POSTER - I

(September 26, 2000)

| Charge, spin, lattice fluctuations and stripes theory | |
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| PI-1/ H. Breitzke Structure of the Cu NQR spectrum in Hg-1223 between 4.2 K and 145 K | PI-12/ S. Kato Phase diagram of stripe order in the extended Hubbard model |
| PI-2/ D. Di Castro Metallic stripes in Oxygen doped La ₂ CuO ₄ | PI-13/ H.V. Kruis Spin-charge separation in 1+1 dimensions as hidden order |
| PI-3 / A. T. Savici Spin freezing and superfluid density in superconducting Stage-4 La ₂ CuO _{4.12} | PI-14/ I. L. Novikov Topological model of the charge and magnetic stripes in La _{2-x} Me _x CuO ₄ (Me=Ba,Sr,Ca) |
| PI-4/P. Starowicz Low temperature magnetic order and the insulator to metal transition in the $Y_{1-x}Ca_xBa_2[Cu_{0.992}^{57}Fe_{0.008}]_3O_{6.1}$ system studied by Mössbauer spectroscopy | PI-15/ Z. Nussinov Topologically disordered stripe phases |
| PI-5/ K. B. Garg Polarised EXAFS study of in-plane distortion in a Pr-doped BSCCO (2212) single crystal | PI-16/ E. Piegari Superconducting fluctuations in a two-gap model for underdoped cuprates |
| PI-6 /Y. Horibe In-plane modulation and electronic phase separation in $La_2CuO_{4+\delta}$ | PI-17/ T. Sakai Mechanism of stripes in t-J model |
| PI-7/ M. Bosch Do shifting Bragg peaks of cuprate stripes reveal fractionally charged kinks? | PI-18/ G. Seibold <i>Fermi surface and photoemission lineshape of</i> <i>incommensurate CDW systems</i> |
| PI-8/ S. Caprara <i>Charge modulation and neutral-ionic transition in</i> <i>mixed-stack donor-acceptor crystals: a slave-boson</i> <i>approach</i> | PI-19 / G.A. Ummarino A model for charge stripes in the framework of Eliashberg theory |
| PI-9/ L. Capriotti <i>Commensurate versus incommensurate spin-</i> <i>ordering in the triangularHubbard model</i> | PI-20 / S. Varlamov Spin and charge density waves in layered cuprates |
| PI-10/ I. Eremin Theory for INS in high- T_c superconductors: doping and temperature dependence of the two characteristic frequencies | PI-21/ P. Wrobel Single-particle spectral weight in the antiferromagnetic stripe phase |
| PI-11/ B. Hosseinkhani Stripes as anyon Mott insulators | PI-22/ M. Zacher Stripes in doped antiferromagnets: single-particle spectral weight |

Structure of the Cu NQR spectrum in Hg-1223 between 4.2 K and 145 K

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An extremely low noise RF preamplifier cooled with liquid Helium has been developed and is used to perform Cu NQR measurements for Hg-1223 at temperatures from 4,2 K to 140 K. The Hg-1223 sample has $T_c = 134$ K. At temperatures from 4.2 K to 40 K the spectra are centred at 15 MHz with a spectral width of approximately 2 MHz, similar to the Cu NQR spectra of the other members of the HgBa₂Ca_{n-1}Cu_nO_{2n+2+δ} series. At temperatures T = 40 K and below, the structure of the Cu NQR spectra exhibit some features indicating an unresolved splitting but they can still be fitted quite well by a set of two ^{63/65}Cu lines one would expect for the 1223 structure. The spectra at 80 K and above clearly show a structure that can not be fitted suitable by a set of two ^{63/65}Cu lines. However, a fit with a set of four ^{63/65}Cu lines instead of two ^{63/65}Cu lines is in a good agreement with the experimental results. Furthermore, the spectra at 80 K, 85 K and 90 K show a strong variation in their structure with respect to each other. However, all three spectra can be fitted by a set of four ^{63/65}Cu lines. This behaviour indicates a structural change like the formation of a superstructure, as discussed for other high-T_c compounds, instead of a simple disorder in the crystal lattice.

Keywords: Cu NQR, Hg-1223, superstructure.

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Metallic stripes in oxygen doped La₂CuO₄

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We have investigated the charge ordering in an oxygen doped La_2CuO_4 . The competition of an electronic crystal of short strings of doped charges with a superconducting phase of long stripes was observed by x-ray diffraction using synchrotron radiation. The superconducting phase shows diffuse diffraction peaks with an incommensurate period of about 48 unit cells and stripes of length longer than 600 Å. The doped charges at the critical doping 1/8 are self trapped into a crystal of ordered strings of finite length of about 60 Å and a commensurate period of 4 lattice units.

