

Session 1:  
Inhomogeneous and Strongly Correlated Materials with Novel Electronic Properties  
(ISCM)

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# Oxide High-Temperature Superconductors: Multiscale Systems of Local Distortions Correlated in Elastic Media

**Alan Bishop**

A qualitative change is taking place in our understanding of many “strongly correlated” electronic materials, based on evidence that multiscale (spatial and temporal) complexity is both intrinsic and functional. This complexity is fundamental to the science of synthesis-structure-property relations, and its control opens the path to predictive design of new generations of technological materials. A large and significant class is provided by transition metal oxides (TMOs), including HTC cuprates and bismuthates, colossal magnetoresistance manganites, and perovskite ferroelectrics. Here, directional (d) bonding and strong (oxygen) polarizabilities and (oxygen-metal) charge-transfers, lead to “landscapes” of sensitive, inhomogeneous ground and metastable states (and associated glassy dynamics). We describe inhomogeneities in such TMOs both at atomic scales (charge/spin localization and perovskite unit cell distortions) and mesoscale structural textures (twinning, tweed, etc.). We suggest that these seemingly disparate scales can correlate into a “system” of functional scales, as a central consequence of strong elasticity in TMOs. For instance, in HTC cuprates, local pairing sites (Jahn-Teller (JT) bipolarons with strong c-axis- ab-plane coupling through perovskite buckling) are induced by hole doping, and are then the source (via a local “compatibility” bonding constraint) of long-range, anisotropic elastic fields. The coexistence of short- and long-range interactions results in intrinsic multiscale patterns (landscapes), including correlations of JT pairing centers into fibrillar and clump patterns — at sufficient doping levels and low temperature, these form correlated percolation channels.

In short, this is a multiscale “system” scenario for HTC oxides (and bismuthates), in which local pairing induces elastic strains which self-consistently induce coherent superconductivity — macroscopically but (at least below optimal doping) inhomogeneously.

# Synergetic coupling of spin, charge and lattice in high temperature superconductors

**T. Egami**

Presently the majority opinion on the mechanism of high-temperature superconductivity (HTSC) is that it is purely an electronic phenomenon involving spin, and could be explained by a  $t$ - $J$  Hamiltonian. However, various experimental results indicate strong phonon involvement. In the conventional theory the spin and phonon mechanisms conflict against each other, with spin preferring the  $d$ -wave and phonon the  $s$ -wave. We propose that a synergetic coupling of spin, charge and phonon could contribute to enhance the  $d$ -wave superconductivity. We discuss a close analogy in the charge-phonon coupling between the cuprates and the ferroelectric titanates and show that phonon-induced charge transfer explains the strong softening of the Cu-O bond-stretching mode, through inelastic neutron scattering and the exact diagonalization calculation on a Hubbard model. We propose a novel spin, charge and phonon coupling mechanism through the phonon-induced spin-polarized charge transfer. While the usual spin-phonon coupling through the modification of  $J$  by the atomic distance is small, this mechanism can be very strong for the Cu-O bond-stretching mode and could bring about a synergetic effect of the HTSC mechanism.

# Recent Neutron and X-Ray Scattering Studies of Complex Oxides

**M. Greven**

Quantum phase transitions in the presence of quenched disorder are at the forefront of research in the field of strongly correlated electron systems, yet there have been relatively few experimental model systems. Complementary magnetometry, neutron scattering, and numerical experiments demonstrate that the randomly diluted square-lattice Heisenberg antiferromagnet  $\text{La}_2\text{Cu}_{1-p}(\text{Zn,Mg})_p\text{O}_4$  is an excellent model material for site percolation in the quantum-spin limit  $S = 1/2$  [1]. Measurements of the ordered moment and spin correlations provide important quantitative information for tests of theories for this complex quantum-impurity problem. Quantum Monte Carlo for the bilayer Heisenberg antiferromagnet indicates that the properties of  $\text{La}_2\text{Cu}_{1-p}(\text{Zn,Mg})_p\text{O}_4$  near the percolation threshold are controlled by the effective proximity to a new quantum critical point [2]. It is furthermore demonstrated that as-grown, non-superconducting  $(\text{Nd,Ce})_2\text{CuO}_4$  at low and intermediate Ce doping is a good model material as well [3].

Historically, neutron scattering has been the tool of choice for measurements of phonons. We demonstrate the feasibility of using inelastic x-ray scattering to measure phonon dispersions in small, high-quality single crystals of complex oxides. Specifically, we report on measurements of the phonon dispersion of the electron-doped superconductor  $\text{Nd}_{1.86}\text{Ce}_{0.14}\text{CuO}_4$  along the  $(\pi, 0, 0)$  and  $(\pi, \pi, 0)$  high-symmetry directions [4]. Compared to the undoped parent compound, the two highest longitudinal optical phonon branches, associated with the Cu-O bond stretching and out-of-plane oxygen vibration, are shifted to lower energies. Moreover, an anomalous softening of the bond-stretching mode is observed near  $(0.2, 0, 0)$ . This anomaly resembles neutron scattering results for the hole-doped high-temperature superconductors and indicates the presence of a significant electron-phonon coupling.

[1] O.P. Vajk et al., *Science* 295, 1691 (2002); cond-mat/0211033.

[2] O.P. Vajk and M. Greven, *Phys. Rev. Lett.* 89, 177202 (2002).

[3] P.K. Mang, M. Greven, and O.P. Vajk (unpublished)

[4] M. d'Astudo et al., *Phys. Rev. Lett.* 88, 167002 (2002); cond-mat/0210700.

