity, the system proved to be rather complex, with a Quantum Critical Point (due to the underlying antiferromagnetic order* located very close to the superconducting critical field $H_{c2}$. Is the new SC phase FFLO, or is it magnetic in origin? I will present Cd-doping data that shows that at the HFLT phase is suppressed by the minute amount of impurities, few hundred parts per million. At this concentration, the average distance between impurities is close to twice the superconducting coherence length $\xi$, making $\xi$ the characteristic length of the HFLT state. We conclude, therefore, that our investigations support the FFLO scenario.

Keywords: unconventional superconductivity, inhomogeneous superconductivity, FFLO

# 28 July Monday 21:30-23:00

## Special Session 1.
## on FeAs Superconductors

- **S. Tajima**
- **H. A. Mook**
- **R. Caivano**
- **H.-J. Grafe**
- **J. Ashkenazi**
- **I. Eremin**

# Introduction to FeAs superconductors

S. Tajima

*Department of Physics, Osaka University*
*Machikane-yama 1-1, Toyonaka, Osaka 560-0043, Japan*

# Magnetic and Structural Order versus superconductivity in the Iron-based layered $LaO_{1-x}F_xFeAs$ systems

H.A. Mook

*Neutron Science Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

mookhajr@ornl.gov

The recent discovery of superconductivity in the rare-earth (R* iron-based oxide systems $RO_{1-x}F_xFeAs$ has generated enormous interest because these materials are the first non-copper oxide superconductors with Tc exceeding 50 K. Here we use neutron scattering to demonstrate that LaOFeAs undergoes an abrupt structural distortion below ~150 K, changing the symmetry from tetragonal (space group P4/nmm* to monoclinic (space group P112/n* at low temperatures, and then followed with the development of long range SDW-type antiferromagnetic order at~134 K with a small moment but simple magnetic structure. Doping the system with fluorine suppresses both the magnetic order and structural distortion in favor of superconductivity. Therefore, much like high-Tc copper oxides, the superconducting regime in these Fe based materials occurs in close proximity to a long-range ordered antiferromagnetic ground state.

# Competition between superconductivity and the structural tethragonal orthorombic transition in in FeAs superconductors

R. Caivano*, M. Fratini, A. Puri,
A. Ricci, A. Bianconi[1]

*Università "La Sapienza" Roma, Dipartimento di Fisica, P.le Aldo Moro 2*

rocchina.caivano@roma1.infn.it

The study of new superconductors compounds FeAs has shown that this materials has a superconductive phase that depends on doping and on the rare-earth [1] and that the non superconductive compounds show a structural tetragonal orthorhombic phase transition [2-4]. In this scenario we discuss the competition between superconductivity and the structural tetragonal orthorhombic transition in NdOFeAs compound and we show that the continous structural phase transition competes with the superconductive phase. Therefore by controlling the internal chemical pressure in new materials it should be possible to push toward zero the critical temperature $T_0$ of the structural phase transition in order to get superconductors with higher $T_c$.

key words: quantum coherence, structural phase transition, layered HTSC.

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# $^{75}$As Nuclear Magnetic Resonance studies of superconducting $LaO_{1-x}F_xFeAs$

H.-J. Grafe *[1], D. Paar [1,2], G. Lang [1], N. J. Curro [3], B. Büchner [1]

[1]*IFW Dresden, Institut für Festkörperforschung, Helmholtzstrasse 20, D-01069 Dresden, Germany.*
[2]*Department of Physics, Faculty of Science, University of Zagreb, P. O. Box 331, HR-10002 Zagreb, Croatia*
[3]*Department of Physics, University of California, Davis, CA 95616, USA*

* h.grafe@ifw-dresden.de

We have performed $^{75}$As Nuclear Magnetic Resonance (NMR* and Nuclear Quadrupole Resonance (NQR* measurements on powders and aligned powders of the new $LaO_{1-x}F_xFeAs$ superconductor [1]. In the normal state, we find a strong doping dependence of the As NQR frequency that increases with increasing F doping, similar to the $^{17}$O quadrupole frequency in the high $T_c$ cuprates, suggesting that the As quadrupole frequency is a measure of the charge carrier doping. From the As NMR experiments on aligned powders [2], we find a strong temperature dependence of the spin shift and Korringa behavior of the spin lattice relaxation rate. In the superconducting state, we find evidence for line nodes in the superconducting gap and spin-singlet pairing. Our measurements reveal a strong anisotropy of the spin lattice relaxation rate, which suggest that superconducting vortices contribute to the relaxation rate when the field is parallel to the c-axis but not for the perpendicular direction.

Keywords: high temperature superconductivity, pseudogap, nuclear magnetic resonance and relaxation, oxypnictides

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[2] H.-J. Grafe et al., arXiv: 0805.2595

# Why Should We Expect Similarities Between the Physics of the Iron-Oxypnictides and of the Cuprates

J. Ashkenazi*

*Department of Physics, University of Miami, Coral Gables, FL 33124, USA*

* jashkenazi@miami.edu

Mossbauer spectroscopy suggests[1] that iron atoms are magnetic within the superconducting (SC* state of the iron-oxypnictides. LDA+DMFT electronic-structure calculations suggest[2] that their five Fe d orbitals are subject to strong intra-atomic correlations, and contribute at the vicinity of $E_{F.}$ Consequently, it should be assumed that low-energy excitations, at (electron-doped* SC stoichiometries of this system, are characterized by an atomic Fe d occupation which fluctuates between those of 6 and 7 electrons.

The auxiliary-particle method can be applied to this case, assigning boson states for integer-spin six-electron atomic configurations (of different Fe d orbitals and their spins*, and fermion states for half-integer-spin seven-electron atomic configurations. Within this method, the sum of the numbers of such bosons and fermions in each Fe site must be constrained to be 1. This constraint is imposed in terms of a Lagrange Bose field, similarly to the approach applied by the author to the high $T_C$ cuprates, in another contribution to this conference.

This results in the existence of many similarities between the iron-oxypnictides and the cuprates, including the occurrence of high-$T_C$ superconductivity. A prediction is made that dynamical spin (and associated charge* inhomogeneities occur in SC oxypnictides, and that they are characterized by wave vectors around those of the SDW in the undoped stoichiometry (with the two alternative directions of orthorhombic axes*.

Keywords: superconductivity, oxypnictides, cuprates, auxiliary particles.

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A. O. Shorikov et al., cond-mat/0804.3283.

# Theory for magnetic excitations in novel superconductors with Fe-based layered structure

Ilya Eremin[1,2*], Maxim Korshunov[1,3]

*[1] Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany*
*[2]Institut für Theoretische Physik, TU Braunschweig, 38106 Braunschweig, Germany.*
*[3]L.V. Kirensky Institute of Physics, Siberian Branch of RAS, Krasnoyarsk, Russia.*

* email: ieremin@mpipks-dresden.mpg.de

Based on the effective four-band model we analyze the spin response in the normal and superconducting state of the novel Fe-pnictide superconductors. While the normal state spin excitations are dominated by the continuum of the interorbital antiferromagnetic fluctuations and the intraband spin density wave fluctuations, the unconventional superconductivity yields different feedback. The resonance peak in form of the well-defined spin exciton occurs {\it only} for the interband scattering at the antiferromagnetic momentum, ${\bf Q}_{AFM}$, for the extended s-wavesuperconducting order parameter and it disappears rapidly for ${\bf q} <{\bf Q}_{AFM}$. The resonance feature is extremely weak for the $d_{x2-y2}$-wave order parameter due to specific Fermi surface topology of these compounds. The essential difference between extended s-wave and $d_{x2 -y2}$-wave symmetries for the magnetic excitations can be used for experimental determination of the superconducting wave function
symmetry.

Keywords: 1D spin chain system; Quantum Tunneling of Magnetization

# 29 July Tuesday 8:30-10:30

## Session 9

- **A. Bishop**
- **M. Greven**
- **P. Bourges**
- **M. Fujita**
- **Ch.Niedermayer**

# Heterogeneity in Strongly Correlated Quantum Matter: Origins, Signatures and Consequences (LA-UR-08-1374*

Alan R. Bishop

*Los Alamos National Laboratory, Los Alamos NM (USA**

* email: arb@lanl.gov

A substantial change is presently taking place in experimental and theoretical approaches to large classes of "strongly correlated" materials, reflecting growing evidence that multiscale spatio-temporal complexity (including filaments and clusters* is frequently both intrinsic and functional, and further that intimate relationships between hierarchies of functional scales constitute essential "Systems" or "Networks". This complexity provides qualitatively new avenues for predictive design of technological materials, including intrinsically nanoscale structures.

In a search for underpinning concepts and principles, we suggest that the prevalence of local constraints and coexisting short- and long-range forces are keys to some major class of materials with emergent "landscapes" of spatio-temporal patterns and associated glassy dynamics and statistics. We review our recent work in these directions in the context of elesticially-driven textures in (a* directionally-bonded electronic materials [(1*], including superconducting, magnetoresistant and ferroelectric oxides; and (b* bubble opening patterns in DNA[(2*]. We emphasize the importance of coordinated suites of experimental probes being applied to establish the networks of functional scales: microscopic to mesoscopic to macroscopic.

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

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# Recent neutron scattering results for the high-temperature superconductors $Nd_{2-x}Ce_xCuO_{4+\delta}$ and $HgBa_2CuO_{4+\delta}$

M. Greven*

*Department of Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford, CA 94305, USA*

* greven@stanford.edu

High-temperature superconductivity develops near antiferromagnetic (AF* phases, and it is possible that magnetic excitations contribute to the superconducting (SC* pairing mechanism. In order to assess the role of antiferromagnetism, it is essential to understand the doping and temperature dependence of the two-dimensional AF spin correlations. The
phase diagram is asymmetric with respect to electron and hole doping, and for the comparatively less-studied electron-doped materials, the AF phase extends much further with doping and it appears to overlap with the SC phase: the archetypical compound $Nd_{2-x}Ce_xCuO_{4+\delta}$ shows bulk superconductivity above x~0.13, while evidence for AF order has been found up to x~0.17. However, our new inelastic magnetic neutron scattering measurements point to the distinct possibility that superconductivity does not co-exist with genuine long-range antiferromagnetism [1]. We furthermore show evidence that the pseudogap phenomenon in the electron-doped materials arises from a build-up of AF spin correlations. Our latest results for the AF spin excitations force us to conclude that recent claims for the existence of a magnetic resonance in the electron-doped cuprates have to be reinterpreted [2].

In a separate effort, we have succeeded in growing sizable single crystals of $HgBa_2CuO_{4+\delta}$, the single-layer hole-doped compound with the highest superconducting transition temperature [3]. Careful characterization demonstrates the high quality of our crystals [4]. Our inelastic neutron scattering results reveal that the magnetic resonance occurs at a rather high energy [3,5]. Finally, we discuss very recent polarized neutron diffraction data that clearly reveal the existence of "hidden" magnetic order in the pseudogap phase of $HgBa_2CuO_{4+\delta}$ [6].

Keywords: High-temperature superconductivity, pseudogap, spin correlations, magnetic order, neutron scattering

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[6] Y. Li, V. Balédent, N. Barisic, Y. Cho, B. Fauqué, Y. Sidis, G. Yu, X. Zhao, P. Bourges, and M. Greven (manuscript in preparation*.

# Magnetic order in the pseudogap state of high-$T_c$ cuprates

Philippe Bourges*

*Laboratoire Léon Brillouin, CEA-CNRS, CEA-Saclay, 91191 Gif-sur-Yvette, France*

*philippe.bourges@cea.fr

One of the leading issues in high-$T_c$ superconductors is the origin of the pseudogap phase in underdoped cuprates. Using polarized elastic neutron diffraction, we identify a novel magnetic order in the $YBa_2Cu_3O_{6+x}$ system [1]. The observed magnetic order preserves translational symmetry as proposed for orbital moments in the circulating current theory of the pseudogap state. Subsequent measurements [2] in an $YBa_2Cu_3O_{6.6}$ sample, that displays very high oxygen order and an exceptionally sharp superconducting transition, confirm the first result. The temperature of the transition is that expected for the pseudogap suggesting that the pseudogap is directly connected with the magnetic order. To date, it is the first direct evidence of a hidden order parameter characterizing the pseudogap phase of high-$T_c$ cuprates.

Keywords: Cuprates, neutron diffraction, pseudogap

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# Neutron-scattering study of impurity effect on stripe correlations in La-based 214 high-$T_c$ cuprate

M. Fujita*[1] M. Enoki[2] K. Yamada[3]

*[1]Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*
*[2]Department of Physics, Tohoku University, Sendai, Miyagi 980-8578, Japan*
*[3]WPI-Advanced Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*

*e_mail: fujita@imr.tohoku.ac.jp

We review a systematic neutron-scattering study of impurity effect on the stripe correlations in the low-temperature-tetragonal (LTT* phase of $La_{1.875}Ba_{0.125}Cu_{y}Zn_{1-y}O_{4}$ (Zn-LBCO* and in the low-temperature-orthorhombic (LTO* phase of $La_{1.88-y}Sr_{0.12+y}Cu_{1-y}Fe_{y}O_{4}$ (Fe-LSCO*. In the former system, the superlattice peaks originated from both spin-density-wave (SDW* and charge-density-wave (CDW* orders were observed in y=0 and 0.03 samples. The broader peaks from SDW and CDW orders in the y=0.03 sample indicate the degradation of stripe correlation by Zn-doping. With decreasing the temperature, SDW and CDW orders simultaneously appear at 50 K and 30 K in the y=0 and 0.03 samples, respectively. On the other hand, in the latter system, CDW order was detected in the 0.005 and 0.01 samples, while no well-defined CDW peak was observed in the sample with y=0. Therefore, the CDW order is induced by Fe-doping in the LTO phase and the correlation quickly destroys by a smaller amount of doped Fe ions than by that of Zn. The incommensurability for the CDW order (ε* was found to be 0.224±0.002 r.l.u., which is approximately twice of that for SDW order (δ* of 0.115±0.003 r.l.u.. The relation of $\varepsilon \approx 2\delta$ is the same for SDW and CDW orders observed in the LTT phase of Zn-LBCO, suggesting that the similar stripe correlations can exist in the La-214 system, irrespective of crystal structure. Similarity and difference between Zn- and Fe-doping effects on the spin correlations, and the universality of stripe correlations will be discussed.