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Spin freezing and superfluid density in superconducting Stage-4 $La_2CuO_{4.12}$

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Zero-field (ZF) and transverse-field (TF) μ SR measurements have been performed on a superconducting stage-4 La₂CuO_{4.12} crystal. Measurements were done on the same crystal sample used for neutron scattering by Lee et al [Phys. Rev. **B** 60 (1999) 3643], in which they found incommensurate magnetic peaks developing below T_C~T_N~42K. The Bessel function oscillating line shape of ZF data and the similar component in TF results are evidence of incommensurate spin modulation magnetic ordering.

As found by Savici et al [Physica B 289-290 (2000) 338], the static magnetic order below T_N produced internal magnetic field only at a finite fraction V_M of the muon sites; V_M increased gradually with decreasing temperature from 0% at $T \sim T_N$ to ~ 40 % at T_0 . This possibly indicates that the static spin freezing is confined to a limited volume of the specimen. The magnetic field penetration depth λ has been determined by using the signal from the remaining muon sites without large internal field.

We will report the analyses of ZF and TF results, to elucidate the interplay between magnetism and superconductivity in this system, and compare the results with the simulation of local field distribution corresponding to a few possible patterns of spin modulation.

Keywords: Superconductivity, Magnetic site fraction, µSR.

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Low temperature magnetic order and the insulator to metal transition in the Y_{1-x}Ca_xBa₂[Cu_{0.992}⁵⁷Fe_{0.008}]₃O_{6.1} system studied by Mössbauer spectroscopy

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Deoxygenated $Y_{1-x}Ca_xBa_2[Cu_{0.992}^{57}Fe_{0.008}]_3O_{6.1}$ compounds with the calcium content of x=0.05, 0.08, 0.12, 0.16, 0.2, 0.26 were prepared by the standard ceramic method what was followed by the reduction in argon. The system exhibit insulator to metal transition revealed by the measurements of electrical resistivity. The onset of superconductivity is visible in the sample with x=0.26.

The oxygen deficiency in the samples is advantageous for the interpretation of Mössbauer spectra because only two doublets corresponding to two chemically inequivalent positions appear at room temperature, whereas the spectra of samples with variable oxygen content would exhibit higher number of doublets.

The influence of doped holes on low temperature antiferromagnetic order is investigated. Low temperature spectra consist of two sextets with relative ratio changing with hole concentration. The sextets are broadened, their shape and temperature dependence indicate the existence of magnetic order fluctuations with the relaxation time slightly higher than the observation time of the method ~ 10^{-7} s. The first sextet is much broadened due to relaxation phenomena and more difficult to analyse. The hyperfine magnetic field in the second sextet decreases with Ca and holes doping. The line width of this sextet broadens with doping what may be interpreted as the increase of inhomogeneity or shortening of the relaxation time while the system is driven to the metallic and superconducting region.

Keywords: magnetic order; Mössbauer measurements; insulator-metal transition; Ca doping.

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Polarised EXAFS study of in-plane distortion in a Pr-doped BSCCO (2212) single crystal

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Polarised EXAFS measurements on the Cu K edge in a Pr-doped BSCCO (2212) insulating single crystal have been made at room temperature at the SRRC, Taiwan. Measurements have been confined to only the E//a, E//a^45 and E//b directions within the Cu-O₂ plane as most of the action is here. While the spectra in the E//a and E//b look very similar, the E//a^45 spectrum does look a little different. EXAFS analysis shows that Cu-O distances as well as the Debye Waller factor values in different directions turn out to be slightly different indicating a possibility of presence of some in-plane distortion. This appears to be very much in agreement with our XANES results on this system and our EXAFS results on Pr-doped YBCO (123) system reported earlier, which also indicate the presence of some distortion. Presence of Pr is speculated to be the cause for producing this distortion. This would be discussed in some detail taking into account the possibility that Pr, besides quenching holes, may also be displacing the in-plane oxygens.

Keywords: EXAFS, Pr-doped BSCCO(2212), distortion.