# Impurity effects on the stripes and superconductivity in $\text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}(\text{Zn,Ni})_y\text{O}_4$

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In order to clarify the relation between the stripe correlations and superconductivity, we have carried out the muon-spin-relaxation and magnetic-susceptibility measurements around  $x = 0.115$  in the Zn- or Ni-substituted  $\text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}(\text{Zn,Ni})_y\text{O}_4$ , changing  $y$  finely up to 0.10. The competition between the magnetic order and superconductivity has been exhibited clearly. That is, the volume fraction of the superconducting state estimated from the susceptibility measurements in one sample is in good correspondence to that of the fast fluctuating region of Cu spins estimated from the measurements. These results can be interpreted in terms of the development of the so-called Swiss cheese model. That is, both Zn and Ni tend to pin rather long-range dynamical spin correlation such as the dynamical stripe around themselves so that the superconductivity is destroyed around Zn and Ni. Moreover, it has been found that the area of the non-superconducting and slowly-fluctuating or statically stabilized region of Cu spins is larger around Zn than around Ni, suggesting that the pinning by the nonmagnetic impurity Zn is stronger than that by the magnetic impurity Ni. This may be the reason why the Zn substitution destroys the superconductivity in the high-Tc cuprates more markedly than the Ni substitution.

# Effect of lattice and impurities on transport properties of cuprates

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We calculate the influence of transverse fluctuations on the longitudinal dynamics in the striped phase of cuprates by using the bosonization technique. First, we analyze only the transverse modes, which are equivalent to a quantum spin-1 chain. The phase diagram for a quantum spin-1 chain was determined numerically by den Nijs and Rommelse, who found six different phases. By treating the spin-1 problem as two coupled spin-1/2 chains and using the bosonization technique, Schulz obtained only five different phases. We review Schulz calculations and generate the full phase diagram from this formalism. Then, we introduce a coupling between the longitudinal and transverse modes. We find that a longitudinal charge density wave instability can arise if the stripe is quarter filled and the underlying lattice potential has a zigzag symmetry [1]. Our results shed light on the as yet not understood connection between the formation of a low-temperature-tetragonal phase and the subsequent appearance of charge order in high-Tc cuprates and manganites.

In addition, the response of charge stripes to an external electric field applied perpendicular to the stripe direction is studied within a diagrammatic approach for both weak and strong pinning by random impurities. The sound-like mode of the stripes described as elastic strings moves to finite frequency due to impurity pinning. By calculating the optical conductivity we determine this characteristic energy scale for both a single stripe and an array of interacting stripes [2]. The results explain the anomalous far-infrared peak observed recently in optical-conductivity measurements on cuprates.

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[2] L. Benfatto and C. Morais Smith, preprint.

## Density wave correlations in quasi-1d and 2d cuprates

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$\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  ladder compounds contain linear fragments of copper oxide planes. Holes doped into these ladders pair and superconduct at high doping concentrations, while insulators are known to result from low hole concentrations. The competition between insulating states and superconductive pairing has emerged as a key feature of the high- $T_c$  problem. Using transport and Raman scattering we identify the insulating state of self-doped ladders as a weakly pinned, sliding density wave (DW) that persists to well above room temperature. We compare low-frequency Raman and DC and AC transport properties in quasi-1D ladders and 2D cuprates at low doping concentrations and find that for both systems the low energy electrostatics is governed by DW correlations.

Refs:

G. Blumberg et al., Science 297, 584 (2002);

A. Gozar et al., Phys. Rev. Lett. 87, 197202 (2001).

# Nanoscale electronic microstructures in correlated metals from neutron PDF measurements

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We have recently been startled by the realization that many correlated metals are inhomogeneous on nanometer lengthscales, and that this has a profound affect on their properties. The electronic phase separation is often striped in nature. Important examples that I will talk about are cuprate high-Tc superconductors and colossal magnetoresistant manganites. We have used the local structural technique of atomic pair distribution function (PDF) analysis of neutron powder diffraction data to follow this electronic phase separation. I will also discuss how a competition between lattice strain and phase separation can lead to a breakup of the stripe structures into nanometer lengthscale microstructures.

# Role of incoherent lattice fluctuations in superconducting hole doped and electron doped systems and in CMR manganites

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Detailed investigations of incoherent, ultra fast lattice fluctuations are made in hole doped  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ ,  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  and electron doped  $\text{Pr}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$  superconducting systems, using Ion Channeling Technique. A marked difference is seen in the incoherent atomic displacement ( $u$ ) values in these two types of systems. Large fluctuations are seen in the case of both LSCO ( $T_c = 41$  K) and YBCO ( $T_c = 92.5, 65$  and  $45$  K respectively, depending on the value of  $x$ ) systems at the respective superconducting transition temperature ( $T_c$ ) and also above  $T_c$  in certain temperature regions indicating a non-analytic behavior in these two systems. However in the case of electron doped PCCO system ( $T_c = 22$  K) there is certainly an enhancement in the  $u$  value across  $T_c$ , but the shape of the  $u$  vs  $T$  spectrum is quite different. There is a gradual change in the  $u$  value as the temperature is increased to room temperature with a small change in slope around 100 K. However there is a marked change around 200 K in all the three cases. For a better comparison with the PCCO system, measurements are being made in the Zn doped YBCO with  $T_c$  around 22K and also in O under doped YBCO with similar value of  $T_c$ .

The above studies have triggered great interest in transition metal oxides of the type  $\text{R}_{0.7}\text{Me}_{0.3}\text{MnO}_3$  ( $\text{R}=\text{Pr},\text{Nd},\text{La}$  and  $\text{Me}=\text{Ba},\text{Sr},\text{Ca}$ ) systems generally known as CMR manganites. A prominent feature of these materials is a large maximum in resistivity near the ferromagnetic transition temperature ( $T_c$ ). This resistivity is dramatically decreased in the presence of an external magnetic field. A large change in the incoherent atomic displacements is observed across  $T_c$  by ion channeling in these CMR materials, showing a clear correlation with the transport properties. These incoherent fluctuations are very fast and can not be detected by normal neutron or x-ray diffraction studies. Even in the two layered systems like  $\text{La}_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$  ( $x = 0.4$ ) and  $\text{La}_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$  ( $x = 0.3$ ), these ultra-fast incoherent lattice fluctuations are observed across the ferromagnetic transition where a large drop in resistivity is seen. However if we take the case of  $\text{Nd}_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$  where there is no ferromagnetic transition because of charge ordering, and accordingly no in enhancement in the incoherent atomic displacement is seen.