Keywords: Neutron-scattering, stripe correlations, impurity effect

# Tuning competing orders in $La_{2-x}Sr_xCuO_4$ cuprate superconductors by the application of an external magnetic field

Ch. Niedermayer*[1], J. Chang[1], N.B. Christensen[1], J. Mesot1, N. Momono[2], M. Oda[2],M. Ido[2]

[1]*Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institute, Villigen, Switzerland*
[2]*Department of Physics, Hokkaido University, Sapporo 060-0810, Japan*

* email: christof.niedermayer@psi.ch

We report the results of a combined muon spin rotation and neutron scattering study of the effects of an external magnetic field in $La_{2-x}Sr_xCuO_4$ for doping concentrations close to the so-called 1/8 anomaly. Application of a magnetic field drives the system towards a magnetically ordered spin-density-wave state, which dominates a large fraction of the underdoped regime and is fully developed at 1/8 doping. For doping levels beyond 1/8 static magnetism appears only above a strongly doping dependent threshold field $H_c$. We discuss our results in terms of competition between antiferromagnetic and superconducting order parameters. The competing spin density wave order may be driving the reconstruction of the Fermi surface into electron and hole pockets.

# 29 July Tuesday 11:00-12:40

## Session 10

- **I. Bozovic**
- **J. Fink**
- **P. Abbamonte**
- **Y. J. Kim**
- **A. Baron**

# Insights in High-$T_c$ Sperconductivity from the Study of Cuprate Heterostructures

I. Bozovic*, G. Logvenov, A. Gozar, V. Butko, A. Bollinger, O. Pelleg, H. J. Shim, P. Chaudhari, N. Bozovic and Z. Radovic

*Brookhaven National Laboratory, Upton NY 11973, USA*

*bozovic@bnl.gov

Using molecular beam epitaxy, we synthesize atomically smooth HTS thin films, multilayers and superlattices.[1] Such heterostructures enable novel experiments that probe the basic physics of HTS. For example, we have established that HTS and anti-ferromagnetic phases separate on Ångstrom scale, while the pseudo-gap state apparently mixes with HTS over an anomalously large length scale ("Giant Proximity Effect").[2]
In this talk, I will review our most recent experiments on such films and superlattices, including XRD, AFM, angle-resolved TOF-ISARS, high-resolution TEM, transport, resonant X-ray scattering, low-energy muon spin resonance, ultrafast photo-induced RHEED, and ultra-high magnetic field (up to 75 T) measurements, as well as a study of SIS junctions. The results include an unambiguous demonstration of strong coupling of in-plane charge excitations to out-of-plane lattice vibrations[3] and the discovery of interface HTS.

Keywords: cuprate films, interface superconductivity

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# Charge order in $La_{1.8\_x}Eu_{0.2}Sr_xCuO_4$ studied by resonant soft X-ray diffraction

J. Fink*[1]

[1]*Leibniz-Institute for Solid State and Materials Research Dresden, P.O. Box 270116*
*D-01171 Dresden, Germany*
*and*
*BESSY, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany*

*J.Fink@ifw-dresden.de

Resonant soft X-ray scattering with photon energies near the O K and the Cu $L_3$ edges has been used to study the charge ordering in the system $La_{1\cdot 8\_x}Eu_{0.2}Sr_xCuO_4$ as a function of temperature for x = 0.125 and = 0.15. Because the ionic radius of Eu ions is much smaller than that of La ions there is a large corrugation of the $CuO_2$ planes which stabilizes static stripe ordering. This offers the unique possibility to study static stripe-ordering at high temperatures. From the superstructure diffraction intensities a doping dependent incommensurate ordering can be derived for the charge carriers and for the lattice distortions caused by the ordering of charge carriers. The charge ordering occurs in the present system at $T_{CO}$ ~ 90 K well below the phase transition into the low-temperature tetragonal phase $T_{LTT}$ = 125 K. On the other hand charge ordering occurs well above the temperatures where spin ordering can be detected by neutron diffraction ($T_{SO}$ ~ 45 K). This clearly indicates that charge ordering and not spin interaction is the primary driving force for the formation of stripe-like phases in two-dimensional doped cuprates. Furthermore the incommensurability vector increases with increasing doping concentration. This is not compatible with nesting scenarios for charge ordering in these systems.

*Work done in collaboration with: E. Schierle, E. Weschke, J. Geck, D. Hawthorn, H. Wadati, H.-H. Hu, H. A. Dürr, N. Winzent, B. Büchner, G.A. Sawatzky*

Keywords: charge ordering, stripes, resonant X-ray scattering.

# Unusual valence band order in Zn-doped $La_{2-x}Sr_xCuO_4$

A. Rusydi[1], J. C. Lee[2], S. Smadici[2], J. C. Lee[2], S. Wang[2], P. Abbamonte [2,*], M. Enoki[3], M. Fujita[3], M. Rübhausen[1], K. Yamada[3]

[1]*Institute for Applied Physics, University of Hamburg, D-20355 Hamburg, Germany*
[2]*Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, IL 61801, USA*
[3]*Institute for Materials Research, Tohoku University, Katahira, Sendai 980-8577, Japan*

*abbamonte@mrl.uiuc.edu

We have observed unusual charge order, in both the valence and structural channels, with resonant soft x-ray scattering (RSXS* and neutron diffraction in several single crystals of $La_{1.95}Sr_{0.05}Cu_{0.95}Zn_{0.05}O_4$ (ZLSCO*. The order is diagonal, i.e. running 45° from the Cu-O bonds, and persists nearly to room temperature. In a detwinned crystal the order was observed to be unidirectional and mainly electronic (though a structural component is clearly visible*, with a period $11.9a_o$, where $a_o$=5.4Å is the orthorhombic lattice parameter. This period is approximately half that of the observed magnetic order [1] so is consistent with a 'stripe' picture [2]. In a twinned crystal with the same stoichiometry, a series of five superlattice reflections, with temperature-dependence similar to that of the untwined crystal, was observed at overtones of the spatial frequency (0.011, 0, 0*. The lower order overtones were observed to be mainly structural. All orders had very long persistence lengths of $\xi \sim 300a_o$. We interpret these superstructures as arising from a complex interplay between a valence electron instability and soft phonon modes, enhanced by the Zn disorder potential.

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# X-ray scattering study of charge stripes in $La_{2-x}Ba_xCuO_4$

Young-June Kim,[1]* J. H. Kim,[1] G. D. Gu,[2] C. S. Nelson,[2] T. Gog,[3] and D. Casa[3]

[1] *Department of Physics, University of Toronto, 60 St. George St. Toronto, ON M5S 1A7, Canada*
[2] *Brookhaven National Laboratory, Upton, NY 11973, USA*
[3] *Argonne National Laboratory, Argonne, IL*

*yjkim@physics.utoronto.ca

We report a comprehensive x-ray scattering study of charge stripe ordering in $La_{2-x}Ba_xCuO_4$ (x ~ 1/8), for which the bulk superconducting $T_c$ is greatly suppressed. Strong superlattice reflections corresponding to static ordering of charge stripes were observed in this sample. We found that the charge order in this sample is described with one-dimensional charge density waves, which have incommensurate wave-vectors (0.23, 0, 0.5) and (0, 0.23, 0.5) respectively on neighboring $CuO_2$ planes. The structural modulation due to the charge stripe order is simply sinusoidal, and no higher harmonics were observed. Just below the structural transition temperature, short-range charge density wave correlation appears, which then develops into a large scale charge ordering around 40 K, close to the spin density wave ordering temperature. However, this charge ordering fails to grow into a true long range order, and its correlation length saturates at ~23 nm, and slightly decreases below about 15 K. In addition, we report our observation of the unusual magnetic field dependence of the charge order correlation length. Specifically, in the superconducting phase the charge order correlation length increases as the magnetic field greater than ~5 T is applied. These observations will be discussed in connection with recent theoretical developments.

Keywords: Charge stripe; LBCO; magnetic field; incommensurate charge order

# Phonons in High-$T_c$ Superconductors by Inelastic X-Ray Scattering

Alfred Q.R. Baron*

*Materials Dynamics Laboratory, SPring-8/RIKEN*
*Facilities and Utilization Division, SPring-8/JASRI*

*baron@spring8.or.jp

We will present measurements of phonons in High-$T_c$ superconductors via Inelastic X-Ray Scattering. The focus will be on the comparison of ab-initio LDA calculations to the measured IXS spectra, in several different materials. This allows one to pinpoint some of the phonon anomalies in the materials, and, in, some sense, gauge the relative size of the phonon anomaly. Recent results will be presented.

# 30 July Wednesday 8:30-10:30

## Session 11

- **T. Egami**
- **S. Sugai**
- **B. O. Wells**
- **D. F. McMorrow**
- **K. Kumagai**

# Nano-Scale Phase Separation in the Cuprates

T. Egami[1,2] and B. Fine[1,3]

[1]*Department of Physics and Astronomy, University of Tennessee, Knoxville, TN, USA*
[2]*Oak Ridge National Laboratory, Oak Ridge, TN, USA*
[3]*Institute for Theoretical Physics, University of Heidelberg, Heidelberg, Germany*

egami@utk.edu

The nature of the pseudo-gap state is one of the central mysteries of the cuprate physics. Based upon careful evaluation of the effect of the long-range Coulomb interaction we argue that it is highly probable that the pseudo-gap state arises because of the nano-scale phase separation into a doped Mott-Hubbard insulator and a Fermi-liquid phase [1]. The phase-separation occurs in the phase diagram surrounded by the metal-insulator transition line ($p \sim 0.06$) and the pseudo-gap temperature line ($p \sim 0.25$). The quantum critical point corresponds to the phase line in the mean-field approximation ($p \sim 0.13$), but in reality it is never attained because of phase-separation. This picture is consistent with the Fermi-arc behavior observed by ARPES. Recent spin-polarized neutron scattering results on a YBCO6.6 single crystal support this view. They show that the magnetic phase is a spin-glass with a very short spin correlation length. It is possible that charges also self-organize into a local two-dimensional order. We suggest that the spin-glass phase offers a hospitable environment for the spin-singlet bipolarons, and phonon-induced charge transfer between the metallic phase and the magnetic phase with bipolarons produces high-temperature superconductivity.

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# Independent Control of Low-Energy Resonant States and Polaron States by the Zn-Doping and the Structural Transition in $La_{2-x}Sr_xCuO_4$ and $La_{2-x}Ba_xCuO_4$

S. Sugai*[1], T. Adachi[2], K. Sugiura[1], T. Takahashi[1], K. Obara[1], Y. Takayanagi[1], and Y. Koike[2]

[1]*Department of Physics, Faculty of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*
[2]*Department of Applied Physics, Graduate School of Engineering, Tohoku University, 6-6-05 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan*

*sugai@cc.nagoya-u.ac.jp

Low-energy electronic states are created as carriers are doped in high temperature superconductors. The states are composed of two different origins, the resonant states created by pure electronic interactions at $E_F$ and the polaron states created by electron-phonon interactions. The resonant states are reduced by the substitution of Zn for Cu, because the antiferromagnetic correlation is disturbed. On the other hand the polaron states are reduced by the structural change from LTO to LTT together with the reduction of the lowest energy $B_{3u}$ phonon peak in LBCO with $x \approx 1/8$. The independent control of the resonant states and the polaron states confirms the existence of two different electronic states near $E_F$. The resonant peak has a gap structure the energy of which increases with increasing carrier density, but it is not the superconducting gap, because it survives even at room temperature. The superconducting coherent peak is created in the polaron states exactly below $T_c$. The energy is almost constant in the underdoped phase indicating that the pairing symmetry is s or d(xy) in the underdoped phase.

Keywords: LBCO with $x \approx 1/8$, Zn-doped LSCO, resonant states, polaron

# Properties of Phase Separated, Super-Oxygenated $La_{2-x}Sr_xCuO_{4+y}$

B. O. Wells[1*], S. B. Emery[1], H. E. Mohottala[1], J.I. Budnick[1], W.A.Hines[1] ,
Ch. Niedermayer [2], L. Udby[3], K. Lefmann[3], N.H. Andersen[3], J. W. Lynn[4], F.C.Chou[5]

[1] *University of Connecticut, Storrs CT 06269, USA*
[2] *Paul Scherrer Institute, CH-5232 Villigen, Switzerland*
[3] *Risoe National Laboratory, DK-4000 Roskilde, Denmark*
[4] *National Institute of Standards, Gaithersburg, MD 20899, USA*
[5] *National Taiwan University, Taipei 106, Taiwan*

* wells@phys.uconn.edu

Previously, we have reported an electronically driven phase separation in superoxygenated $La_{2-x}Sr_xCuO_{4+y}$, with various Sr contents, forming separate magnetic and superconducting regions.[†] The phase diagram for the oxygen doped material consists of four line phases, alternating magnetic and superconducting phases. These phases are: the undoped antiferromagnetic insulator, a Tc=30K superconductor, the magnetically ordered 1/8$^{th}$ doped striped phase with Tm=40K, and an optimally doped Tc=40K superconductor. Investigating these fully phase separated materials gives us an avenue toward understanding the widely-reported inhomogeneities in high temperature superconductors. Magnetic hysteresis measurements reveal that there is substantially less flux pinning in the phase separated, O doped samples compared to the more extensively studied Sr doped samples with similar average hole densities. We attribute this to a length scale effect for the inhomogeneity present – typically of nm range in Sr doped $La_2CuO_4$ but too large to form pinning sites in fully phase separated, super-oxygenated $La_2CuO_{4+y}$. A further set of experiments concerns magnetic neutron diffraction studies that show an increase in incommensurate magnetic peak intensity with applied magnetic field. This effect has been detected in several 214-type superconductors and is usually discussed in terms of a model of competing, and coexisting, magnetic and superconducting phases. Phase separated, super-oxygenated $La_2CuO_{4+y}$ also shows such enhancement, though the magnitude of the effect seems to be a strong function of which phases are present. We discuss how this affects the expected magnetic-superconducting phase diagram.

This work is supported by the US-DOE through contract DE-FG02-00ER45801.

Keywords: high temperature superconductivity, phase separation, phase diagrams

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# Quantum Criticality in a Model Spin Ladder

Ch. Rüegg[1], B. Thielemann[2], K. Kiefer[3], K.W. Krämer[4], H.M. Ronnow[5], J. Mesot[2], D. F. McMorrow[1]

[1]*London Centre for Nanotechnology, University College London, United Kingdom*
[2]*Laboratory for Neutron Scattering, Paul Scherrer Institute, Switzerland*
[3]*BENSC, Hahn--Meitner Institute, Berlin, Germany*
[4]*Department of Chemistry and Biochemistry, University of Bern, Switzerland*
[5]*Laboratory for Quantum Magnetism, EPFL, Switzerland*

d.mcmorrow@ucl.ac.uk

One prevalent view of cuprate superconductors is that stripe formation effectively partitions the copper oxide planes into a system of weakly coupled spin ladders. Thus as well as being of interest in its own right, the physics of spin ladders is also germane to our understanding of the role of magnetic fluctuations in high-$T_c$ superconductors. Here we report on an extensive set of thermodynamic and neutron scattering experiments on $(Hpip)_2CuBr_4$ ($Hpip=C_5H_{12}N$), which establish this material as the best realisation to date of a spin ladder in the strong coupling limit. The study of this material is further facilitated by the low value of the exchange coupling – of order 1 meV – which allows us to investigate for the first time the full field-temperature phase diagram, including the existence of two field-induced quantum critical points.

