SESSION 16

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Microscopic origin of the pseudogap

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By paying attention to the distortion effects of the CuO_6 octahedra or CuO_5 pyramids in the underdoped cuprates, Kamimura, Hamada and Ushio [1] have recently clarified the key features of the many-electron electronic structures of underdoped cuprates based on the first principles cluster calculations. According to them, a metallic state of the underdoped cuprates is characterized by the alternating appearance of the Zhang-Rice spin-singlet state and the Hund's coupling spin-triplet state in the spin-correlated region of local antiferromagnetic ordering due to the localized spins around Cu sites. This eloctron-spin state is now called "Kamimura-Suwa model", which differs from the ordinary Fermi liquid theory. As a result the area of the Fermi surfaces is proportional to the doping concentration in the underdoped region and thus the Fermi surface is small. When the hole concentration increases beyond the optimum doping to the overdoped region, the spin-correlation length decreases so that the local antiferromagnetic ordering disappears. Thus the Fermi surfaces change from small ones to larger ones at a certain concentration x_c in the overdoped region, where the latter is assumed to be treated by the ordinary Fermi liquid at the begining. We will show that the temperature T'nax called "high-energy" pseudogap below which the spin susceptibility exhibits a broad peak, reflecting 2D antiferromagnet, corresponds to a first-order-like phase transition from the phase consisting of small Fermi surfaces to the phase consisting of large Fermi surfaces. We have also calculated the hole concentration dependences of the electronic entropy and of the electronic specific heat for LSCO and compared the results with those observed by Loram et al [2]. By this comparison we find that the Kamimura-Suwa model explains well quantitatively the experimental results in the underdoped region while the results calculated by the LDA energy band structure give very small entropy in the overdoped region compared with the experimental results. In this context we contracted the bandwidth of the conduction band in the LDA band by 1/6 so as to reproduce the experimental results. Thus we coclude that not only in the underdoped region but also in the overdoped region the hole carriers behave like heavy Fermions with the effective mass of 6 times heavier than the free electron mass due to both the electron correlation and the electron-phonon interaction.

[1] H. Kamimura, T. Hamada and H. Ushio, to be published in Physica C (2000)
[2] J. W. Loram et al., J. Phys. Chem. Solids 59 (1998) 2091.

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Superconducting correlations in metallic dots

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Progress in nanofabrication has recently allowed to detect signatures of superconducting correlations in individual metallic dots, with level spacing comparable to the superconducting correlation energy.
The universal properties of such systems can be described by the BCS pairing hamiltonian, in the canonical ensamble. Pairing correlations are strong (nonperturbative) even for ultrasmall grains and drive the crossover to BCS superconductivity when the level spacing becomes small enough.
The low energy physics turns out to be expressed in terms of universal functions of the ratio between the level spacing and the correlation scale (which becomes the BCS gap in the bulk limit). This allows a quantitative description of the full crossover behavior.
We studied the thermodynamics of superconducting dots. We addressed thequestion of observable features of superconducting correlations in the regime of large level spacing (ultrasmall grains).
In particular grains with an odd number of electrons show a reentrant behavior of the spin susceptibility vs. temperature, which is a "smoking gun" of the combined of parity effects and pairing correlation, even for ultrasmall grains.

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Local polarization, electron stripe, and high-T_c superconductivity in layered cuprates

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We examine the possibility of high-T_c superconductivity mediated by the elementary excitation of an electron stripe which is realized by stabilizing local polarizations mainly caused by the *c*-displacement of ions on the CuO_2 plane, where the ion displacement is easily realized due to the smallness of the *c*-axis force constant, compared with that of other typical perovskite crystals, such as $BaTiO_3$. Under the translation invariance of the electronic state of the electron stripe, itinerant and localized electrons (and holes) can coexist in the stripe phase, where the localized electrons are aligned antiferromagnetically along the stripe. If the antiferromagnetic state is partially violated by the itinerant electrons (or holes), the superconductivity for T_c around 100 K can be realized, due to the enhancement of the coupling constant, with the corresponding characteristic "Debye" temperature being estimated as about 300 K. This indicates that the electron stripe caused by the local polarization should play a consequential role in high-T_c superconductivity.

Keywords: *local polarization, itinerant and localized electrons, antiferromagnetic stripe.*

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Quantum interference mechanism and analytical Hartree-Fock "parquet" stripe phase solutions for the Hubbard model

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quantum interference mechanism of the stripe phase instability in quasi one-dimensional (1D) repulsive electron system is proposed. It is shown that away from half filling periodic lattice potential causes cooperative condensation of the spin and charge superlattices via quantum interference of the scattered electrons wave-functions. 1D renormalization group analysis ("parquet"), specially modified for the case of the two coupled order parameters, indicates transient-scale correlations resembling the mean-field pattern (S. Mukhin 1997,1998,2000). An exact self-consistent analytical solution for the spin-charge solitonic superstructure in quasi-one-dimensional electron system is obtained in the framework of the Hubbard model for a hole doping close to the half-filling of the electron band (S. Matveenko and S. Mukhin 2000). A transition from a weak coupling (spin- charge-density waves) to a strong coupling ground state (solitonic spin- and charge superlattices) with decreasing hole concentration is demonstrated explicitly. These results reveal possible microscopic mechanism of the stripe phase ordering, which mainly relies on the local (onsite) electron interactions.

Keywords: *stripe phase, Hubbard model, coupled spin-charge fluctuations, solitonic superlattice.*

References

[1] S.I. Mukhin, J. Phys. Chem. Solids 59, 1846 (1998); cond-mat/9811409; Phys. Rev. B (2000) in publication.
[2] S.I. Matveenko and S.I. Mukhin, Phys. Rev. Lett. (2000) in publication; cond-mat/9912487.

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Topological defects and the spin glass phase of cuprates

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Recent experiments have shown the existence of incommensurate correlations in the spin glass phase of $La_{2-x}Sr_xCuO_4$. We argue that this spin glass phase is a state with random distributed charges which act as polarizable dipolar frustration centers to the antiferromagnetic environment. While any kind of charge order is absent, the spins have an instability to a phase with spiral and thus incommensurate spin correlations. We study the role of disorder in the spiral state within a continuum field theory and propose that the spin glass phase of cuprates is due to the proliferation of topological defects of a spiral distortion of the antiferromagnet order. Our theory explains straightforwardly the short range nature of the incommensurate correlations in this phase. We further show via a renormalization group calculation that the collinear O(3)/O(2) symmetry is unstable towards the formation of local non-collinear correlations in presence of disorder. A critical disorder strength is identified beyond which topological defect proliferate which leads to glassy behavior at low temperatures.

Keywords: *Spin glass, incommensurate phases, spiral correlations.*

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Electronic structure of the striped phase in $La_{2-x-y}Nd_ySr_xCuO_4$

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Using dynamical mean-field theory for the two-dimensional Hubbard model [1] we have previously demonstrated the stability of populated domain walls in static striped phases. In order to investigate in detail the electronic structure of $La_{2-x-y}Nd_ySr_xCuO_4$ [2] we use a realistic model Hamiltonian for populated domain walls in doped antiferromagnets. This allows us to derive analytic results for the momentum dependent single-particle gap induced by stripe order, and to study the consequences of dislocations and long range hopping matrix elements for the electronic structure in this class of materials.

Keywords: *Metallic stripes electronic structure pseudogap.*

References

[1] M. Fleck et al., Phys Rev. Lett. 84, 4962 (2000).
[2] X J. Zhou et al., Science 286, 268 (1999); A. Ino et al., cond-mat/0005370.

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