All these measurements will be discussed in the light of the existing theories of high temperature superconductivity and CMR manganites.

# Is there a narrow collective conductivity mode in the cuprate oxides?

**S. Sridhar**

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A systematic set of microwave measurements on several oxides - cuprate superconductors, CMR manganites and striped nickelates - has yielded new insights into their electrodynamic properties. A cohesive picture is emerging that the electrodynamics at these sub-optical frequencies is dominated by collective charge transport and also manifests signatures of lattice instabilities at specific temperatures.

In the superconducting state below  $T_c$  of all the cuprates, including BSCCO,  $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+d}$ ,  $\text{HgBa}_2\text{CuO}_{4+d}$ ,  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+d}$  and  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ , the microwave data clearly are incompatible with the quasiparticle response of a pure d-wave superconductor. Instead, we have successfully modeled the data in terms of a non-quasiparticle scenario, according to which the electrodynamic response is ascribed to a collective mode, similar to the dynamic response of a density wave in low dimensional materials. Such a density wave can well arise from an inhomogeneous electronic state.

The collective mode dynamics is also observed above  $T_c$ , in terms of an anomalous plasmon-like response implying negative permittivities ( $\text{Re}(\epsilon(\omega)) < 0$ ) at microwave frequencies in the pseudogap state of the cuprate superconductors. The microwave plasmon arises from a charge collective mode characterized by a low plasma frequency and extremely low damping, distinctly different from those observed at optical frequencies.

Another feature common to several oxides, including the parent members of the cuprate superconductors and the nickelates, is the observation of dielectric transitions at characteristic temperatures that we associate with lattice instabilities. In  $\text{La}_2\text{CuO}_{4+x}$  and  $\text{La}_{5/3}\text{Sr}_{1/3}\text{NiO}_4$  these occur at common temperatures 32K and 245K, and are signatures of local lattice octahedra instabilities occurring in these isostructural perovskite oxides. These results also indicate that inhomogeneous electronic states, such as charge stripes and oxygen ordering, are strongly connected to underlying lattice instabilities.

$\text{MgB}_2$  presents a considerably different picture in terms of the microwave response in the superconducting state. Sample quality has been rapidly improving and in some high quality films we observe directly an exponential dependence on temperature of the surface resistance and the penetration depth. The resulting gap obtained from the measurements is approximately 1.92 meV, substantially smaller than the mean field value, but consistent with value of the smaller of the two gaps reported by other techniques.

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# Evolution of temperature dependent local Cu-O displacements from underdoped to overdoped La-Sr-Cu-O superconductor

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Advanced experimental probes of local and instantaneous structure have provided evidences for the importance of local structural fluctuations in the inhomogeneous superconductors with high transition temperature. Here we have studied temperature dependent local structure of superconducting  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (0.105, 0.13, 0.15, 0.20) single crystals by Cu K-edge extended x-ray absorption fine structure (EXAFS) measurements with polarization parallel to the in-plane Cu-O bonds. We find that, while underdoped crystals ( $x=0.105, 0.13$ ) show anomalous temperature dependence, similar to the case of optimally doped system ( $x=0.15$ ), overdoped crystal ( $x=0.20$ ) does not reveal such anomaly. Correlated Debye-Waller factor (DWF) of the Cu-O bonds (distance broadening) has been used as an order parameter to determine characteristic local displacements in the  $\text{CuO}_2$  plane. The amplitude of temperature dependent step-like increase in the DWF at low temperature decreases with increasing doping. It has been discussed that decreasing electron-lattice interaction with increasing doping, shown by angle resolved photoemission measurements, is closely related to the evolving anomalous local  $\text{CuO}_2$  distortion and charge inhomogeneity with doping in the  $\text{CuO}_2$  plane of high  $T_c$  oxides. The results on A15 ( $\text{Nb}_3\text{Ge}$  intermetallic) and C15 ( $\text{CeRu}_2$ ) intermetallic systems are also presented discussing the similarities and differences with respect to the importance of local electron-lattice interactions in these materials.

# Beyond mean field approaches: Nanoscale heterogeneity and properties of complex materials

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One of the fundamental bases of condensed matter physics is periodicity and the corollary attribute of homogeneity down to the scale of the unit cell. These aspects of crystalline materials have their historical origins in the diffraction pattern and associated crystal lattice. Recently, however, attention has been given to the more accurate description of diffraction as representing the long range average structure of the coherent fraction of a crystalline solid. The actual arrangement of atoms on smaller length scales may therefore deviate significantly from the one determined by conventional crystallographic approaches. In correlated and transformational materials that possess multiple states with similar energies, collective behavior among sites exhibiting lattice distortions, amplified by dynamic effects such as charge ordering and static ones such as fluctuations in local composition, may even result in nanophase separation as sets of dozens or hundreds of atoms adopt conformations different from that of their host. Many of the compelling properties of complex materials, one characteristic of which is unit cell stoichiometries that differ from their chemical compositions, may therefore result from this nanoscale heterogeneity instead of from traits inherent to their homogeneous descriptions. Using a combination of local structure measurements, modeling, and calculations, we have been able to identify these kinds of behaviors in, e.g., NiMn, Pu alloys,  $\text{PuO}_{2+x}$ , etc., and have made progress in evaluating the actual arrangements of atoms in complex materials and its effect on structure factors and other larger scale properties.