# NMR study of a FFLO state of $CeCoIn_5$ in a perpendicular and a parallel field

K. Kumagai*[1], T. Oyaizu[1], N. Kondoh[1], Y. Furukawa[1], H. Shishido[2], Y. Matsuda[2]

[1*] *Division of Physics, Faculty of Science, Hokkaido University, Sapporo 060-0810, Japan*
[2*] *Department of Physics, Kyoto University, Kyoto 606-8502, Japan*

*kumagai@phys.sci.hokudai.ac.jp

We have studied NMR of a heavy-fermion superconductor $CeCoIn_5$ which is believed to host a Fulde-Ferrell-Larkin-Ovchinnkov (FFLO) state. We direct our attention to newly-discovered SC state of $CeCoIn_5$ in a perpendicular field (H_ab-plane) as well as in a parallel field (H//ab), and present clear evidences for the FFLO state in both cases as well. NMR spectra at the Co, In(1), and In(2) sites have been measured in a wide frequency range for H_ab. Upon entering the new SC state at high field and low temperature region, NMR spectra change dramatically below $T(H_c)$ in the case of H_ab as well as H//ab. A well-separated double peak structure persists down to the lowest temperature (70~mK), which indicates the appearance of a nordal plane structure of superconducting order parameter. We find the critical field $H_{FFLO}$ separating the FFLO and the BCS state lies in a very narrow range between 4.65 T and 4.70 T below $T_c(H)$. We discuss also strong Pauli paramagnetic effects on the temperature and field dependences of the Knight shift in the vicinity of the first order transition at $H_{C2}$.

Keywords: NMR, FFLO state, $CeCoIn_5$

# 30 July Wednesday 11:00-12:40

## Session 12

- **H. Mook**
- **Y. Uemura**
- **S. Tajima**
- **A. Lanzara**
- **G. LeLay**

# Observation of Magnetic Order in a $YBa_2Cu_3O_{6.6}$ Superconductor

H. A. Mook,[1] Y. Sidis,[2] B. Fauqué,[2] V. Balédent,[2] and P. Bourges[2]

[1] *Neutron Scattering Science Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6393 U.S.A.*
[2] *Laboratoire Léon Brillouin, CEA-CRNS, CEA-Saclay, 91191 Gif sur Yvette, France*

mookhajr@ornl.gov

The pairing mechanism that permits superconductivity in the copper oxides remains unknown, largely because there is little understanding of the state of matter (pseudogap) from which the superconductivity emerges. The transition to the pseudogap is observed by a number of techniques, but no heat capacity signature is found. However, recent evidence suggests that the transition breaks time-reversal symmetry signifying a transition to a new state. Here we report neutron scattering measurements on a highly perfect crystal of $YBa_2Cu_3O_{6.6}$ that shows broken symmetry that arises from a magnetic state with an onset at 235K, the temperature expected for the pseudogap transition. The moment is found to be about 0.1 $\mu_B$ and have a correlation length of at least 75 Å. We found the critical exponent for the magnetic transition to be (0.37+/-0.12). This may provide an explanation for the lack of a specific heat divergence at the pseudogap as some transitions of this type do not show such a divergence.

# Puzzles in Superfluid Density of the Cuprates: Nodal Gap ? K-T ? Collective Mode ?

Yasutomo J. Uemura

*Physics Department, Columbia University, New York, NY 10027, USA*

tomo@kirby.phys.columbia.edu

Superfluid density is a very important parameter of superconductivity. The absolute values of the superfluid density and its relationship to Tc can be used for discussing energy scales and condensation mechanisms [1,2]. Temperature dependence of the superfluid density is related to the thermal process of depleting superconducting order parameter. Recently, some detailed experimental studies of superfluid density have been reported in very thin 2-d films [3,4] and high-quality 3-d single crystals [5] of very underdoped YBCO and similar 123 systems via induction, field effect, and microwave methods. The former exhibits behavior typical to Kosterlitz-Thouless (K-T) transition: i.e., jump of the superfluid density at Tc with the absolute values below Tc following general K-T relationship. Almost no temperature dependence of superfluid density was observed for films with Tc lower than 20 K, reminiscent of the case of superfluidity in thin film He. In contrast, the 3-d single crystals exhibit marked temperature dependence of superfluid density with the absolute values at T = 0 much larger than that for a film systems having comparable Tc, and sub-linear dependence of Tc on superfluid density at T = 0.

The markedly different temperature dependence of the superfluid density indicates that the process of depleting order parameter is different between the 2-d and 3-d specimens of the cuprates. We would like to discuss the origin of these behviours, and compare three fundamentally different processes of depleting order parameter: (a) pair-breaking excitations of nodal quasi particles; (b) Kosterlitz-Thouless process in low-dimensional systems; and (c) roton-like collective mode excitations related to dynamical soft mode towards competing spin-charge stripe state [2]. It should be noted that (b) and (c) are both pair non-breaking processes which cause phase fluctuations to condensed bosons. We wish to answer questions such as, how the absence of temperature dependence of superfluid density in thin films can be compatible with nodal pair breaking? Why 2-d and 3-d look so different ? ….

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[5] D.M. Broun et al., Phys. Rev. Lett. 99 (2007) 237003

# Effects of pseudo-gap disappearance on electronic state in high-$T_c$ cuprates

Setsuko Tajima

*Department of Physics, Osaka University*
*Machikane-yama 1-1, Toyonaka, Osaka 560-0043, Japan*

tajima@phys.sci.osaka-u.ac.jp

We present the systematic studies for pair-breaking peaks in Raman scattering spectra, anisotropic resistivity, anisotropy ratio of upper critical field and Zn-substitution effect on resistivity, focusing on the electronic change in the overdoped regime. All these physical quantities show qualitative changes at a certain doping level where the pseudo-gap seems to collapse.

The changes of pair-breaking peaks in Raman scattering spectra do not take place monotonically but there exist a critical doping at which the changes occur rapidly. The critical doping level is $p \approx 0.19$ for $YBa_2Cu_3O_y$. This is close to the point where the pseudo-gap energy at T=0K becomes zero.

The trace of pseudo-gap in $\rho_a$ and $\rho_c$ diminishes at $p \approx 0.18$, but the incoherent charge transport along the c-axis seems to survive even at higher doping where no pseudo-gap opens. The anisotropy ratio $\gamma$ of upper critical field was determined from $\rho(T,H)$ and/or magnetization. As carriers are doped, $\gamma$ rapidly decreases and eventually reaches a very small value (~3, the band calculation value) at $p \approx 0.19$.

The Zn-substitution effect on $\rho_c$ is completely different from that on $\rho_a$ when the pseudo-gap opens. In the underdoped regime, Zn-substitution tends to suppress the pseudo-gap, while no clear Zn effect is observed in the optimally and slightly overdoped regime with $p<0.19$. The latter is the other evidence for an incoherent transport along the c-axis at these high doping levels.

*This is a collaborative work with T. Masui, T. Hiramachi, K. Nishikawa, K. Nagasao, Y. Uraike, and H. Eisaki.*

Keywords: high $T_c$ superconductors, overdoped state, pseudo-gap, charge transport

# The effect of strain on the quasiparticle dynamics of single layer Bi2201

Alessandra Lanzara

*University of California, Berkeley*
*Material Science Division, Lawrence Berkeley Laboratory, Berkeley- CA*

* email: alanzara@lbl.gov

Angle resolved photoemission spectroscopy measurements were performed in single layer $Bi_2Sr_{1.6}Ln_{0.4}CuO_{6+delta}$ by varying the radius of the Ln lanthanide atoms. A large range of increasing lattice strains leading to the extinction of the superconducting gap was studied. We discuss how strain modifies the nodal and antinodal quasiparticles dynamics and how this modifies the physics of Fermi arcs and two gaps picture.

# Metallic Silicon Nanowires

C. Léandri[1], P. De Padova[2], B. Aufray[1] and G. Le Lay*[1]

*[1]CINaM-CNRS, Campus de Luminy, Case 913, F-13288 Marseille cedex 09, France*
*[2]ISM-CNR, via del Fosso del Cavaliere, 00133 Roma, Italy*

lelay@crmcn.univ-mrs.fr

We will present a detailed investigation by STM/STS and High-Resolution Synchrotron Radiation Photoelectron Spectroscopy on a massively parallel array of straight Si nanowires (SiNWs), lying flat on a Ag(110) surface. These novel silicon nano-objects are metallic and atomically precise; they possess a magic width of just 1.6 nm and show quantized electronic states. Furthermore, they reveal a surprising symmetry breaking and a substrate mediated cross talk, which induces their chiral organization in magnetic-like domains. The spectroscopic signature of these SiNWs is unique: narrowest Si 2p core-level lines, allowing to identify for the first time a Coster-Kronig process. These SiNWs can self-organize by lateral compaction to form a one-dimensional grating at the molecular scale. The metallic nature of these SiNWs, along with their peculiar atomic structure, have lead us to a search for low dimensional superconductivity.

Keywords: silicon nanowires, electronic & structural properties

# 30 July Wednesday 15:30-17:00

## Session 13

- **P. Calvani**
- **E. Liarokapis**
- **Ch. Renner**
- **A. Keren**
- **D. B. Tanner**
- **N. E. Phillips**

# Charge-Order Excitations in the sub-Terahertz Conductivity of Oxides

R. Sopracase[1], A. Nucara[1], G. Gruener[2], P. Maselli[1], M. Ortolani[3], J. Garcia[4], U. Schade3, P. Calvani[1]*

*[1]CNR-INFM Coherentia & Dipartimento di Fisica, Università La Sapienza, Roma, Italy. [2]LEMA, Université F. Rabelais, Tours, France. [3]BESSY, Berlin, Germany. [4]CSIC & Universidad de Zaragoza, Zaragoza, Spain.*

*paolo.calvani@roma1.infn.it

The reflectivity of different manganites showing commensurate charge order (CO) below a characteristic temperature $T_{CO}$ has been measured at different temperatures down to 5 $cm^{-1}$ (0.15 THz). These very low frequencies were attained by using the Coherent Synchrotron Radiation extracted from the storage ring BESSY when working in the so-called $\alpha$-mode.

Below $T_{CO}$, both in polycrystalline $La_{n/8}Ca_{1-n/8}MnO_3$ (n = 6,7) and in a single crystal of $Nd_{1/2}Sr_{1/2}MnO_3$, one observes the opening of a mid-infrared gap and characteristic resonances at frequencies well below 1 THz. In the case of n = 6, the resonance causes a jump as large as 20% in the reflectivity around 0.3 THz.

Those resonances are discussed in terms of the existing models for the collective excitations of charge density waves (CDW). The present observations confirm that sub-Terahertz spectroscopy is a unique tool to investigate such excitations in charge clusters or stripes, which are otherwise hardly detectable, as it was already pointed out in previous works on the cuprates [1, 2].

Keywords: Terahertz, charge order, manganites

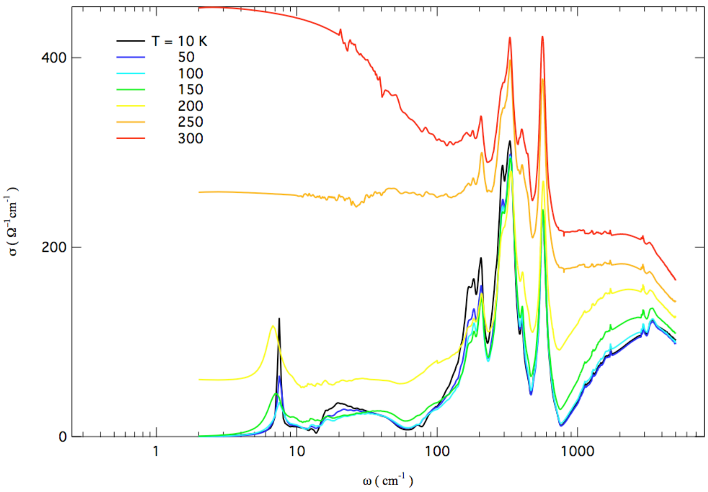



Fig. 1. Optical conductivity of $La_{3/4}Ca_{1/4}MnO_3$ showing, in the low-temperature CO phase, both the opening of a gap and the insurgence of a resonance below 10 $cm^{-1}$ (0.3 THz). The peaks between 100 and 700 $cm^{-1}$ are phonon lines.

[1] A. Lucarelli et al., Phys. Rev. Lett. **90**, 037002 (2003).
[2] M. Ortolani et al., Phys. Rev. B **73**, 184508 (2006).

# Tuning the phase separation in manganite thin films

A. Antonakos[1], D. Lampakis[1], G. H. Aydogdu[2], H.-U. Habermeier[2], M. Filippi[3], W. Prellier[3], and E. Liarokapis[1]

[1]*Department of Physics, National Technical University of Athens, GR-15780 Athens, Greece*
[2]*Max-Planck-Institute for Solid State Research, D-70569, Stuttgart, Germany*
[3]*Laboratoire CRISMAT, CNRS UMR 6508, ENSICAEN, 6 Bd. Marechal Juin, F-14050 Caen Cedex, France*

eliaro@central.ntua.gr

We have studied several methods for tuning the phase separation in manganite thin films. By varying the external (pressure, temperature, magnetic field) and internal (epitaxial strains, film thickness, and doping) conditions in the $R_{1-x}Ca_xMnO_3$ (R=La, Pr) compounds grown on different substrates, we have investigated the effects on the Raman and IR spectra. We have found that the charge ordered (CO) phase in $Pr_{1-x}Ca_xMnO_3$ (PCMO) occurs in the region 0.75>x>0.3 in the temperature range 220-260 K ($T_{CO}$) that depends on the amount of Ca doping and it is optimized for x=0.5. Within this CO phase, there is a magnetic transition to an antiferromagnetic insulating (AFI) phase at temperature $T_N<T_{CO}$. At the phase boundary (x=0.5) on $La_{1-x}Ca_xMnO_3$ (LCMO), the bulk compound is a paramagnetic (PM) insulator and undergoes first a ferromagnetic (FM) transition and a simultaneous AFM and CO transition at lower temperatures. We have proved that a combination of film thickness, Ca doping, and substrate strain can be chosen to tune the electrical and transport properties of the films and manipulate the CO state. By our systematic Raman and IR studies under varying conditions, we investigate certain modes and extract direct information about the amount of the Jahn-Teller (JT) distortions, the CO state, and the strain or pressure induced phase separation in the manganite thin films.