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In-plane modulation and electronic phase separation in La₂CuO₄₊

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The stripe structure is a consequence of a competition between the electronic phase separation and the Coulomb interaction between holes. If the Coulomb interaction is screened, the electronic phase separation should be realized. In La₂CuO_{4+δ}, it is expected that the Coulomb interaction can be screened by an in-plane modulation along the CuO₂ layer, which is due to extra oxygen ions. Hole-rich regions in the separation can be also detected as those with the LTT tilting of the CuO₆ octahedra. In order to examine the presence of the separation, we have investigated crystallographic features of a La₂CuO_{4.045} single crystal by transmission electron microscopy.

Specimens for the observation were prepared by an Ar-ion thinning of the single crystal at the temperature of liquid nitrogen, because the in-plane modulation can be stabilized, due to surface effect. In-situ observations were performed by using an H-800 electron microscope with a liquid He holder.

In electron diffraction patterns below about 110K, there were 100-type forbidden reflections, which are indicative of the appearance of the LTT-tilting region. In areas with a specimen thickness of about 50nm, the 100-type reflection has an ellipsoid shape elongated along the [110] direction. From an analysis of the elongated reflection, it is concluded that the two-dimensional electronic phase separation should occur below about 110K in La₂CuO_{4.045}.

Keywords: La₂CuO₄₊, electronic phase separation, transmission electron microscopy

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Do shifting Bragg peaks of cuprate stripes reveal fractionally charged kinks?

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The stripe phases found in correlated oxides can be viewed as an ordering of the solitons associated with doping the Mott-insulating state. Inspired by the recent observation that the stripes tilt away from the main axis of the crystal lattice in the regime x > 1/8, we propose that a new type of stripe phase is realized in the large doping regime. This new phase should be viewed as a doped version of the microscopically insulating x < 1/8 stripes. The topological excitations associated with the extra doping are fractionally charged kinks along the stripes whose motions make the stripe fluctuate.

We argue that the directional degree of freedom of the kinks might order, causing the stripe phase to tilt. Quantitative predictions follow for the doping dependence of the tilt angle, which in turn can be used to determine the fundamental charge quantum associated with the stripe phase.

Keywords: stripes, neutron-scattering, fractional charge.

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Charge modulation and neutral-ionic transition in mixed-stack donor-acceptor crystals: a slave-boson approach

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Crystals composed of alternated donor and acceptor atoms or molecules are often found either in the quasi neutral or in the ionised configuration as a result of the competition between ionic and covalency effects. A suitable slave-boson approach is introduced to describe the low-energy properties of these systems. A neutral-ionic transition is found within a mean-field approach, which is first-order when the Coulomb energy in the ionized phase is taken into account. The results are compared with real-space renormalization-group calculations.

Keywords: Charge modulation, neutral-ionic transition.

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Commensurate versus incommensurate spin-ordering in the triangular Hubbard model

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We investigate the metal-insulator transition in the half-filled Hubbard model on a twodimensional triangular lattice using both the Kotliar-Ruckenstein slave-boson technique, and exact numerical diagonalization of finite clusters. Contrary to the case of the square lattice, where the perfect nesting of the Fermi surface leads to a metal-insulator transition at arbitrarily small values of U, always accompanied by antiferromagnetic ordering, on the triangular lattice, due to the lack of perfect nesting, the transition takes place at a finite value of U, and frustration induces a non-trivial competition among different magnetic phases. Indeed, within the mean-field approximation in the slave-boson approach, as the interaction grows the paramagnetic metal turns into a metallic phase with incommensurate spiral ordering. Increasing further the interaction, a linear spindensity-wave is stabilized, and finally for strong coupling the latter phase undergoes a first-order transition towards an antiferromagnetic insulator.

Keywords: Incommensurate magnetic ordering, metal-insulator transition.

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Theory for INS in high-T_c superconductors: doping and temperature dependence of the two characteristic frequencies

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Inelastic neutron scattering (INS) below T_c reveals two characteristic frequencies which are attributed to magnetic coherence [1] and the so-called resonance peak [2]. Calculating the spin susceptibility within RPA and using the one-band Hubbard Hamiltonian we determine the doping and temperature dependence of these two characteristic frequencies ω_0 and ω_{res} at which $\chi''(\mathbf{q}, \omega)$ and the resonance peak appear, respectively. We show that only for *d*-wave symmetry pairing both ω_0 and ω_{res} are present, however for *s*-wave pairing only ω_{res} occur. We further present results for the doping dependence of ω_{res}/k_BT_c . Bilayer effects on nesting properties as well as the momentum dependence of ω_0 are also investigated. It is remarkable that for a spin-fluctuation-induced pairing both frequencies can be explained in a good agreement with experiment within such a unified theory.