# Lattice and charge inhomogeneities in perovskite type transition metal oxides

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Transition metal oxides with complex perovskite type structures are well known to undergo a variety of instabilities which are either structural ones or charge/spin related. Since the oxygen ion  $2p^2$  state is unstable as a free ion, hole doping of these systems is of vital importance in order to virtually stabilize the  $O^{2-}$  ion and provide a substantial energy gain. Since a complete stabilization cannot be achieved, transition metal – oxygen p – d charge transfer effects are crucial and dynamical hybridisation plays an important role. Modelling these types of compounds consequently requires to include strong electron-phonon interactions which are unconventional since multi – phonon – density – density interactions play a dominant role. By explicitly incorporating these terms and solving the complex problem on the lattice, unusual “extra” dynamics on top of the ordinary phonons result, which give rise to phonon anomalies at incommensurate wave vectors. Due to the strong coupling between electrons and phonons substantial anomalies occur in the electronic energies which can be related to charge density wave formation and unconventional superconductivity.

The results are discussed for actual systems and relations to experimental data presented.

# Nanoscale phase separation, colossal magnetoresistance, and stripes in cuprates

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Recent developments in the context of theory and experiments for manganites will be reviewed. It will be argued that the presence of nanoscale phase separation is at the heart of the CMR phenomenon [1]. These effects are not limited to manganites, but they appear in other compounds as well, such as the high- $T_c$  cuprates. Results of a spin-fermion model show the presence of stripes in this context, and tendencies toward d-wave pairing.

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# Giant Dielectric Permittivity of Electron-Doped Manganite Thin Films, $\text{Ca}_{1-x}\text{La}_x\text{MnO}_3$ ( $0 \leq x \leq 0.03$ )\*

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Measurements of the low-frequency ( $f < 100\text{kHz}$ ) in-plane permittivity ( $\epsilon'$ ) of epitaxial thin films of  $\text{Ca}_{1-x}\text{La}_x\text{MnO}_3$  ( $x \leq 0.03$ ) in the range  $4\text{K} \leq T \leq 300\text{K}$  reveal giant effective values of the permittivity,  $\epsilon' \sim 10^4 - 10^7$ , with weak  $T$  dependence for  $T > 200\text{K}$ . This phenomenon is attributed to an internal barrier-layer capacitor (BLC) structure, with insulating boundary layers at grain boundaries between semiconducting grains. The measured values of  $\epsilon'$  exceed those of conventional two-phase BLC materials based [1] on  $(\text{Ba,Sr})\text{TiO}_3$  as well as recently discovered [2]  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$  and doped NiO [3]. Consistent with this picture is an increase in  $\epsilon'$  with the bulk conductivity of the grains through electron (La) doping.

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# Tunneling studies on the electronic excitation spectrum of Bi2212

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Using Bi2212/vacuum/Bi2212 (BVB) junctions fabricated by STM, we have examined the  $T$  dependence of tunneling spectrum over a wide hole-doping range. It has been demonstrated that in the normal-state electronic excitations, there exist two kinds of pseudogaps (PG's) with different characteristic energies. The smaller energy-scale PG (SPG), which is comparable to the SC gap in magnitude, is some kind of precursor of superconductivity, while the larger energy-scale PG (LPG), which is 3 to 4 times larger than the SC gap, seems to be due the gradual development of antiferromagnetic (AF) spin fluctuations. In this talk, we will focus on the following behavior of the electronic excitation spectrum across  $T_c$ .

- i) The SPG evolves smoothly into the SC gap below  $T_c$ , as reported in earlier tunneling experiments. This fact strongly supports the contention that the SPG will be a precursor of superconductivity.
- ii) In the tunneling spectrum, a depression of spectral weight, the so-called “dip-structure”, appears in the energy region just outside the SC gap below  $T_c$ . The dip-structure is consistent with a drastic change in the electronic dispersion curves around  $(\pm\pi, 0)$  and  $(0, \pm\pi)$  across  $T_c$ , which has recently been reported in ARPES experiments by Gromko *et al.* It has also been found in the present study that the dip-structure develops gradually as a function of decreasing temperature below  $T_c$  and its development is saturated at low temperatures. The  $T$  dependence of dip-structure is in good agreement with that of the intensity of neutron scattering due to the AF resonance mode with a characteristic energy of  $\sim 40$  meV and also similar to that of the intensity of neutron scattering due to a phonon mode. This finding suggests that the dip-structure in the electronic excitation spectrum, which appears in accordance with the SC transition, will be due to the strong couplings of electrons around  $(\pm\pi, 0)$  and  $(0, \pm\pi)$  with a combined magnon and phonon collective mode.
- iii) In underdoped Bi2212, the high-energy spectral feature, reflecting the LPG, changes from a broad hump to a clear hump across  $T_c$ , accompanied by a shift of its position toward lower energies, suggesting that the LPG will also be modified in accordance with the SC transition.

# Imaging Nanoscale Phase Segregation in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$

**Eric W. Hudson**

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Recently, a variety of experimental measurements have begun to suggest that the electronic structure of high temperature superconductors is inhomogeneous on very short length scales. Using scanning tunneling microscopy, we have probed superconductivity at the atomic scale in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ , both in its native state and perturbed by intentionally doped, single atom impurities. After an introductory review of scanning tunneling microscopy, I will discuss some results of these studies. In particular, I will focus on spatial variations of the local density of states and how maps of these variations reveal the presence of electronically distinct nano-domains. I will also describe the local effects of individual Ni atoms embedded in these domains, and explain their power as “superconductivity markers.” Finally, I will discuss more recent results from oxygen doping dependent studies.

This project was carried out in collaboration with K.M. Lang (NIST Boulder), J.E. Hoffman (U.C. Berkeley), V. Madhavan (Boston College) J.C. Davis (Cornell), S.H. Pan (University of Houston), H. Eisaki (AIST Tsukuba) and S. Uchida (Tokyo University).