# Scanning tunneling microscopy and spectroscopy of manganites Ordered electronic phases in manganites

Ch. Renner[1,2*], B. Bryant[2], G. Aeppli[2]

[1] *Department of Condensed Matter Physics and NCCR Materials with Novel Electronic Properties, University of Geneva, 24 Quai E.-Ansermet, 1211 Geneva 4, Switzerland.*
[2] *LCN, University College London, 17-19 Gordon Street, London WC1H 0AH, England.*

* christoph.renner@physics.unige.ch

Competing energy scales in correlated electron materials lead to real space ordering of electronic degrees of freedom (charge, spin and orbital state) and phase separation. We shall present a selection of STM results where such effects have been observed in perovskite and bilayer manganese oxides. Charge ordering (CO) in perovskite manganites is accompanied by substantial lattice distortions as observed in high resolution STM micrographs. These images further give clear evidence for site centered charge distribution and are not compatible with bond centered scenarios. Stripe phases observed on the same samples differ in two remarkable ways from the above CO regions: atomic resolution is systematically absent and the tunneling spectroscopy gap is about a factor 2 smaller.

Keywords: Scanning tunneling microscopy, Manganites, Charge ordering, Stripes

Ch.Renner, G.Aeppli, B.G.Kim et al., Nature **416**, 518 (2002)
Ch.Renner, G.Aeppli and H.M.Rønnow, Material Science and Engineering C **25**, 775 (2005)
H.M.Rønnow, Ch.Renner, G.Aeppli et al., Nature **440**, 1025 (2006)

# A magnetic analog of the isotope effect in cuprates

Rinat Ofer, Yuval Lubashevsky, Amit Kanigel, Amit Keren*

*Department of Physics, Technion-Israel Institute of Technology, Haifa 32000, Israel*

*keren@physics.technion.ac.il

Since the discovery of superconductivity in the cuprates, it has been speculated that their pairing mechanism is due to magnetic interactions. However, this was never demonstrated in the laboratory. Such a demonstration would require an experiment similar to the isotope effect in metallic superconductors, namely, a measurement of $T_c$ versus the in-plane super-exchange J, with no other structural changes.
We have done this experiment using the $(Ca_xLa_{1-x})(Ba_{1.75-x}La_{0.25+x})Cu_3O_y$ system with its 4 different families (x) having different $T_c^{max}$. For each family, we measured the Néel Temperature $T_N$, the anisotropies of the magnetic interactions, the spin glass temperature $T_g$ of underdoped samples, and the superconducting carrier density $n_s$ using _SR. We determine the level of disorder by NMR, and the level of doping with NQR. The pseudogap temperature T* is obtained from susceptibility measurements. Finally, we extracted lattice parameters by neutron diffraction.
We major finding is that $T_c$=cJ(x)$n_s$(y) where c~1, and that J varies between families due to changes in the oxygen buckling angle. We also show that T* scale with the maximum $T_N$ of each family. These results demonstrate experimentally that the pairing and the pseudogap in the cuprates stems from magnetic interactions.

Keywords: Néel, superconductivity, cuprates, muSR, NQR, NMR, pseudogap.

# Phase separation in manganite thin films

D.B. Tanner,* Naveen Margankunte, Tara Dhakal, and Amlan Biswas

*Dept. of Physics, University of Florida, Gainesville, FL 32611, USA*

*tanner@phys.ufl.edu

Optical studies of phase separated manganite thin films show clear evidence for phase-separation effects. These thin films were prepared by laser ablation. Infrared reflectance measurements were performed for a range of temperatures from 10 to 300 K. Particular attention was given to the narrow temperature range where the insulator-metal transition occurs. Measurements were also made in magnetic fields up to 18T. The optical constants (optical conductivity and dielectric constant) were extracted by fitting the measured reflectance to a Drude-Lorentz dielectric function, using exact thin-film optics and the measured properties of the substrate. Spectral weight analysis shows that the growth of low energy oscillator strength occurs well above the Curie temperature, indicating phase coexistence in the hysteresis regime seen in resistivity measurements. Application of magnetic field at low temperatures leads to melting of the insulating phase, and converts most of the film to ferromagnetic metal. When the field is removed much of these new metal regions remain. The strain introduced by the choice of substrate is believed to have an important influence on this behavior. An effective medium approach to the optical properties will be discussed.

*This research was supported jointly by NSF grant DMR-0305043 and DOE contract DE-AI02-03ER46070.*

# Superconductivity and Charge Density Wave Order in $Na_{0.35}CoO_2 \cdot 1.3H_2O$

R. A. Fisher[1], H. Fu[1], D.-H. Lee[1], N. Oeschler[1], N. E. Phillips*[1], R. J. Cava[2], M.-L. Foo[2]

[1]*LBNL and University of California, Berkeley*
[2]*Princeton University*

*nephill@berkeley.edu

Specific-heat measurements on $Na_{0.35}CoO_2 \cdot 1.3H_2O$ have shown the evolution and ultimate disappearance of superconductivity with increase in the concentration of pair breaking centers. Comparison with neutron diffraction results[a] suggests the identification of O vacancies as the pair breaking centers. For two superconducting samples, with $T_c \sim 4.5$ K, the specific heat is characteristic of two-band, two-gap superconductivity. The pair breaking takes place preferentially in the band in which the pairing interaction is weaker, the small-gap band. An increase in the pair breaking changes the relative contributions of the two bands to the superconducting condensate, an effect that is quantitatively characterized by the specific-heat data. Greater increase in the pair breaking weakens the superconducting pairing interaction to the point that it gives way to a competing order, and there is a different transition, characteristic of CDW order, near 7 K. The 7-K specific-heat anomaly is consistent with a CDW on 1/4 of the Fermi surface and an order parameter with a temperature dependence similar to that of the BCS transition. A theoretical study using a band-structure fit to ARPES data for $Na_{0.3}CoO_2$ supports the presence of CDW order. Under renormalization group flow an onsite plus nearest-neighbor Hubbard interaction leads to an effective low-energy electron-electron interaction containing scattering processes that favor a CDW with waves of period $3^{-}$a, where a is the lattice constant. A mean-field analysis confirms that this effective low-energy interaction can lead to real-space density modulations with period $3^{-}$a.

Keywords: Superconductivity; Non-magnetic pair breaking; CDW order

[a]P. W. Barnes, M. Avdeev, J. D. Jorgensen. D, G. Hinks, H. Claus, and S. Short, Phys. Rev. B **72**, 134515 (2005).

# 30 July Wednesday 17:30-19:30

## Session 14

- **B. Dora**
- **M. J. Lawler**
- **E. Kim**
- **J. J. Rodriguez Nuñez**
- **B. Fine**
- **A. S. Mishcenko**
- **T. Ord**

# Inelastic scattering from local vibrational modes

B. Dora*, M. Gulacsi

*Max Planck Institute for the Physics of Complex Systems, Dresden, Germany*

* dora@kapica.phy.bme.hu, dora @kps.mpg.de

We study a nonuniversal contribution to the dephasing rate of conduction electrons due to local vibrational modes. The inelastic scattering rate is strongly influenced by multiphonon excitations,
exhibiting oscillatory behaviour. For higher frequencies, it saturates to a finite, coupling dependent value. In the strong coupling limit, the phonon is almost completely softened, and the inelastic cross section reaches its maximal value. This can be a possible, magnetic field insensitive contribution to the dephasing time in mesoscopic systems, in addition to magnetic impurities.

# Theory of the nematic to smectic quantum phase transition in electronic systems

Kai Sun,[1] B. M. Fregoso,[1] M. J. Lawler,*[2,3] and E. Fradkin[1]

[1]*Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL, 61801 USA*
[2]*Department of Physics, Applied Physics and Astronomy, The State University of New York at Binghamton, Binghamton, NY 13902 USA*
[3]*Department of Physics, University of Toronto, Toronto, ON M5S 1A7 Canada*

* michael.lawler@utoronto.ca

In this talk I will present a theory of the quantum melting of electronic stripes. Such stripes arise in the phenomenology of cuprate superconductors near 1/8th doping and in the the higher Landau levels of quantum Hall systems. To describe the stripes, we consider a phenomenological model that couples bosonic translational (smectic) and orientational (nematic) order parameters to gapless fermions in the spirit of Hertz's original treatment of the metallic ferromagnetic quantum critical point. We find that the phase transtiion between these two phases can be continuous and critical or Goldstone modes generally drive the electrons into a non-Fermi liquid regime. The continuous nature of the phase transition is particularly surprising for it is quite unlike the MacMillian-De Gennes classical counter part where a fluctuation induced 1st order transition is generically predicted.

Keywords: nematic, stripe, quantum phase transition

# Dynamical Layer Decoupling in a Stripe-Ordered High-Tc Superconductor

E. Berg[1], E. Fradkin[2], E.-A. Kim [1], S. Kivelson[1], V. Oganesyan[3], J. Tranquada[4], and S. C. Zhang[1]

*[1]Department of physics, Stanford University, Stanford, USA._[2]Department of Physics, University of Illinois at Urbana-Champaign, Urbana, USA. [3]Department of Physics, Yale University, New Haven, USA.*
*[4]Brookhaven National Laboratory, Upton, USA*

* eunahkim@stanford.edu

In the stripe-ordered state of a strongly correlated two-dimensional electronic system, under a set of special circumstances, the superconducting condensate, like the magnetic order, can occur at a nonzero wave vector corresponding to a spatial period double that of the charge order. In this case, the Josephson coupling between near neighbor planes, especially in a crystal with the special structure of $La_{2-x}Ba_xCuO_4$, vanishes identically. We propose that this is the underlying cause of the dynamical decoupling of the layers recently observed in transport measurements at x=1/8.

Keywords: stripe, high Tc, dynamical decoupling

# s–wave Superconductivity and the Isotope Exponent vs the number of carriers in a triangular lattice: applied pressure.

J. J. Rodríguez-Núñez*[1] A. A. Schmidt[2] V. K. Giménez[3]

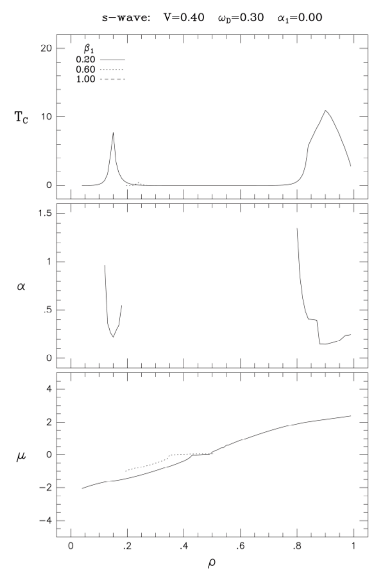
[1]*Laboratory SUPERCOMP, Physics Department, Faculty of Science, University of Carabobo, Campus de Bárbula, P. O. Box 129, Valencia 2001; Venezuela.*
[2]*Departamento de Matem´atica, UFSM, 97105-900 Santa Maria, RS, Brazil.*
[3]*Liquid Crystal Institute, Kent State University, Kent 44242, Ohio–USA.*

* email: jjrn01@cantv.net

We propose a band structure for a triangular lattice with nearest neighbor hopping, in terms of parameters $\alpha_1$ and $\beta_1$ which depend on applied pressure, as follows,

$$\in(\vec{k})/2t = -\cos(k_x) + \alpha_1 \cos(\frac{k_x}{2} + \frac{\sqrt{3k_y}}{2}) + \beta_1 \cos(\frac{k_x}{2} - \frac{\sqrt{3k_y}}{2}). \quad (1)$$

where $t$ is our scale of energy. For $\alpha_1 = \beta_1 = 1$, we recover the sodium cobalt oxyhidrate compound discovered by Takada, Sakurai et al, Nature 422, 453 (2003).
Such a lattice is a representation of the compound, $Na_xCoO_2 \bullet yH_2O$ (Sodium Cobalt Oxyhydrate), which is superconducting at a critical temperature of Tc ≈ 5 K. We have calculated Tc and μ *vs* n, where n is the number of carriers, for several values of the tight binding parameters which depend on pressure, distorting in this way the geometry of the original lattice. Doing this we have verified that all the $T_{c,max}$'s are related, one–to–one, to the logaritmic singularities which appear in the free density of states, N(ω) *vs* ω.
Additionally, this paper is devoted to the calculation of the isotope exponent, α *vs* n for several values of $\alpha_1$ and $\beta_1$. α is defined by means of the ionic isotopic mass, M, as $T_c \propto M^{\alpha}$ . We have found that the α *vs* n, for $T_c \neq 0$, changes non–monotonically. Experimental tests of the isotope exponent are called for to test the validity of our theoretical prediction.




We present in Fig. 1 results for several values of 1 and 1.

*FIG. 1: $T_c/t$ vs ρ = n/2 (upper figure), μ/t vs ρ (middle figure) and α vs ρ (lower part)*

# Phase separation in cuprates: a theoretical criterion and some possible scenarios.

Boris Fine

*Institute for Theoretical Physics, University of Heidelberg*

B.Fine@thphys.uni-heidelberg.de

I present a rigorous measure of the tendency towards phase separation inthe systems exhibiting phase transitions or crossovers controlled bycharge carrier concentration[1]. This measure is devised for thesituations when the quantitative knowledge of various contributions tofree energy is incomplete, and is applied to evaluate the chances of electronic phase separation associated with the onset ofantiferromagnetic correlations in high-temperature cuprate superconductors. This analysis indicatesthat cuprates are realistically close to the threshold of phaseseparationónanoscale-limited in-plane or even macroscopic with chargedensity varying between adjacent crystal planes. I then discuss thepossible dimensionality of the in-plane phase separation scenarios bycomparing the standard one-dimensional stripe interpretation of elastic scattering experiments in 1/8 doped lanthanum cuprates with two two-dimensional interpretations. One of them is known as grid[2,3] and the other one is the lattice of magnetic vortices[4]. Both can induce a 4x4 charge modulation similar to the one detected by scanning tunneling spectroscopy. The case of magnetic vortices, however, is favored against grid by a recent spin polarized neutron scattering experiment by Christensen et al.[5].

[1] B. V. Fine and T. Egami, Phys. Rev. B, v. 77, 014519 (2008).
[2] B. V. Fine, Phys. Rev. B, v.70, 224508 (2004).
[3] B. V. Fine, Phys. Rev. B, v.75, 014205 (2007).
[4] B. V. Fine, Phys. Rev. B, v.75, 060504 (2007).
[5] N. B. Christensen et al., Phys. Rev. Lett. v. 98, 197003 (2007).

# Interplay of magnetic correlations and electron-phonon coupling in the underdoped phase of cuprates: Diagrammatic Monte Carlo study.