Keywords: *spin-fluctuation-induced pairing mechanism, inelastic neutron scattering, resonance peak, magnetic coherence.*

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Stripes as anyon Mott insulators

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Although there is a growing body of evidence for the existence of stripes in high- T_c cuprate superconductors, their precise microscopic nature is still subject to debate. After all, stripes emerge on the same scale as the superconductivity. We focus on the possibility of hidden time-reversal symmetry breaking in the spin system (flux phases) and within a strong coupling framework we find a possible stripe-like instability which corresponds with an anyon Mott-insulator.

Keywords: Stripes, anyon statistics, flux-phases.

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Phase diagram of stripe order in the extended Hubbard model

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We investigate the temperature dependence of stripe order in the extended Hubbard model with a nearest neighbor Coulomb repulsion (V) on the square lattice within a mean field approximation. For filling n=0.8 and U/t=8.0, the diagonal stripe state is stable against small V at low temperature. For larger V and low temperature, a striped charge-density-wave state with antiferromagnetic order becomes stable. We also discuss the effect of the spin fluctuation on the temperature dependence of the stripe order.

Keyword: stripe order extended Hubbard model, electronic structure.

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Spin-charge separation in 1+1 dimensions as hidden order

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We propose that ordered stripe phases should be viewed as 2+1 dimensional decompactifications of the spin-charge separation phenomenon occurring in 1+1 dimensions. We revisit the doped Hubbard chain, and recast the familiar spin-charge separation as a manifestation of a hidden global Z_2 symmetry: every time a hole is encountered it is squeezed out of the chain and, consequently, the remaining sites toggle from one sublattice to the other. Here, we compute the correlation functions of these "squeezing operators" and argue for a symmetry principle of great generality.

Keywords: stripes, spin-charge separation, symmetry, Hubbard model.

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Topological model of the charge and magnetic stripes in La_{2-x}Me_xCuO₄ (Me=Ba,Sr,Ca)

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In the paper the model of the charge ordering and magnetic ordering in $La_{2-x}Me_xCuO_4$ is suggested. The model assumes that the spin polarons appeare in the compound La_2CuO_4 at the doping. The La substitution leads to the hole appearance in the p-band of the oxygen in CuO_2 plane. This carrier is in the medium of the magnetic moments of Cu_{+2} ions and orientates the magnetic moments of the neighboring Cu_{+2} ions in antiparallel to it's own moment. At the temperature drop the regions between polarons are to have antiferromagnetic ordering. The polaron structure is in accordance with the medium structure to decrease the system's energy, because the internal polaron structure is the antiferromagnetic structure. Also the polarons are mobile, therefore they occupy the special positions in the antiferromagnetic structure of the medium. These reasons lead to fact that the spin polarons are arranged in the space, forming the charge and magnetic stripes.

It is obtained that the wave vector of the charge superlattice $Q_s = 0.4$ [p,p] and the wave vector of the magnetic superlattice $Q_M = 0.2$ [p,p] at x = 0.1. At unique doping x = 1/8 $Q_M=0.125$ [p,0] and $Q_s = 0.25$ [p,0]. The structure of the stripe superlattices disintegrates at x>0.25. At 1/8<x £ 0.25 the stripe structure is not changed.

Keywords: high temperature superconductivity, La-based compound, spin polaron, superlattice.

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Topologically disordered stripe phases

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As a sequel to statements regarding the ordered stripe phases as manifestations of decompactified versions of 1+1 dimensional spin-charge separation (see the poster by H. V. Kruis *et al.*), here we examine spin and charge excitations in the presence of defects. Charge (stripe) dislocations frustrate spin-charge separation. We formulate this frustration in geometric terms: Charge dislocations act as sources of gravity for the spin texture. We find that non-trivial Berry phases emerge in certain instances. In the continuum limit, we map the *ab* plane onto the complex plane and examine the resulting analytical structure for the various disordered stripe phases. We also extend some of the results introduced in H. Kleinert's treatise on stresses and defects in classical elasticity to the quantum case (2+1 dimensional) and compute correlation functions in various disordered phases.

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Keywords: stripes, spin-charge separation, dislocations, Berry phases.