# Dramatic Effect of Inhomogeneities on Electron-Phonon Coupling in Exotic Superconductors.

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The maximum superconducting transition temperature due to a phonon-mediated interaction was estimated by McMillan in 1967 to be about 30 K. This estimate follows from the sum-rule on the electron-ion interaction  $V(q)$ , given by  $V(0)=Z/N(E_F)$ , which applies to a homogeneous electron gas, as treated by the Bohm-Pines-Nozieres theory. In "exotic" superconductors, this e-g theory breaks down completely, either because of the extreme inhomogeneity of the e-g (fullerenes), or because of an extremely inhomogeneous ionic polarizability (cuprates, organics, etc.), that has the lattice periodicity (and therefore Bloch's theorem applies). The wavevector  $G$  which characterizes this inhomogeneity is larger than  $2k_F$ , therefore the e-g cannot follow the inhomogeneity, and sees the average polarizability, which is extremely large (the perovskites being almost ferroelectric). As a result, the electron-electron interaction is screened-out by the ionic polarizability. This enhances the electron-ion potential (for ions situated in regions of small ionic polarizability) and thus the electron-phonon coupling, by a large amount, and consequently the maximum superconducting transition temperature (due to the BCS phonon-mediated mechanism) increases to about 200 K in cuprate-like materials.

Experimental support for this theory is provided by the STM measurements of Davis & Pan, who found that the (Debye) screening-length in BiSCCO is about 14 Å, (instead of about 0.5 - 1 Å), i.e. there is virtually no screening of the potential due to inhomogeneities (interstitials, vacancies) by the e-g. Also, neutron-diffraction experiments by Egami et al show that some very specific phonon mode is abnormally softened; this mode interacts selectively with the polarizable units (apex oxygens, and Bi or chain-Cu atoms). Thus, the role of the phonon-mediated interaction should be reconsidered, because of the extreme inhomogeneity characteristic of exotic superconductors.

# Hole phase separation in underdoped cuprate superconductors

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There is considerable evidence, especially from recent STM measurements of the Davis group, that the hole density is inhomogeneous in the under-doped cuprate high temperature superconductors. It has also been suggested by Uemura, and others, that the over-doped system is also inhomogeneous, this to explain the decreasing condensate fraction manifest in the Uemura plot. This talk describes a new formulation for the t-J model which has been developed by Barnes and Maekawa. The spins have a flux ground state related to Anderson's RVB state. In addition to the gap associated with this flux-RVB state is a charge pseudo gap of the type described by the Bogoliubov theory of  $^4\text{He}$ . The interplay between these two gaps and the infrared cut-off associated, roughly speaking, with Cooper pair formation determines the phase diagram. It is an important result that the effective hopping matrix elements for the spin particles is  $J-2xt$ , i.e., exhibits a competition between the anti-ferromagnetic  $J$  and the hole induced ferromagnetic process reflected by the term  $-2xt$ . This competition would result in a quantum critical point (QCP) near optimal doping if it were not for superconductivity. What it *does* do is lead to an instability towards hole separation in the underdoped region. There is no such effect in the overdoped region, *however* the theory predicts that condensed bosonic and fermionic holes coexist in a fashion which is consistent with the experimental data. This effect is quite different from stripe formation although it has a similar experimental signature to short-range-time-fluctuating-stripes.

The theory was originally devised to describe a rather subtle bi-layer splitting of the condensate peak observed, by the Shen group, in ARPES for the bi-layer Bi-materials. Our prediction for the decomposition of the ARPES spectra made on the basis of our theory was later verified by experiment. The famous hump-dip-peak seen in ARPES and tunneling has a natural explanation in terms of our approach.

# Competing degrees of freedom in the physics of high temperature superconductors

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Here we report a detailed study of temperature, doping and momentum dependence of the quasiparticle dynamics and scattering process in high temperature superconductors using high-resolution angle resolved photoemission spectroscopy (ARPES).

A detailed doping and temperature dependence study is reported and similarities between different families are discussed.

# Direct ARPES Studies on In-Situ Grown LSCO-214 Superconducting Films: Strain and Enhanced Superconductivity

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We have successfully performed angle resolved photoemission spectroscopy on a series of epitaxial  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) superconducting thin films grown in-situ by laser deposition on (001)- $\text{SrLaAlO}_4$  substrates. Our measurements are the first direct probing of the low energy electronic structure of any high  $T_c$  superconductor under different degree of epitaxial (compressive) strain. In optimally doped films (0.15% Sr content), we clearly measure the band dispersion along  $K_x$  and the Fermi level crossing before the Brillouin zone boundary, in sharp contrast to the flat band remaining well below the Fermi level for unstrained samples. Surprisingly, the associated reduction of the density of states does not diminish the superconductivity, but actually enhances the critical temperature by about 6 degrees to 44K (as compared to  $T_c=38\text{K}$  in unstrained films or single crystals). Based on our systematic measurements, we determine the evolution of the Fermi surface in LSCO-214 with both doping and the strain and critically discuss the relevance of our results for the evolving theory of high temperature superconductivity.

## Do apical oxygens have any role in high $T_c$ superconductivity?

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High  $T_c$  superconductivity is believed to occur in the  $\text{CuO}_2$  planes that are common to high  $T_c$  superconductors. Even though the apical oxygens are adjacent to the  $\text{CuO}_2$  planes, their role has been largely ignored on the reasoning that the apical oxygen driven states are far away from the Fermi energy. However, this has not been experimentally proven. In this talk, experimental results on  $\text{Sm}_2\text{CuO}_4$  and  $(\text{Na,Ca})_2\text{CuO}_2\text{Cl}_2$  by ARPES and XAS will be presented. The parent compound of an electron doped superconductor  $\text{Sm}_2\text{CuO}_4$  shows a quite different dispersion from that of  $\text{Ca}_2\text{CuO}_2\text{Cl}_2$  which can be hole-doped. XAS results on Na doped  $\text{Ca}_2\text{CuO}_2\text{Cl}_2$  will also be discussed.