Andrei S. Mishchenko*[1,2]

[1]*Cross-Correlated Materials Research Group, RIKEN, 2-1 Hirosawa, Wako, Saitama, 351-0198, Japan*
[2]*Russian Research Centre "Kurchatov Institute", 123182 Moscow, Russia*

*andry.mishenko@aist.go.jp

The angle resolved photoemission spectra (ARPES) and optical conductivity (OC) of the underdoped high temperature superconductors is studied in the framework of the low density limit of the t-J-Holstein model in which hole in the antiferromagnetic background is coupled to optical phonons. The ARPES and OC is calculated by Diagrammatic Monte Carlo technique using well justified non-crossing approximation for magnetic degrees of freedom while performing exact summation of the lattice dynamical variables.
It is shown that both magnetic excitations of the t-J model and strong coupling to phonons are important to explain the ARPES and OC in the underdoped compounds. Strong coupling to phonons leads to the transfer of the spectral weight of ARPES from the narrow quasiparticle peak to the broad Franck-Condon shake-off band which maximum, nevertheless, copies dispersion of a hole in the pure t-J model without coupling to phonons. The infrared OC of the underdoped compounds reveal, both in theory and experiment, the two band structure with low energy band arising due to phonon scattering and high energy peak emerging because of complex process of simultaneous emission of magnon and several phonons.
It is shown that analysis of ARPES and OC data for larger dopings suggests fast decrease of the electron-phonon coupling strength with doping having universal dependence of the coupling strength on the in-plain hole-doping concentration.

*Author acknowledges collaboration with N. Nagaosa, Z.-X. Shen, J. Zaanen, T.P. Devereaux, G. De Filippis, V. Cataudella, C. Bernhard, K.W. Kim, K.M. Shen, X.-J. Zhou.*

Keywords: ARPES, optical conductivity, underdoped cuprates

# Relaxation of superconducting fluctuations in a two-component scenario with intra- and interband pairings

T. Örd*, K. Rägo

*Institute of Physics, University of Tartu, 4 Tähe Street, 51010 Tartu, Estonia*

*teet.ord@ut.ee

We study the peculiarities of the relaxation of superconducting fluctuations in a two-component (two-band) model. The following interactions between carriers have been taken into account: interband pair-transfer coupling, intraband effective attractions of electron-phonon nature, and intraband Coulomb repulsions. These interactions are active in the different regions of momentum space. The free energy functional of a two-component superconductor have been derived on the basis of the microscopic model and the corresponding system of Ginzburg-Landau-Khalatnikov equations have been obtained. By separating the critical and non-critical variables, appearing as certain linear combinations of the superconducting band order parameters, the relaxation channels associated with these degrees of freedom have been established. As a result, one can distinguish two time scales in the damping of the fluctuations of superconducting order parameters in the class of two-band models with interband coupling. The behaviour of the relaxation times as functions of intra- and interband interactions has been analyzed in detail. The possible applications for magnesiumdiboride and copper-oxide systems are discussed.

Keywords: two-component superconductors, fluctuations, relaxation times, intra- and interband interactions

# 30 July Wednesday 21:30-23:00

## Special Session 2.
## on FeAs Superconductors

- **Y. Uemura**
- **A. V. Boris**
- **W. Malaeb**
- **T. Kroll**
- **T. Mizokawa**
- **J. Mustre de Leon**

# Introduction to Magnetism amd Superconductivity in FeAs Superconductors

Yasutomo J. Uemura

*Physics Department, Columbia University, New York, NY 10027, USA*

# Signatures of Electronic Correlations in Optical Properties of $LaO_{1\_x}F_xFeAs$

A.V. Boris,*[1,2] S.S.A.Seo,[1] N.N. Kovaleva, [1,2] J.S. Kim,[1] P.Popovich,[1] Y. Matiks,[1] R.H. Kremer, [1] and B. Keimer[1]

*[1]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart, Germany [2]Department of Physics, Loughborough University, Loughborough, United Kingdom*

* A.Boris@fkf.mpg.de

The relevance of electronic correlations to the unusual properties of a new family of Fe-based high-temperature superconductors in the normal and superconducting states is highly debated at the deficiency of experimental data. Recent theoretical and experimental advances have demonstrated that optical conductivity study is an exclusive probe to explore the strength of electronic correlations in transition metal oxides [1-5]. We report temperature dependences of the optical dielectric response of the F-doped superconducting $LaO_{0.9}F_{0.1}FeAs$ with $T_c$ = 26 K and the undoped LaOFeAs polycrystalline samples, measured by ellipsometry over a wide range of temperatures (5 - 350 K) and photon energies extending from the far infrared into the deep ultraviolet (0.01 - 6.5 eV). The optical conductivity spectra are dominated by a sequence of interband optical transitions, Fe3d-Fe3d, As4p-Fe3d, O2p-Fe3d, and O2p-La5d, and, in overall, look very similar for both samples. Contrary to the theories which predict large Fe3d density of states at the Fermi level, the far-IR conductivity is at the limit of a "dirty" metal ( ~ 100-200 $\Omega^{-1}cm^{-1}$), and the estimated effective number of the free charge carriers is only ~ 0.03-0.05 electrons per Fe atom. This may imply that the band is strongly renormalized by electronic correlations while most of its spectral weight is transferred into a broad Hubbard band at higher energy ~ U, in agreement with the recent DMFT calculations [1,3]. In further support of this interpretation, our optical conductivity spectra show significant temperature-driven transfer of the spectral weight from low energies to the broad optical band above ~ 4 eV with increasing temperature in the superconducting $LaO_{0.9}F_{0.1}FeAs$. In contrast, the temperature-dependent redistribution of the spectral weight in the undoped LaOFeAs is restricted at low energies < 1.5 eV. The ellipsometric data show continuous opening of the pseudogap at hω δ 0.8 eV in both samples with decreasing temperature. In addition, the undoped LaOFeAs reveals gapping at lower energies δ 0.15 eV and shows anomalies in the far-IR conductivity at the magnetic transition temperature $T_{SDW}$ ~ 150 K.

[1] K. Haule and G. Kotliar, Preprint at arxiv:0804.3283 (2008); [2] A. Comanac et al., Nature Physics **4**, 287 (2008); [3] K. Haule and G. Kotliar, Phys. Rev. B **76**, 104509 (2007); [4] A.V. Boris et al., Science **304**, 708 (2004); N.N. Kovaleva et al., Phys. Rev. Lett. **93**, 147204 (2004).

Keywords: superconductivity, optical conductivity, electronic correlations, oxypnictides.

**Core- and valence-level spectra of La(O1-xFx)FeAs as revealed by x-ray photoemission spectroscopy**

W. Malaeb *[1], T. Yoshid [a]1,
T. Kataoka [1], A. Fujimori1, Y. Kamihara [2],
M. Hirano [2], and H. Hosono [2].

[1]*Department of Physics and Department of Complexity Science and Engineering, University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan*
[2]*ERATO-SORST and Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan.*

malaeb@wyvern.phys.s.u-tokyo

Superconductivity was recently discovered in the iron-based layered compound La(O1-xFx)FeAs with a transition temperature of ~ 26 K [1]. Having a tetragonal crystal structure with the LaO and FeAs layers stacked along the c-axis, this compound is considered to show highly two-dimensional (2D) physical properties similar to cuprates.
Although a lot of research has been focused on this compound since its discovery, a systematic understanding of its electronic structure has not yet been achieved. Photoemission spectroscopy is one of the most powerful tools to study the electronic structure of solids. In this work, we have used x-ray photoemission spectroscopy and report core-level and valence-band spectra of the parent compound LaOFeAs as well as the fluorine-doped compound La(O1-xFx)FeAs (x=0.06) which shows superconductivity below ~26 K. From these measurements, we could observe the core-level spectra and also a clear Fermi edge in the valence band spectra. When compared with other iron compounds like FeS and Fe7Se8 for example [2], Fe 2p core-level spectra indicate an itinerant behavior rather than strong electron correlation. Based on these results, we shall discuss the electronic structure of the iron-based superconductors as weakly correlated itinerant d-electron systems.

Keywords: LaOFeAs, superconductivity, XPS.

[1] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. 130 (2008) 3296.
[2] K. Shimada, T. Mizokawa, K. Mamiya, T. Saitoh, A. Fujimori, K. Ono, A. Kakizaki, T. Ishii, M. Shirai and T. Kamimura, PRB 57 (1998) 8845.

# On the electronic structure of electron and hole doped LaOFeAs

T. Kroll *[1], A.Koitzsch [1], D. Inosov [1],
S. Bonhommeau [2], T. Kachel [2], H.A. Duerr [2], J. Werner [1], G. Behr [1], A. Kondrat [1],
J.E. Hamann-Borrero [1], C. Hess [1], R. Klingeler [1], J. Fink [1,2], M. Knupfer [1],
and B. Buechner [1]

*[1] IFW Dresden, Helmholtz Strasse 20, 01069 Dresden, Germany*
*[2] Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H. (BESSY), Albert-Einstein-Straße 15, 12489 Berlin, Germany*

t.kroll@ifw-dresden.de

The newly found superconducting material LaOFeAs has raised large scientific efforts. In this contribution, we will present new details on the electronic structure of electron and hole doped LaOFeAs. Based on various spectroscopic methods such as XAS, PES, and optics, as well as LDA and multiplet calculations, we search for a coherent picture of the electronic structure for various doping levels. This data is supported by transport and magnetic measurements wich lead to a further insight into the underlying physics of this interesting new system.

Keywords: FeAs, Spectrosco, electronic structure

# Electronic Structure study of LaOFeAs: Orbital Degeneracy and Excitonic Instability

T. Mizokawa and T. Sudayama

*Department of Complexity Science and Engineering & Department of Physics, University of Tokyo, 5-1-5 Kashiwanoha, Chiba 277-8581, Japan*

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

We report an electronic-structure study of LaOFeAs using unrestricted Hartee-Fock and self-energy calculations on a multi-orbial d-p model for the FeAs layer. We have analyzed relationship between the yz/zx orbital degeneracy and the excitonic instability in the undoped FeAs layer. Also we would like to discuss effect of electron doping on the Fermi surface geometry.

Keywords: FeAS layer, orbital degeneracy, excionic insulator

# Density of states in quaternary iron arsenide rare earth oxides

J. Mustre de León

*Departamento de Física Aplicada, Cinvestav-Mérida, Mérida, 97300 México.*

mustre@cinvestav.mx

We have used a real-space full multiple scattering formalism in order to calculate partial density of states in AOFeAs compounds (A=rare earth). We study the influence of having a different rear earth atom. We used La, Sm, Nd and Pr-based compounds. We performed these calculations in clusters containing approximately 200 atoms. These calculations use a self-consistent calculation of electronic charge densities. However, they are done within a spherical muffin-tin approximation for the scattering potentials. We present correlations between the atomic size of the rear earth and characteristic features of the density of states in the neighborhood of the estimated Fermi energy.

# 31 July Thursday 8:30-10:30

## Session 15

- **Aeppli**
- **Zaanen**
- **Krueger**
- **Seibold**
- **Carlson**
- **Lichtenstein**

Gabriel Aeppli

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

gabriel.aeppli@ucl.ac.uk

## Fermionic quantum criticality and the fractal nodal surface

J.Zaanen and F.Krueger

*Instituut Lorentz for Theoretical Physics, Leiden University, Leiden, The Netherlands*

*jan@lorentz.leidenuniv.nl

The fermion sign problem, i.e. the inability of theoretical physics to deal systematically with problems of large numbers of interacting fermions, is the central problem of condensed matter physics. This problem is particularly manifest dealing with quantum critical states involving fermions, like the ones found in heavy fermion metals and the normal state of high Tc superconductors, since the standard description in terms of path integrals is wrecked by the signs. But an alternative description is Ceperley's constrained path integral where the sign problem turns into a problem of constraints that is related to the nodal structure of the wave function. Resting on this formalism we have discovered a genuinely scale invariant fermionic state: it turns out that Feynman's hydrodynamical backflow wavefunction for fermions is characterized by a fractal nodal structure and we show explicitly that this reproduces the hallmark of (heavy) fermionic criticality: the divergence of the mass of the Fermi-liquid quasiparticles in the approach to the critical point where the Fermi surface vanishes.

# Pacifying the Fermi-liquid: battling the devious fermion signs.

J. Zaanen [1], F. Krueger [*1], J.-H. She [1], D. Sadri [1], and S. I. Mukhin [2]

[1] *Instituut Lorentz for Theoretical Physics, Leiden University, Leiden, The Netherlands*
[2] *Moscow Institute for Steel and Alloys, Moscow, Russia*

[*] krueger@lorentz.leidenuniv.nl

Dealing with fermionic degrees of freedom the path-integral mapping of the quantum many body system to an equivalent statistical physics problem fails due to the infamous minus signs rendering the path integral non probabilistic. As a consequence, the only fermionic systems we fully understand are the ones that, in a scaling sense, turn into a free gas of fermionic quasiparticles. Obviously, this Fermi liquid wisdom does not apply if we are facing metallic states with a scale invariant quantum dynamics as observed in the high-Tc superconductors or the heavy fermion compounds. Some time ago, Ceperley discovered an alternative representation of the fermionic path integral in which the minus signs are self-consistently translated into a constraint structure (the nodal hypersurface) acting on an effective bosonic dynamics. Recently, we demonstrated that within this language the workings of Fermi-Dirac statistics and scale invariance can be reconciled (see contribution Zaanen). Here we investigate the workings of the Ceperley path integral in the case of the Fermi liquid which turns out to be a rather complicated affair. In particular, we establish an analogy to a Mott insulator in a harmonic trap living in momentum space. Going back to real space, we discuss the topological properties of the nodal cells, and suggest a new holographic conjecture relating Fermi liquids in higher dimensions to soft-core bosons in one dimension.

## Spin excitations in the spin glass phase of cuprates

G. Seibold [*1], J. Lorenzana [2]

[1] *Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany*

[2] *Center for StatisticalMechanics and Complexity, INFM, Dipartimento di Fisica,*
*Università di Roma La Sapienza, P. Aldo Moro 2, 00185 Roma, Italy*

*email: goetz@physik.tu-cottbus.de

Recent inelastic neutron scattering experiments on LSCO compounds indicate a continuous evolution of the spin response from the metallic (superconducting) into the insulating spin glass phase. In both regimes the spectra show the characteristic “hour-glass” dispersion consisting of low energy incommensurate spin fluctuations and a high energy AF-like response. Based on the time-dependent Gutzwiller approximation of the Hubbard model we investigate the possibility wether the diagonal incommensurate spin scattering in the spin glass phase of lanthanum cuprates may originate from the suceptibility of these materials towards stripe formation.

Calculation of the dynamic spin response for stripes in the diagonal phase yields good agreement with available experimental data. At higher energies the spectra bear a strong resemblance with the excitations of the undoped compound thus providing an understanding for the evolution of magnetic scattering from the antiferromagnet to the 'universal spin response' observed in cuprate materials.

Keywords: stripes, spin fluctuations, Hubbard model

# Stripe Switching Noise in Cuprate Superconductors

Erica W. Carlson

*Purdue University, Dept. of Physics, 525 Northwestern Ave., West Lafayette IN 47907-2036, USA*

* email@ ewcarlson@physics.purdue.edu

An electron nematic is a translationally invariant state which spontaneously breaks the discrete rotational symmetry of a host crystal. In a clean square lattice, the electron nematic has two preferred orientations, while dopant disorder favors one or the other orientations locally. In this way, the electron nematic in a host crystal maps to the random field Ising model (RFIM). This model captures the physics of thermal fluctuations in local stripe orientation in cuprate superconductors in the presence of quenched disorder. We discuss the consequences of this for noise and hysteresis in transport anisotropy, superfluid density, and scanning tunnelingmicroscopy.

# Dual Fermion Approach to HTSC

H. Hafermann*[1], S.Brener[1], A. N. Rubtsov[2], M. I. Katsnelson[3] and A. I. Lichtenstein[1]

[1]*Institute of Theoretical Physics, University of Hamburg, 20355, Hamburg, Germany*
[2]*Department of Physics, Moscow State University, 119992 Moscow, Russia*
[3]*Institute for Molecules and Materials, Radboud University of Nijmegen, 6525 ED Nijmegen, The Netherlands*

*hartmut.hafermann@physnet.uni-hamburg.de

The recently developed dual fermion approach is a fully renormalized diagrammatic expansion around the well-established dynamical mean field theory (DMFT). It allows to treat non-local correlations beyond the mean-field level. We apply this approach to the 2D Hubbard model. Already the lowest order non-local correction to the DMFT reproduces the antiferromagnetic pseudogap. We formulate the Bethe-Salpeter equations for the full vertex in the particle-hole and particle-particle channels and introduce an approximation for practical calculations. At half filling, we calculate the spin-spin susceptibility and find a suppression of the Néel temperature as compared to DMFT due to the incorporation of the fluctuations. We further present results for the temperature- and doping dependence of the leading eigenvalue of the Bethe-Salpeter equation for the particle-particle channel. Perspectives of the application of a cluster generalization of the approach to HTSC are discussed.

Keywords: 2D Hubbard model, strongly correlated electrons, superconductivity

# 31 July Thursday 11:00-12:40

## Session 16

- **F. Marsiglio**
- **P. Banascky**
- **C. De Morais Smith**
- **D. Poilblanc**
- **M. Machida**

# What the optical sum rule tells us about superconductivity

F. Marsiglio

*Dept. of Physics, University of Alberta, Edmonton, AB*

frank.marsiglio@phys.ualberta.ca

The optical sum rule has been used to infer novel physics in the cuprate superconductors, both in the normal state and in the superconducting state. This talk will provide an overview of what is known, and of some of the pitfalls in the interpretation of the data. The main conclusion is that an anomaly at Tc points towards a new paradigm in superconductivity.

# Ground Electronic State of Superconductors: T-Dependent Antiadiabatic State at Broken Symmetry

Pavol Bañacky

*Faculty of Natural Science, Institute of Chemistry, Chemical Physics division, Comenius University, Mlynská dolina CH2, 84215 Bratislava, Slovakia and S-Tech a.s., Dubravská cesta 9, 84105 Bratislava, Slovakia*

banacky@fns.uniba.sk

For different types of superconductors, $MgB_2$, $YBa_2Cu_3O_7$, $YB_6$, and corresponding nonsuperconducting analogues, $AlB_2$, $YBa_2Cu_3O_6$, $CaB_6$, it has been shown that superconducting compounds at the equilibrium high-symmetry nuclear geometry, in contrast to the nonsuperconducting analogues, are characteristic by the band structure fluctuation at Fermi level due to electron coupling to respective phonon mode(s). This kind of band structure fluctuation is connected to dramatic decrease of Fermi energy (chemical potential). Consequently, the original adiabatic state ($\omega / E_F << 1$) that corresponds to equilibrium high-symmetry nuclear geometry has been changed to antiadiabatic state ($\omega / E_F \geq 1$) at distorted geometry related to nuclear vibration displacements in respective phonon mode(s). At these circumstances, the Born-Oppenheimer approximation (BOA) is not valid. It means not only breakdown of the Migdal theorem, but also impossibility to calculate nonadiabatic corrections by means of perturbation theory (vertex corrections) to the unperturbed adiabatic ground state. This effect should be the crucial reason of the problems of current microscopic theories of superconductivity. These are based on the assumption of the validity of the adiabatic BOA that is correct, in case of superconductors, only for high symmetry adiabatic metal-like structures at temperatures above $T_c$.

Based on the nonadiabatic theory of electron-vibration interactions, which from the very beginning treats electrons and nuclei on the same footing, i.e. electronic state is treated to be dependent not only on the instantaneous nuclear positions Q but also on the instantaneous nuclear momenta P, it has been shown that system in antiadiabatic state can be stabilized by nonadiabatic electron-phonon interactions. Stabilization effect in antiadiabatic state is due to strong dependence of the electronic motion mainly on the instantaneous nuclear kinetic energy – nuclear momenta P, i.e. on the effect that is negligibly small on the adiabatic level within the BOA. In this way, it can be shown that the electronic ground state is not the adiabatic state at the equilibrium high-symmetry nuclear geometry, but more stable is antiadiabatic state at distorted nuclear geometry. On the lattice scale, antiadiabatic state is geometrically degenerate at broken translation symmetry with fluxional nuclear configurations in respective phonon mode(s) that drive transition from adiabatic into antiadiabatic state. It means that there are an infinite number of displaced nuclear positions in the involved phonon mode(s), while the ground state energy of system is the same. It enables formation of mobile bipolarons that can move over lattice without dissipation at the presence of external electric field.

Antiadiabatic results strongly indicate necessity of reconsideration of the current understanding of microscopic mechanism of superconducting state transition.

# Inhomogeneous and striped RVB superconductors

Manuela Capello[1] and Didier Poilblanc[1]*

1 Laboratoire de Physique Théorique, CNRS & Université Paul Sabatier, 31062 Toulouse, France

*didier.poilblanc@irsamc.ups-tlse.fr

Properties of non-uniform RVB superconductors are investigated using large-scale Variational Monte Carlo (VMC) simulations of the t-J model. Striped superconductors consist of arrays of domail walls (DW) with enhanced (reduced) charge density (d-wave pairing) [1,2]. Remarkably, such states exhibit coexisting modulated superconducting, charge and valence bond orders. We have investigated two scenarios in which the superconducting regions on each side of the DW could be in- [1] or out-of-phase [2]. It has been shown that a lattice orthorhombic distortion (occurring in the low-temperature tetragonal phase of several High-temperature superconductors) helps to stabilize striped phases. Impurities are also expected to lead to inhomogeneous ground states. We apply our VMC framework to investigate the modulations of the charge density, the bond strength and the superconducting order in the vicinity of bond or site impurities [3]. Results will be discussed in the context of recent experiments (including STM/STS experiments) on underdoped cuprate superconductors.

[1] Manuela Capello, Marcin Raczkowski, Didier Poilblanc, arXiv:0801.2722.
[2] Marcin Raczkowski, Manuela Capello, Didier Poilblanc, Raymond Fresard, Andrzej M. Oles, Phys. Rev. B 76, 140505(R) (2007).
[3] M. Capello and D. Poilblanc, in preparation (2008).

# Staggered-Vortex Superfluid of Ultracold Bosons in an Optical Lattice

Lih-King Lim[1], A. Hemmerich[2], and C. Morais Smith[1*]

[1]*Institute for Theoretical Physics, University of Utrecht, Utrecht, the Netherlands*
[2]*Institute fur Laser-Physik, Universitat Hamburg, Hamburg, Germany*

* c.demorais@phys.uu.nl

We show that the dynamics of cold bosonic atoms in a two-dimensional square optical lattice produced by a bichromatic light-shift potential is described by a Bose-Hubbard model with an additional effective staggered magnetic field. Besides the known uniform superfluid and Mott insulating phases, the zero-temperature phase diagram exhibits a novel kind of finite-momentum superfluid phase, characterized by a quantized staggered rotational flux. An extension for fermionic atoms leads to an anisotropic Dirac spectrum, which is relevant to graphene and high-Tc superconductors.

Keywords: BEC, cold atoms, staggered-flux-phase

# Stripe Formation in Fermionic Atoms on 2-D Optical Lattice: DMRG Studies for Repulsive Hubbard Ladders

M. Machida[1], M. Okumura[1], S.Yamada[1] and Y. Ohashi[2]

[1]*CCSE, Japan Atomic Energy Agency, 6-9-3 Higashi-Ueno, Taito-ku, Tokyo 110-0015, Japan and JST(CREST) Honcho, Kawguchi, Saitama 332-0012 Japan*
[2]*Institute of Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba 332-0012 Japan and JST(CREST) Honcho, Kawguchi, Saitama 332-0012 Japan*

machida.masahiko@jaea.go.jp

In order to predict strongly-correlated behaviors of atomic Fermi gas loaded on two-dimensional (2-D) optical lattice, we employ the parallel density matrix renormalization group method and examine 2-D repulsive (mainly square and triangular for comparison) Hubbard model. In the presentation, we firstly suggest that a box shape trap enables one to observe intrinsic properties of the Hubbard model in a fixed doping in contrast to the conventional harmonic trap bringing about wide spatial variations of atom density profiles. Next, we show atomic density profile on 4-leg repulsive Hubbard model with the open boundary condition realized under the box trap. The variation parameters in the simulation are the doping rate below the half-filling and the repulsive interaction U/t. As a result, we find that stripe formations are universal in a low hole-doping range and the stripe sensitively changes its structure with variations of U/t and the doping rate. A striking feature is that a stripe formed by a pair of holes turns to one by a bi-hole pair when entering a limited strong U/t range. Namely, the stripe like clustering composed of four holes occurs. This feature was theoretically predicted by Chang and Affleck (M.-S.Chang and I.Affleck, Phys.Rev.B76, 054521 (2007)*. Furthermore, a systematic calculation reveals that the Hubbard ladder shows a change from the stripe to the Friedel oscillation with increasing the doping rate.

Keywords: Stripe, Hubbard Model, Optical Lattice, Atomic Fermi Gas

# 31 July Thursday 15:30-17:00

## Session 17

- **Y. A. Soh**
- **M. von Zimmermann**
- **Y. Takada**
- **T. G. Perring**
- **Y. W. Park**
- **J. Mustre de Leon**

# Spin density wave quantization and magnetic domain wall scattering in an antiferromagnet

Yeong-Ah Soh*[1,2]

[1] *Department of Physics and Astronomy, Dartmouth College, Hanover, New Hampshire 03755, USA*
[2] *Department of Materials, Imperial College London, Exhibition Road, London, SW7 2AZ, United Kingdom*

* yeong-ah.soh@dartmouth.edu

The role of magnetic domains and domain walls in determining the electrical properties of ferromagnetic materials has been investigated in great detail for many years, because control over domains offers a means of manipulating electron spin to control charge transport in 'spintronic' devices. In contrast, much less attention has been paid to the effects of domains and domain walls on the electrical properties of antiferromagnets since antiferromagnetic domains show no net external magnetic moment, and so are difficult to manipulate or probe. In this talk, I will present electrical measurements on chromium—a simple metal and quintessential spin density wave antiferromagnet—that show behaviour directly related to spin density wave formation and the presence of antiferromagnetic domains [1]. Our results are potentially of practical importance, in that they reveal tunable electrical effects of film thickness and domain walls that are as large as the highest seen for ferromagnets.

Keywords: quantum size effect, quantum phase transition, spintronics

[1] Ravi K. Kummamuru and Yeong-Ah Soh, Nature 2008 in press.

# Charge stripes in nickelates and cuprates under extreme conditions

Martin v. Zimmermann*[1], M. Hücker[2], M. Debessai[3], J. Schilling[3], and G. Gu[2]

*[1]Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany.*
*[2]Materials Science Physics Department, Brookhaven National Laboratory, Upton, New York, USA.*
*[3]Department of Physics, Washington University, St. Louis, Missouri, USA*

* martin.v.zimmermann@desy.de

The relation between stripe order and materials physical properties, in particular to electronic transport and superconductivity is still under debate. By exposing the material to extreme conditions, i.e. electric field or pressure, the ground state properties are manipulated. The response of static charge stripe order to this different ground state is studied using the bulk probe of high energy x-ray diffraction. In the orthorhombic nickelate $Nd_{1.67}Sr_{0.33}NiO_4$, no evidence is found for a deformation or sliding of charge stripes under high electric field, contradicting indications from nonlinear conductivity measurements. In the cuprate $La_{0.875}Ba_{0.125}CuO_4$, pressure strongly affects the stability of the low temperature tetragonal (LTT) phase and the transition temperature into the superconducting phase. Thus pressure provides an ideal tool to study the interplay between LTT-distortion and stripe order. Implication for the pinning of stripes are discussed.

Keywords: charge stripe order, x-ray diffraction, pressure

# Mechanism of Superconductivity in Graphite Intercalation Compounds Including $C_6Ca$

Yasutami Takada*

*Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan.*

*takada@issp.u-tokyo.ac.jp

More than a quarter of century ago, I proposed a theory (YT, J. Phys. Soc. Jpn. **51**, 63 (1982)* to explain the superconductivity in the first stage graphite-alkali metal intercalation compounds $C_8M$ (M = K, Rb, or Cs). In the theory, the three-dimensional interlayer electrons are identified to superconduct with the aid of both the acoustic and the optic phonons in which the negatively charged carbon layers oscillate, respectively, in phase and out of phase with the positively charged alkali metal layers to give strong polar couplings with the electrons. In my talk, I will report the result obtained by applying the same theory to the recently discovered superconductors $C_6Ca$ and $C_6Yb$, in which the metal layers are charged twice as large as the case of $C_8M$, giving a much stronger electron-phonon interaction. I also suggest the maximum transition temperature to be expected in this kind of compounds.