# Photoemission study of diluted magnetic semiconductors and layered transition-metal oxides

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By using x-ray photoemission spectroscopy (XPS) and x-ray absorption spectroscopy (XAS), we have studied the electronic structures of diluted magnetic semiconductors ( $\text{Zn}_{1-x}\text{Mn}_x\text{O}$ ,  $\text{Ga}_{1-x}\text{Mn}_x\text{As}$ ) and some two-dimensional  $t_{2g}$  systems ( $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ ,  $\text{NaCo}_2\text{O}_4$ ,  $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_9$ , and  $\text{Ca}_3\text{Co}_4\text{O}_9$ ) that are ferromagnetic or are close to ferromagnetic instability. The valence band XPS and Co 2p XAS data of  $\text{NaCo}_2\text{O}_4$ ,  $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_9$ , and  $\text{Ca}_3\text{Co}_4\text{O}_9$  [1-3] show that  $\text{Co}^{3+}$  and  $\text{Co}^{4+}$  have low-spin configurations. The O 1s XAS data of  $\text{NaCo}_2\text{O}_4$ ,  $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_9$ , and  $\text{Ca}_3\text{Co}_4\text{O}_9$  show that the holes are mainly located in the  $a_{1g}$  orbital. Since the lobe of the  $a_{1g}$  orbital is directed to the  $c$ -axis that is perpendicular to the Co-O triangular lattice, the  $a_{1g}$  band is expected to be very flat and strongly affected by the electron-electron and electron-lattice interactions [4]. Probably, the almost localized  $a_{1g}$  electron is responsible for the enhanced thermopower commonly observed in the layered Co oxides [1-3] and the ferromagnetism at low temperature found in  $\text{Bi}_2\text{Sr}_2\text{Co}_2\text{O}_9$  [2] and  $\text{Ca}_3\text{Co}_4\text{O}_9$  [3]. The  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$  system has a rich phase diagram including superconductor, paramagnetic metal, antiferromagnetic insulator, and paramagnetic insulator phases [5]. In  $\text{Sr}_2\text{RuO}_4$ , the Ru 3d core level XPS has a double-peak structure that can be attributed to the well-screened and poorly-screened peaks. Also the O 1s core level has a similar double-peak structure. In order to examine the relationship between the spectral line shape and the metal-insulator transition, we have performed XPS measurement changing composition and surface sensitivity. We will compare the  $t_{2g}$  systems with that of diluted magnetic semiconductors [6] and discuss their electronic structure in a systematic way.

This work has been done in collaboration with A. Fujimori, S. Hirata, K. Okazaki, Y. Hitsuda, T. T. Tran, M. Kurokawa, H. Yagi, T. Nambu, J. Okabayashi, O. Rader, L. H. Tjeng, H.-J. Lin, C. T. Chen, N. Nücker, S. Schuppler, H.-J. Noh, S.-J. Oh, S. Nakatsuji, H. Fukazawa, Y. Maeno, R. Kitawaki, I. Terasaki, S. Lambert, C. Michel, Y. Suzuki, Y. Miyazaki, T. Kajitani, I. Tsukada, T. Yamamoto, and K. Uchinokura.

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# Stripe-like Inhomogeneities, Spectroscopies, Transport and Pairing in the High $T_c$ Cuprates

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Theoretical calculations, and a variety of experimental data, support an approach to the high- $T_c$  cuprates which is based on dynamical stripe-like inhomogeneities, and the existence of both large- $U$  and small- $U$  orbitals in the vicinity of  $E_F$ . Such an approach, where the major aspects within a  $\text{CuO}_2$  plane are treated by a  $t-t'$  model, is applied. The solution introduces a state where three types of carriers coexist: polaron-like "stripions" carrying charge, and consisting primarily of large- $U$  orbitals in charged stripes; "quasi-electrons" (QE's) carrying charge and spin, and consisting of hybridized large- $U$  and small- $U$  orbitals; and "svivons" carrying spin and lattice distortion.

Under this approach the observed systematic behavior of spectroscopic and transport properties (including the resistivity, Hall constant, and thermoelectric power) in the cuprates is understood. The AF/stripe-like inhomogeneities result from the Bose condensation of the svivon field, and the observed neutron-scattering resonance mode represents its excitations towards the restoration of non-magnetic homogeneity. The renormalization of the electron bands close to  $E_F$  results in anomalous bandwidths and a "kink"-like behavior observed by ARPES.

High  $T_c$  pairing results from transitions between pair states of stripions and QE's through the exchange of svivons, causing large gain in inter-stripe hopping of stripions. It is dominated by  $t$ -hopping processes and requires stripes oriented along the Cu-O bonds. The pairing symmetry is of the  $d_{x^2-y^2}$  type; however there is phase reversal of QE pairs through the charged stripes, resulting in features characteristic of an  $s$ -type pairing component when tunneling between different  $\text{CuO}_2$  planes occurs. Incoherent pairing results in the existence of a pseudogap phase of incoherent pairs, and the Uemura limit, in underdoped cuprates.

For low doping levels the stripes are diagonal, and inter-stripe hopping occurs through  $t'$  processes, resulting in the observed appearance of states on  $E_F$  at point  $(\frac{\pi}{2}, \frac{\pi}{2})$ , but no SC pairing. For higher doping levels the stripes become oriented along the Cu-O bonds, and also  $t$  processes contribute to inter-stripe hopping, resulting in the observed appearance of states on  $E_F$  around points  $(\pi, 0)$  and  $(0, \pi)$ , and SC pairing.

The sharp coherence peak above the SC gap results from stripion+svivon excitations, with spin periodicity contributing to the restoration of non-magnetic homogeneity. The spectral weight of this peak is transferred from high-energy states (as observed) which are involved in the formation of the AF/stripe-like inhomogeneities. It is proportional to the superfluid density, which has a maximum for slightly overdoped cuprates, as is reflected also in the "boomerang" behavior of the Uemura plots. This maximum corresponds to a half-full stripion band. Non-magnetic homogeneity (and coherence) is restored in the normal state of overdoped cuprates, at low temperatures.