Keywords: graphite-intercalation, phonon mechanism, superconductivity

# Antiferromagnetic Fluctuations and Polaron Correlations in the Layered Colossal Magnetoresistive manganites

T.G. Perring*[1], D.T. Adroja[1], G. Aeppli[2], P.Manuel[1], T. Kimura[3] , D.Prabhakaran[4] and Y. Tokura[5]

[1]*ISIS Facility, CCLRC Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK*
[2]*London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London, UK*
[3]*Osaka University, 1-3 Machikaneyama, Osaka 560-8531, Japan*
[4]*Department of Physics, Oxford University, Oxford, OX1 3PU, UK*
[5]*Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan*

*t.g.perring@rl.ac.uk

Two different short-range orderings were independently discovered a few years ago in the ferromagnetic colossal magnetoresistive bilayered manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$, x=0.4: one is short-range, short-lived antiferromagnetic fluctuations[1], which involve the magnetic degrees of freedom, the other is short-range correlations of polarons[2], which are related to the lattice degrees of freedom. Results will be presented of a comprehensive study of the temperature and magnetic field dependency of these short-range dynamic orderings for other layered manganites: both with different hole doping per Mn site, x=0.30 and x=0.35, and in $(La_{0.6}Nd_{0.4})_{2-2x}Sr_{1+2x}Mn_2O_7$, x=0.4, with same doping but in which the ferromagnetc ordering temperature has been reduced to 30K and the resistivity at the lowest tempratures in the ferromagnetic state is $10^2$-$10^3$ greater than the other cases. The antiferromagnetic fluctuations and polaron correlations seen earlier for x=0.40 are also observed to coexist with the ferromagnetic critical scattering in the paramagnetic phase and diappear in the metallic-like phase, whether that be by the application of temperature, magnetic field, and in the case of $(La_{0.6}Nd_{0.4})_{2-2x}Sr_{1+2x}Mn_2O_7$, by switching between phases at 10K on increasing magnetic field at 3.5T. The intensity tracks that of the resistivity both as a function of magnetic field and temperature, and the results indicate that both the antiferromagnetic fluctuations and polaron correlations are closely related phenomena in the layered CMR manganites.

Keywords: Manganites, magnetoresistance, spin dynamics, polarons

[1] T.G. Perring et al., Phys. Rev. Lett. **78** (1997) 3197.
[2] L. Vasiliu-Doloc et al., Phys. Rev. Lett. **83** (1999) 4393.

# Interacting two fluids model in high $T_c$ superconductors: Thermoelectric power

Jun-Sung Kim and Yung Woo Park*

*Department of Physics and Astronomy & Nano Systems Institute - National Core Research Center, Seoul National University, Seoul 151-747, Korea*

* ywpark@phya.snu.ac.kr

The thermoelectric power (TEP) measurement results for both hole-doped and electron-doped cuprate superconductors are reviewed. The anomalous temperature dependent TEP results in the normal states are analyzed with the configuration entropy for the interacting two fluids of bound pairs and independent carriers, which are akin to the resonance superfulidity or shape resonance in atomic scattering resonance theory. The effect of lattice in the interacting two fluids is discussed to understand the high $T_c$ superconductivity.

Keywords: high $T_c$ superconductors, thermoelectric power, interacting two fluids model, shape resonance

# Polaronic behavior and Metal-Insulator Transition in Rare-Earth Nickel Oxide Perovskites

J. Mustre de León[1*], M. Acosta-Alejandro,[2] M. Medarde[3]

*[1]Department Departamento de Física Aplicada, Cinvestav-Mérida, Mérida, 97300 México. _Universidad Juárez Autónoma de Tabasco, Cunduacán, Tabasco, 86690, México. Laboratory for Developments and Methods, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland.*

* mustre@cinvestav.mx

X-ray absorption near edge structure (XANES) measurements at the Ni-K edge of $PrNiO_3$ across the metal insulator transition show that a change in the local lattice structure accompanies such transition. Theoretical calculations of the XANES show that the observed features of the spectra are consistent with the orthorhombic structure, reported by neutron diffraction, in the metallic phase. However, for the insulating phase a change in the local symmetry, consistent with a monoclinic structure, is required to reproduce the spectra. This local symmetry change, yields to two nickel sites with different local environment, and implies a strong electron-lattice interaction at the local level. The structure implies the presence of a Ni-site with long Ni-O bonds, consistent with a Jahn-Teller distortion. [1] These results indicate that even in the large size rare earth ion compounds of the family $RNiO_3$ a change in the symmetry centered at Ni occurs across the metal insulator transition, at least at the local scale. This change of symmetry implies the presence of an inhomogeneous local atomic structure in the insulating phase, similar to that present in other transition metal oxides, like high-temperature cuprate superconductors. We discuss the relevance of these results to models implying the presence of polaron in these oxides.

Keywords: polaron, lattice distortion, anomalous isotopic shift

[1] M. Acosta Alejandro, J. Mustre de León, M. Medadrde, Ph. Lacorre, K. Konder, P.A. Montano, Phys. Rev. B 77, 085107 (2008).

# 31 July Thursday 17:30-19:30

## Session 18

- **N. Kirova**
- **R. Hackl**
- **K. Maki**

# Long range and local instabilities in sliding or strained charge density waves.

N. Kirova *

*Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS, UMR 8502, F-91405 Orsay Cedex, France.*

*kirova@lps.u-psud.fr

Charge density wave (CDW) is a crystal of singlet electronic pairs, which is typically formed in low dimensional conductors. The CDW can be strained by applied voltage or by charge transfer at junctions, or by an electric field which can also put the CDW into sliding. Strains can give rise to local or long range modulational instabilities. Their recent identification (D.LeBolloch et al) was provided by a new method of coherent micro diffraction, which is accessible at the modern synchrotron irradiation sources. In the Blue Bronze $K_{0.3}MoO_3$ the individual dislocations where identified. Most recently it was found that under the electric field the system develops a very long wave, 1_m scale, and surprisingly coherent periodic unharmonic superstructure. We compare theories of plausible scenarios of the observed phenomena, related to formation of solitonic lattices or dislocation arrays. We address also direct observations of individual solitons, provided recently (C.Brun and Z.Wang) by the STM in another CDW compound – $NbSe_3$.

Keywords: charge density wave, soliton lattice, dislocations

# Evolution of electronic interactions in $La_{2-x}Sr_xCuO_4$

L. Tassini[1], B. Muschler[1], W. Prestel[1], R. Hackl*[1], M. Lambacher[1], A. Erb[1],

Seiki Komiya[2], Yoichi Ando[3], M. Fujita[4]

[1]*Walther Meissner Institut*
*Bayerische Akademie der Wissenschaften, 85748 Garching, Germany*
[2]*Central Research Institute of Electric Power Industry, 2-11-1 Iwato-kita, Komae, Tokyo 201-8511 Japan*
[3]*Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan*
[4]*Institute for Chemical Research, Kyoto University, Gokasho, Uji 610-0011, Japan*

*hackl@wmi.badw.de

We present Raman scattering results on $La_{2-x}Sr_xCuO_4$ in the doping range $0 \leq x \leq 0.3$. The electronic contribution to the spectra depends on the light polarizations, on temperature, and on doping. For strongly overdoped non-superconducting samples (x = 0.26 and 0.30) the spectra are well reproduced in terms of a conventional Fermi liquid with completely isotropic electron dynamics. The first strong renormalization of the spectra is observed at the anti-nodal points ($B_{1g}$ symmetry) at the onset of superconductivity between x = 0.26 and 0.25 ($T_c$ = 10 K). In the entire superconducting range (0.05 < x < 0.26) the nodal spectra ($B_{2g}$ symmetry) show little variation with doping while the anti-nodal ones undergo three additional transitions at approximately x = 0.20, 0.15, and 0.13 where a strong anisotropy sets in, a response from charge-ordering fluctuations appears and the pair-breaking peaks fade away, respectively. Below x = 0.05 we find clear evidence also in the Raman spectra that the stripe pattern rotates by 45° as observed first by neutron scattering. Since the respective doping levels approximately coincide it seems that the changes in the $B_{1g}$ spectra are linked to the onset of spin fluctuations, and charge ordering phenomena.

Keywords: Cuprates, spin- and charge ordering, electron dynamics, Raman scattering

# Majorana fermion,d-soliton and half quantum vortex(HQV) in triplet superconductors PrOs4Sb12 and CeSi3Pt.

H.Y.Kee[1],Y.Morita[2] and K.Maki[3]*

*[1]Dept. of Physics,University of Toronto,Ontario M5S,1A7,Canada*
*[2]Faculty of Engineering,Gunma University,Kiryu,Gunma 376-8515,Japan*
*[3]Dept. of Physics and Astronomy,University of Southern California,Los Angeles,Ca 90089-0484,USA*

kmaki@usc.edu

We have shown recently triplet superconduvtors UPt3 and Sr2RuO4 havor Majorana fermion associated with Abrikosov's vortex,d-soliton and half quantum vortex(HQV) in the low temperature and low field corner in the B-T phase diagram. Here we establish the similar things for filled skutteride PrOs4Sb12 and the crystal without inversion symmetry CeSi3Pt. In particular we find the stability region of HQVs in these superconductors,compute the Majorana wave function, local quasiparticle density of states and local magnetic field around a pair of bound HQVs. It appears that HQVs are most readily accessible through micromagnetometry and small angle neutron scattering at low temperaures(say T<300-100mK)

# 26-31 July 14:30-15:00

## Poster Session

| | |
|---|---|
| **1P** | **M. Enoki** |
| **2P** | **P. G. Freeman** |
| **3P** | **A. Hamann** |
| **4P** | **T. K. Kopec** |
| **5P** | **W. Malaeb** |
| **6P** | **J. Miranda Mena** |
| **7P** | **F. M. D. Pellegrino** |
| **8P** | **N. Poccia** |
| **9P** | **M. Ricco'** |
| **10P** | **A. Rojo Bravo** |
| **11P** | **S. Sanna** |
| **12P** | **A. Vittorini** |

1P

# Study of spin correlations in $La_{1.76-x}Sr_xCe_{0.06}CuO_4$ with less-corrugated $CuO_2$ planes

M. Enoki*[1], M. Fujita[2], K. Yamada[3]

[1]*Department of Physics, Tohoku University, Sendai, Miyagi 980-8578, Japan*
[2]*Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*
[3]*WPI-Advanced Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*

*enyokin@imr.tohoku.ac.jp

Comprehensive neutron-scattering study on the La214 system has revealed close relationships among the spin correlations, the superconductivity and the crystal structure. In the $La_{2-x}Sr_xCuO_4$ (LSCO) system, which has low-temperature-orthorhombic structure with Bmab symmetry in a wide doping range, the lattice distortion is known to affect the superconductivity and the stability of magnetic order. Therefore, to clarify the intrinsic connection between the high-$T_c$ superconductivity and magnetism, a study on the system without lattice distortion, namely corrugating of $CuO_2$ planes is important. Motivated above the reason, we performed low-energy ($\omega \leq 12$ meV) neutron-scattering on $La_{1.94\_x}Sr_xCe_{0.06}CuO_4$ (LSCCO) with x=0.14 ($T_c$=30 K), x=0.18 ($T_c$=35 K) and x=0.24 ($T_c$=25 K), in which the corrugation of $CuO_2$ planes is relaxed by doping Ce ion, compared with that in LSCO with comparable hole concentrations (p).
In the LSCCO with x=0.18 (p~0.14) and x=0.24 (p~0.20) samples, a clear gap-structure with the edge energy of ~7meV was observed in the ω–dependence of local dynamical susceptibility $\chi''(\omega)$, as is the same results for optimally doped LSCO (x=0.14–0.20). On the other hand, in the x=0.14 (p~0.10) sample, with increasing ω, $\chi''(\omega)$ above 0.5 meV decrease toward the minimum intensity at ~3 meV and turn to increase. This dip-structure in the $\chi''(\omega)$ is contrastive to the almost ω-independent $\chi''(\omega)$ in the underdoped LSCO (x=0.10). Therefore, the structural effect on the spin fluctuations is more prominent in the underdoped region. These results will be discussed in connection with the instability of low-energy spin fluctuations on the flat $CuO_2$ planes.
Keywords : Neutron-scattering, La-214 system, Spin fluctuation

2P

# The Dual Character Magnetism of Charge Stripe Ordered $La_{1.55}Sr_{0.45}NiO_4$.

P.G. Freeman[1], S. R. Giblin[2], A. T. Boothroyd[3], D. Prabhakaran[3], K Hadril[4].

e-mail: freeman@ill.fr

*1. Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France.*
*2. ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom.*
*3. Department of Physics, Oxford University, Oxford, OX1 3PU, United Kingdom.*
*4. Institut für Physikalische Chemie, Universität Göttingen, Tammanstrasse 6, 37077 Göttingen, Germany.*

We studied the magnetism of charge stripe ordered $La_{1.55}Sr_{0.45}NiO_4$ by the combined techniques of neutron diffraction, muSR and mass susceptibility. Magnetic ordering was observed at a lower temperature by muSR than neutron diffraction, indicating a glassy transition to the ordered phase. The magnetic order was observed by neutron diffraction to be of both anisotropic 3D and 2D (without any correlation on the c axis) character, muSR confirmed this to be consistent with a single magnetically ordered spin stripe phase as observed for other doping levels[1]. As with other doping levels of $La_{2-x}Sr_xNiO_4$ a spin reorientation[2] is observed in the x = 0.45, which is enhanced in temperature and magnitude in a similar fashion to the x = 0.5[3] in which 2D checkerboard charge ordering occurs. Our measurements on $La_{1.55}Sr_{0.45}NiO_4$ indicate the enhancement of spin reorientation is not as previously assumed, due to a coupling to checkerboard charge-ordering in the x = 0.5, but appears to be due the loss of c axis spin correlation. We comment on the probable cause of loss of spin correlation along the c axis.

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3P

# Renormalization of the longitudinal bond-stretching phonon branch in $La_{1.95}Sr_{0.05}CuO_4$ probed by inelastic neutron scattering technique

D. Reznik[1], D. Lamago[1], A. Hamann*[1], L. Pintschovius[1]

[1]*Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany*

* andreas-c.hamann@gmx.de

$La_{2-x}Sr_xCuO_4$ becomes superconducting (sc) in a doping range of $0.06 \leq x < 0.3$, where optimal doping of x = 0.15 results in $T_c$ up to 38 K. Neutron scattering experiments focusing on phonon dispersion relations revealed an anomalous renormalization of the longitudinal Cu-O bond-stretching branch in (100)-direction that is only present in the superconducting regime [1] – there also at temperatures above $T_c$. Thus, this effect might be correlated to superconductivity (SC) via enhanced electron-phonon coupling. On the other hand, non-superconducting samples at low doping show antiferromagnetic or stripe order that vanishes close to the onset of SC [2]. The impact of remaining dynamic (fluctuating) stripes on the lattice possibly competing with SC is still puzzling.
We report on our latest neutron scattering measurements on $La_{1.95}Sr_{0.05}CuO_4$ that fit into the picture of that compound: In comparison to the sc-samples the softening of the bond-stretching branch towards the zone boundary becomes less pronounced. Particularly, the anomalous broadening of the phonon lineshape previously reported around q = 0.3 weakens significantly.
In addition to the bond-stretching peak, we observe a second subtle maximum that could easily be misinterpreted either as an intrinsic effect due to exotic physics or as originating from some misoriented domain or even pure statistics and thus corrupt the extraction of the width. We fitted the data using shell model predictions including resolution effects to be convoluted with Lorentzians to extract the intrinsic width. By this means we clearly revealed the role of resolution-based contributions from low-symmetry directions that contaminated our scans, most prominently as the small high-energy peak mentioned above. For a reliable quantitative analysis, such effects turn out to be very crucial - especially since the width is extremely sensitive to the fitting procedure. We compare our data in detail with previous work.

Keywords: High $T_c$ superconductivity, stripes, phonon renormalization, bond stretching branch

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4P

# Emergence of Pairing Interaction in the Hubbard Model in the Strong Coupling Limit

V. A. Apinyan[1,2] and T. K. Kopec*[1]

[1]*Institute for Low Temperature and Structure Research, PO. Box 1410, 50-950 Wroclaw 2, Poland*
[2]*International Max Planck Research School, Nothnitzer Str. 38, 01187 Dresden, Germany*

*e_mail: kopec@int.pan.wroc.pl

The mechanism of superconductivity in cuprates requires the knowledge of bosons mediating the pairing as well as the nature of the paired states. Here, the underlying attraction force appears very puzzling since it is hard to reconcile the microscopic attractive interaction with the completely repulsive bare electron-electron forces. In this work we consider the Hubbard model in a spin-rotationally invariant setting. The original electron operators are presented in the charge-spin-fermion U(1)_SU(2) factorized form. Using the functional field integration formalism we construct the grand canonical partition function of the system. While maintaining the spin-rotational invariance, we rewrite the action of the system by transforming it into new bosonic and fermionic variables with the help of the U(1) and SU(2) gauge transformations and factorize the original electron operators in terms of the emergent gauge fields. We show that these fields play a similar role as phonons in the BCS theory: they provide the "glue" for fermion pairing in the Hubbard system. By tracing out gauge bosons the form of paired states is established and the role of the antiferromagnetic correlations is explicated.

key words: Hubbard model, gauge fields, pairing interactions

**5P**

# Temperature dependence of the chemical potential in $La_{2-x}Sr_xCuO_4$

W. Malaeb[*1], M. Hashimoto[1], M. Takizawa[1], K. Ebata[1], T. Yoshida[1], A. Fujimori[1], H. Eisaki[2], T. Kakeshita[3], T. Sasagawa[4], S. Uchida[1].

[1]*Department of Physics and Department of Complexity Science and Engineering, University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan*
[2]*AIST, Tsukuba, Ibaraki, 305-8568, Japan*
[3]*ISTEC, Koto-ku, Tokyo 135-0062, Japan*
[4]*Tokyo Institute of Technology, Yokohama, Kanagawa, 226-8503, Japan.*

* malaeb@wyvern.phys.s.u-tokyo.ac.jp

A theoretical study based on the t-J model [1] predicts a non-Fermi-liquid-like temperature dependence of the chemical potential and other thermodynamic quantities of strongly correlated electrons. In the high-$T_c$ cuprates $Bi_2Sr_2CaCu_2O_{8+\_}$ (Bi2212), the chemical potential shows strong temperature dependence in low doping region [2]. This is qualitatively consistent with the theoretical study [1], but a large quantitative discrepancy exists.
In the present work, we have performed x-ray photoemission (XPS) measurements on the high-$T_c$ system $La_{2-x}Sr_xCuO_4$ (LSCO) at temperatures ranging from 15K up to 250K. From these measurements, we deduced the temperature dependence of the chemical potential shift as shown in Fig. 1. It is clear that the chemical potential shifts upwards with temperature for the underdoped samples and downwards for the overdoped samples. We shall discuss the origin of these contrasting behaviors and their relationship with thermodynamics.

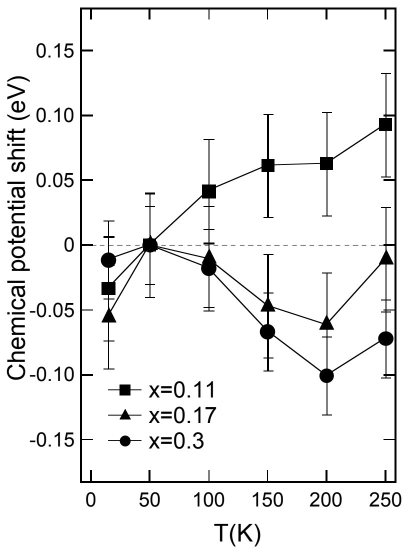


Fig. 1. Temperature dependence of the chemical potential shift in $La_{2-x}Sr_xCuO_4$.

Keywords: chemical potential, strongly correlated electrons, high-$T_c$ cuprates.

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6P

# Bipolaron Jahn-Teller pairing and charge transport in cuprates.

J. Miranda Mena[1], T. Mertelj [1,2], V.V. Kabanov[1] and D. Mihailovic[1,2]

[1] *Josef Stefan Institute, Jamova 39, SI 1001 Ljubljana, Slovenia*
[2] *Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI 1001, Ljubljana, Slovenia*

joaquin.miranda@ijs.si

Recently the mechanism for an intersite pairing was proposed for cuprates [1]. It was shown that two fold degenerated level is coupled to local lattice modes due to finite wavevector Jahn-Teller (JT) coupling. The mechanism was based on the following experimental facts: 1) an incommensurate extra phonon mode observed by inelastic neutron scattering (INS) [2], 2) local distortions measured by EXAFS [3], 3) the interpretation of a Jahn-Teller distortion in the three spin magnetic polaron, measured by electron paramagnetic resonance (EPS) [4]. After elimination of vibrational degrees of freedom the model was reduced to the classical lattice model of polarons interacting via the deformation field and direct Coulomb repulsion. Monte Carlo simulations in a wide range of doping and temperature revealed formations of single pairs, clusters and stripes of different sizes [5,6]. Formation of pairs and clusters is accompanied by a suppression of density of states (DOS) at the Fermi level [7]. In this report, we focus in the charge transport properties that can be deduced from the above model. We present patterns created for selected dopings and their single particle DOS and biparticle DOS at different temperatures. We argue that single particle and pair conductivity may differ. For a better analysis on this issue, we compute the contribution to the electrical conductivity arising from single particle using a variable range hopping model. The general trend is that conductivity has a crossover from 1/T temperature behavior at high temperature to a strong reduction of the conductivity at low temperatures. Finally, the gap magnitude in the calculated DOS and the average pair energy, are discussed in connection to the pseudogap region in cuprates.

7P

# Statistical correlations in an ideal gas of particles obeying fractional exclusion statistics

F.M.D. Pellegrino[1] G.G.N. Angilella[2], N.H. March[3, 4] and R. Pucci[2]

[1]*Scuola Superiore di Catania, Via S. Nullo, 5/i, I-95123 Catania, Italy.*
[2]*Dipartimento di Fisica e Astronomia, Università di Catania, and CNISM, UdR Catania, and INFN, Sez. Catania, Via S. Sofia, 64, I-95123 Catania, Italy.*
[3]*Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium*
[4]*Oxford University, Oxford, England*

After a brief discussion of the concepts of fractional exchange and fractional exclusion statistics, we report partly analytical and partly numerical results on thermodynamic properties of assemblies of particles obeying fractional exclusion statistics. The effect of dimensionality is one focal point, the ratio $\mu/k_B T$ of chemical potential to thermal energy being obtained numerically as a function of a scaled particle density. Pair correlation functions are also presented as a function of the statistical parameter, with 'Friedel' oscillations developing close to the fermion limit, for sufficiently large density.

Ref.: PHYSICAL REVIEW E 76, 061123 (2007)
URL: http://link.aps.org/abstract/PRE/v76/e061123

8P

# Multi-variables phase diagrams of cuprates.

Nicola Poccia, Alessandra Vittorini Orgeas, Michela Fratini, Antonio Bianconi

*Department of Physics, La Sapienza University of Rome, 00185 Roma, Italy*

nicola.poccia@roma1.inf.it

The mechanism allowing a macroscopic quantum coherent phase to survive to the attacks of temperature decoherence effects is attracting interest in many fields from quantum biophysics to quantum computing. There are growing experimental evidences that this mechanism may emerge in the proximity of a quantum critical point [1, 2]. We discuss the phase diagrams of the superconducting order, the structural order, the magnetic order and the charge order in cuprates as a function of doping $\delta$ and internal chemical pressure $\varepsilon$. The order that competes with the superconducting long range order is the polaron electronic crystalline phase called a Wigner polaron crystal [4] in the proximity of the microstrain quantum critical point [3]. The variation of the spin gap energy as a function of microstrain provides a strong experimental support for this proposal [5]. An electronic topological transition driven by the microstrain has been found at doping 0.25, suggesting the importance of a material dependent parameter to control the universal phase diagram of cuprates [6]. A possible interpretation is that energy of different kind of interaction are comparable [7].

key words: cuprates, Wigner Crystal, polaron, quantum critical point, phase diagram.

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9P

# Unconventional isotope effects in superconducting fullerides

M. Riccò[1*], F. Gianferrari[1], D. Pontiroli[1], M. Belli[1], C. Bucci[1], T. Shiroka[1,2]

[1] *CNISM and Dipartimento di Fisica, Università di Parma - Via G.P. Usberti 7/a, 43100 Parma, Italy*
[2] *Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut - CH-5232 Villigen PSI, Switzerland*

*e-mail Mauro.Ricco@fis.unipr.it

Although widely accepted, the phonon mediated, BCS-like theory of superconducting $A_3C_{60}$ fullerides (A = K, Rb, Cs) cannot reproduce correctly all their parameters, even in its strong-coupling, Migdal-Eliashberg limit.
The fundamental difficulty, ascribed to intrinsically close phonon and electron energy scales (respectively at 0.2 and 0.25 eV), has been overcome by dynamic mean field theories (DMFT), which, unlike ME, consider electron-phonon and electron-electron interactions on an equal footing.
The unconventional phenomena predicted in the new framework include, among others, isotope effects on spin susceptibility, totally absent from standard theories.
We have tested these predictions, finding a significant dependence on the isotopic mass in both $T_c$ and, more importantly, in the normal-state Pauli susceptibility $\chi_P$.
The comparative measurement of $\chi_P$ in two different $K_3C_{60}$ samples (85% $^{13}$C-enriched vs. natural abundance), both} by SQUID magnetometry as well as by $^{13}$C NMR Knight shift, definitely confirms the presence of an isotope effect on susceptibility, although a quantitative agreement with theory is still missing.

# 10P

## Self-trapping of particles from singular pockets in the weakly doped AFM Mott insulator.

A. Rojo*[1,2], S. Brazovskii*[2,3]

[1] *CNRS, LPS UMR 8502 , Univ. Paris-Sud, Orsay, France*
[2] *CNRS, LPTMS UMR 8626, Univ. Paris-Sud, Orsay, France*
[3] *L.D. Landau Institute, Moscow, Russia*

* alvaro.rojo@lptms .u-psud.fr

We consider effects of self-trapping of particles added or excited over the insulating state of an antiferromagnetic Mott insulator. The state of an electron or a hole (as appears in ARPES), or of their bound pair (as appears in optics) can be modified by interactions with collective degrees of freedom – deformations of the lattice or of the spin environment. The resulting self-localized state lowers the total particle energy, enhances its effective mass and splits off the electronic level below the nominal insulating gap. We show theoretically that the effect is particularly pronounced for states near the (π,0) type point of the Brillion zone of the $CuO_2$ because of a proximity to the van Hove singularity. The results are clearly important for the electron-doped cuprates where these points correspond to spectrum bottom for electrons. The effect is indirectly important for lightly hole-doped cuprates concerning the spectrum transfer between the nodal arcs and the dark anti-nodal regions.

• key words : AFM Mott state, doped cuprates, ARPES, optics, seltrapping, van Hove singularity

## 11P

# Effect of cation substitution in underdoped high $T_c$ cuprates

S.Sanna*[1], F. Coneri[1], A.Rigoldi[2], G.Concas[2] and R. De Renzi[1]

[1] *CNISM and Physics Department, University of Parma, Italy*
[2] *Physics Department and CNISM, University of Cagliari, Italy*

*Samuele.Sanna@fis.unipr.it

We present an extensive exploration of the phase diagram of $Y_{1-x}A_xBa_2Cu_3O_{6+y}$ ($A=Ca^{II}, Eu^{III}, Nd^{III}$) vs. oxygen at low fixed content of cation substitution (x=0.08). In this system, the cationic radii difference of the substituents induces local distortion on the nearest $CuO_2$ planes. The aim is to identify the specific role of doping, distortion-driven- and Coulomb-driven-disorder by comparing the isovalent and heterovalent substitution of yttrium at the antiferromagnetic-superconducting boundary ($0.2<y<0.4$). The local magnetic and superconducting properties have been studied by performing zero and transverse field μSR on polycristalline samples prepared by the topotactic technique [1].

We show that the disorder opens a window of pure cluster spin glass (CSG) state between the antiferromagnetic and the superconducting phases. In particular the pure CSG is absent in the phase diagram of the sole oxygen doped $YBa_2Cu_3O_{6+y}$ which approaches the clean limit [2,3]. This means that the pure CGS phase is not intrinsic to cuprates in contrast to what is commonly believed, but it is related to the cation substitution. We will discuss the specific behaviour of the isovalent and heterovalent substitution.

The results on $Y_{1-x}Ca_xBa_2Cu_3O_{6+y}$ provide also the evidence that the doping mechanism (cation substitution or oxygen loading) directly determines whether the corresponding injected mobile holes contribute to superconductivity or only to high temperature transport [4]. We argue that this hole tagging is a signature of the complexities of single hole doping in Mott insulators and it calls for a subtler description of the correlated bands than the usual one.

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# Local X-ray writing charge ordered domains and readingin $La_2CuO_{4+y}$

A. Vittorini-Orgeas[1], M. Fratini[1], G. Campi[2], A. Bianconi[1].

*1Dipartimento di Fisica, Università di Roma "La Sapienza", P. le Aldo Moro 2, 00185 Roma, Italy*
*1 Istituto di Cristallografia, CNR, Via Salaria Km 29,300, 00016, Monterotondo St., Roma, Italy*

High- resolution synchrotron x-ray diffraction is used to control and manipolate a short range superstructure in the $La_2CuO_{4+y}$ (y=0. 08) single crystal with a $T_c$=38K. We have observed the effects of the x-ray radiation dose on the diffraction pattern of a quasi bidimensional phase named Q3, associated to a liquid of polarons, as a function of photon flux at low temperature (100 K). These results suggest the possibility of manipulating the nanoscale ordering by x-ray illumination.

*Keywords*: Cuprates, superstructures, ordering, photo induced, x-ray diffraction.

## Presenting Authors