# Study of charge inhomogeneities in the $\text{La}_2\text{CuO}_{4.1}$ system

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We have investigated charge ordering in an oxygen doped  $\text{La}_2\text{CuO}_{4.1}$  crystal by high-resolution x-ray diffraction using synchrotron radiation. Thanks to the high brilliance synchrotron radiation it has been possible to record a large number of weak superstructure spots due to charge ordering around the main peaks of the average structure. The oxygen ordering structure has been separated from the charge ordering features. The charge modulation as a function of temperature and the x-ray incident photon flux is reported. We show that photodoping at 100K induces bubbles of charge stripes. The results are consistent with diagonal stripes in the LTO phase with anisotropic next near neighbour hopping  $t'$ . The data are discussed in the new phase diagram of cuprates at constant doping as a function of Cu-O bond distance (microstrain).

# Non-equilibrium-state x-ray absorption spectroscopy: a local structure study of photo-induced phase transition

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We describe non-equilibrium-state x-ray absorption spectroscopy focusing on local structure of photo-excited states trapped at low temperature. For this purpose, a novel Ge 100 pixel array detector with a packing density of 88% was developed. The local structure of photo-induced phase of Fe(II) spin crossover complex,  $[\text{Fe}(\text{2-pic})_3]\text{Cl}_2\text{EtOH}$  (2-pic=2-aminomethyl pyridine), was investigated at low temperature ( $T < 150$  K). The use of pixel array detector and high-flux synchrotron x-ray source (multipole wiggler) successfully provided x-ray absorption spectra with high quality, *in-situ*, during the photo-excitation. It was found that *the photo-induced phase under optical pumping at low temperature ( $T < 50$  K) has an octahedral geometry with the elongated Fe-N distance ( $2.16 \pm 0.01 \text{ \AA}$ )*, stabilizing the high spin state (S=2) configuration. No indication of symmetry breaking of  $\text{FeN}_6$  clusters upon LS $\leftrightarrow$ HS spin-state switching was observed. It was demonstrated that the technique is a promising means to probe the local structure of non-equilibrium state such as trapped excited states or metastable states.

# Magnetic and Orbital correlations in the electron-doped manganites

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A double exchange model for degenerate  $e_g$  orbitals with intra- and inter-orbital correlations as well as the nearest neighbour Coulomb interactions has been used to study the electron doped manganites  $A_{1-x}B_x\text{MnO}_3$   $x \geq 0.5$ . We show that such a model reproduces the observed phase diagram and orbital ordering in the intermediate bandwidth regime. The Jahn-Teller effect, considered crucial for the region  $x < 0.5$  does not play a major role in this region as observed by Brink and Khomskii [1] in the limit of infinite Hund's coupling. From a realistic calculation with finite Hund's coupling, we show that inclusion of interactions stabilizes the C-phase, the antiferromagnetic metallic A-phase moves closer to  $x=0.5$  while the ferromagnetic phase shrinks. This is in agreement with the recent observations of Kajimoto et al. [2] and Akimoto et al. [3]. The charge ordering close to  $x=0.5$  and the effect of reduction of band-width are also outlined.

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# Jahn-Teller Polaronic Inhomogeneous in Ferromagnetic $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$

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Recently was shown, that the charge carriers in the doped manganites  $(\text{RE})_{1-x}\text{A}_x\text{MnO}_3$  ( $\text{RE} = \text{La, Pr, Nd}$ ;  $\text{A} = \text{Ca, Sr, Ba}$ ) have the properties of polarons. The isolated electron in an  $e_g$ -shell of ions  $\text{Mn}^{3+}$  ( $3d^4$ ) occupies  $3d(x^2 - y^2)$  or  $3d(z^2 - r^2)$  an orbital located inside an oxygen octahedron with Jahn-Teller distortion, that is a  $JT$  polaron. In a high-temperature limit the ensemble of polarons is possible to view as a polaronic fluid, which can be transformed with decrease of temperature to ordered structure of the Jahn-Teller polarons. The polarons in a limit of strong (small) electron - phonon interaction are called as polarons of small (large) radius. The polarons of large radius can rather easily move on a sample due to small effective mass ( $m^* \sim 2-4$ ), thus the distortion of a lattice envelops great area of a crystal. On the other hand polarons of small radius can move on a crystal only by tunneling, or at the expense of jumps, activated by a heat, between locally distorted positions of  $\text{Mn}^{3+}\text{O}_6$  oxygen octahedrons, thus a lattice distortion envelops area from one up to several values of a lattice constant. For a case of intermediate electron - phonon connection, which is implemented in doped manganites, it is expected crossover from a regime of large polarons to small. In this case, the composite phases may coexist in the samples involving the intermediate polarons with  $m^* = 5-10$  and radius  $\sim 5\text{\AA}$ , and also the regions with travelling large polarons and areas of localized small polarons. There are the experimental evidences of ordering  $JT$  polarons in manganites in stripes and ferromagnetic metal areas..

In this paper it was investigated the magnetic  $T$ - $x$  phase diagram of doped  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  compounds by the methods of x-ray diffraction, magnetization in constant magnetic field  $M(T, x)$  and a high-frequency susceptibility  $\chi'_{ac}(T, x)$  for three regime of the calcium doping : weak ( $0 \leq x < x_c$ ), optimum ( $x_c < x \leq 0,4$ ) and strong ( $0,4 \leq x \leq 1,0$ ), where  $x_c \approx 0,1$  is critical concentration of Ca impurity. We established, that for  $x < x_c$  the cooperative Jahn-Teller a lattice distortion at 300K corresponds to tetragonal compression of a unit cell along the  $c$ -axis, whereas for  $x > x_c$  dominate the incoherent disordered strains of oxygen octahedrons. There is the concentration phase transition from ordered distribution of the Jahn-Teller distortions to a distribution with the disordered local distortions of the  $\text{Mn}^{3+}\text{O}_6$  octahedrons, which is attended with sharp changes of the temperature and concentration dependences of magnetic properties of the  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  samples. The obtained experimental results are evidence in a close relationship between the magnetic properties of these compounds with Jahn-Teller distortions dynamics. We have also discussed the following questions: 1. Crystalline structure of doped compounds  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  at 300°K ; 2. Phase transitions in the ferromagnetic and cluster glass like states ; 3. Influence of intermediate electron-phonon interaction on dependence  $T_c(x)$  ; 4. Double phase transition a  $FM$ - $AFM$  induced by charge ordering ; 5. Orbital and charge ordering in  $\text{La}_{1-x}(\text{Sr, Ca})_x\text{MnO}_3$  compounds.

# Role of Inter - site Exchange and Hybrid Interactions in Itinerant Ferromagnetism

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In this work we study the magnetic properties of itinerant electron systems using the Hubbard – like tight binding Hamiltonian along with inter – site exchange and hybrid interactions. We have used the mean – field approximation to deal with the exchange and hybrid interactions. It is found that hybrid interaction is more effective than exchange interaction for the on – set of ferromagnetic state. We have studied the effect of hybrid interaction on various physical quantities at different temperatures. The effective mass ( $m^*/m$ ) of up spin electrons increases slowly as the temperature decreases but below the critical temperature ( $T_c$ ), it decreases rapidly. For down spin electrons effective mass increases slowly as the temperature decreases and below  $T_c$ , it increases more rapidly. Spectral weight ( $n/m^*$ ) for up spin electrons decreases slowly upto  $T_c$  & below  $T_c$ , it increases rapidly. For down spin electrons spectral weight decreases slowly upto  $T_c$  & below  $T_c$ , it decreases rapidly. Our results for both the effective mass & spectral weight are in good agreement with recently observed experimental behaviour in itinerant ferromagnet  $Ga_{1-x}Mn_xAs$  (Singley. et. al., Phys. Rev. Lett. 89, 097203 (2002)). We have also studied variation of the spectral weight and optical absorption with temperature in presence of magnetic field. We found that these two quantities for up spin electrons increase as applied magnetic field increases at all temperatures ( $\sim 4T_c$ ). For down spin electrons these two quantities decrease as applied magnetic field increases.

# A search for extra Lattice distortions in High $T_c$ $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ associated with the Superconductivity

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A large number of intensive studies for physical properties in high- $T_c$  oxide superconductors have been accumulated since the discovery of more than 15 years. However, the origin of such a high superconductivity transition temperature is still wrapped in mystery.

A precision measurement of the temperature dependence of the lattice parameters in a single crystal of  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  was made by Maeta et al. [1-3] by using an X-ray Bond method. In this method systematic errors were avoided by fixing two X-ray counters at symmetrical positions on both sides of the incident X-ray beam and only a single crystal specimen was rotated during a measurement. By adopting this method, it became possible to determine the lattice parameters up to the order of the accuracy of  $10^{-7}$  [4]. From this measurement a spontaneous lattice contraction of  $2.3 \times 10^{-5}$  was found in the ab-plane, while along the c-axis an expansion of  $1.5 \times 10^{-5}$  was observed. Those distortions of the crystal lattice are associated with the appearance of the high- $T_c$  superconductivity.

A careful search has been made for existence of any extra lattice distortion associated with the stripe structure above the transition temperature. However, it was not possible to detect any small distortion of the lattice to the extent of the experimental accuracy.

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# Fluctuations of order parameters in a two-band high- $T_c$ superconductor

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The fluctuations of superconductivity order parameters have been studied in the framework of a two-band model with interband pair-transfer interaction. Two relaxation times and coherence lengths revealing critical and noncritical temperature behaviour near the phase transition point have been obtained on the basis of the free energy derived for spatially inhomogeneous band order parameters. The existence of two relaxation time-scales in the kinetics of superconductivity fluctuations has been observed experimentally in  $Y_1Ba_2Cu_3O_y$  [1,2]. It has been found that the damping of fluctuations is going at first mainly in the fast relaxation channel and, after that, in the slow relaxation channel. The dependencies of relaxation times and coherence lengths vs chemical potential position (doping) have been calculated.

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# The Mesoscopic Mechanics

Artur Sowa

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The Mesoscopic Mechanics (MeM) is a self-consistent mathematical framework for the description of the mesoscopic scale electronic phenomena that occur in two-dimensional systems. The dynamic variable of this theory may be interpreted as an endomorphism of the algebra of observables. The theory admits both relativistic and nonrelativistic formulation. In spite of its nonlinear nature (the nonrelativistic version of) this theory exhibits striking analogies with the Schrodinger picture. MeM emerges from a broader interpretation of the previously introduced by me Nonlinear Maxwell Theory. While the latter is a field theory that provides a unified phenomenological model of such phenomena as the magnetic vortex lattice formation, superconductivity, charge stripes, and magnetic oscillations, the Mesoscopic Mechanics clarifies why the model works vis a vis the fundamental principles. MeM is very explicitly rooted in Quantum Mechanics on one hand and the Quantum Field Theory on the other. However, the formalism and character of this theory are altogether different.

This approach is entrenched in the physics culture best characterized by the following broadly recognized general ideas: To understand the mesoscopic scale electronic phenomena may require concepts that are logically separate from the many-body Schrodinger picture [cf. Laughlin & Pines]. A presence of (intrinsic to the system) topological invariants plays a role in the stability and very nature of some Correlated Electrons phenomena [cf. Laughlin]. It may be necessary to make explicit use of such intrinsic topological invariants in an attempt at error-correcting implementation of Quantum Computation [cf. Freedman].

The Nonlinear Maxwell Theory has been described in the following articles:

- The (fully) Nonlinear Maxwell Theory delineated, *Journal of Geometry and Physics*, VOL. 45, NO. 1-2 (2002), 54-74
- Nonlinear Maxwell Theory and Electrons in Two Dimensions, *Communications in Mathematical Physics* 226 (2002), 559-566
- On an equation arising from the geometry of Riemannian submersions, *Journal fur die reine und angewandte Mathematik* 514 (1999), 1-8
- Magnetic Oscillations and Maxwell Theory, *Physics Letters A* 228 (1997), 347-350