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Superconducting fluctuations in a two-gap model for underdoped cuprates

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A key feature of underdoped cuprates is the presence of a pseudogap in the single particle excitation spectrum above T_c. One possibility is that the pseudogap opening is due to preformed pairs without phase coherence, destroyed by strong superconducting fluctuations. According to the Stripe-Quantum Critical Point scenario for high-T_c superconductors [1,2] the pairing at high temperature is mediated by a strong momentum dependent effective interaction which gives rise to d-wave gap and pseudogap. Moreover the band structure of the cuprates is characterized by fermionic states around the M points $[(0, \pm \pi), (\pm \pi, 0)]$ with low Fermi velocity ("hot spots") and "cold" states, in the arcs of FS about the nodal points, with larger dispersions. We describe the strong momentum dependent electronic properties of the cuprates in terms of a two gap model [3]. In order to investigate the role of fluctuations we start within a standard Ginzburg-Landau approach and we find a bifurcation between T^{*}, the mean field critical temperature, and T_c, the critical temperature renormalized by superconducting fluctuations, as the anisotropy of the interaction is increased. In the extreme strong coupling limit for the hot particles we recover the results of the mixed boson-fermion models [4,5], proposed for the heavily underdoped cuprates. The BCS-BE crossover induced by the increasing strength of the coupling of the hot particles is also followed and quantified by zero temperature mean field calculations of the gap and the chemical potential.

Keywords: superconducting fluctuations, interaction anisotropy, psuedogap, QCP.

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Mechanism of stripes in t-J model

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We consider a possible mechanism of the stripe order in the high-temperature cuprate superconductors, based on the concept of the phase separation in the t-J model. We also calculate some hole-hole correlation functions of finite clusters of the t-J model using the numerical diagonalization, to examine it.

Keywords : stripe, high-Tc cuprate, t-J model.

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Fermi surface and photoemission lineshape of incommensurate CDW systems

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The concept of frustrated phase separation is applied to investigate its consequences for the electronic structure of the high T_c cuprates. The resulting incommensurate charge density wave (CDW) scattering is most effective in creating local gaps in k-space when the scattering vector connects states with equal energy. Starting from an open Fermi surface we find that the resulting CDW is oriented along the (1,0)- and (or) (0,1)direction which allows for a purely one-dimensional or a two-dimensional eggbox type charge modulation. In both cases the van Hove singularities are substantially enhanced and the spectral weight of Fermi surface states near the M-points tends to be suppressed. Remarkably, a leading edge gap arises near these points which, in the eggbox case leaves finite arcs of the Fermi surface gapless. In addition the lineshape in the superconductiong state around the M-points agrees well with experimental data.

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A model for charge stripes in the framework of Eliashberg theory

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In the present work, we extend to the strong electron-boson-coupling regime an idea of V.V. Moshchalkov and V.A. Ivanov (cond-mat 9912091) who allowed for an angular dependence of the coupling in the BCS framework. This dependence is assumed to model the existence of a stripe phase in the electronic properties. It is possible to vary the relative weight of the bosonic contribution and of the Coulomb-repulsion contribution to the coupling ($\lambda_P(\phi)$ and $\lambda_C(\phi)$, respectively) in order to have a remarkable enhancement of T_c .

In the simplest case one can assume that in the $\phi = 0$ direction (parallel to the stripes) only the boson-mediated coupling between quasiparticles is active, while in the direction $\phi = .../2$ (perpendicular to the stripes) the Coulomb repulsion is the only contribution. More complex situations are also possible, where the $(\lambda_P(\phi) \text{ and } \lambda_C(\phi) \text{ dependencies are not so simple and the two components have a modulation in energy. By solving in direct way the modified Eliashberg equations, we examine some of these possibilities and calculate their effect on the values of <math>T_c$ and Δ , and on the behaviour of the quasiparticle density of states. Finally, we investigate whether this model can explain some other phenomena, such as, for example, the presence of a pseudogap in the high- T_c superconductors.

Keywords: Eliashberg theory; stripes; strong electron-boson coupling

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Spin and charge density waves in layered cuprates

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Self-consistent calculations of spin (charge) density wave (SDW/CDW) with s+id order parameters have been performed for bilayered cuprates on the basis of a singlet correlated band model. The smooth development of the pseudogap formation temperature is explained from underdoped to overdoped states and the Fourier amplitudes $\langle S_q \rangle$ (spin) and $\langle e_q \rangle$ (charge) modulations have been calculated (cond-mat/9908297). The CDW frequencies $\omega(q)$ have been calculated. A clear zero-level crossing is found along $(0,\pi)$ to (π,π) direction, but no such crossing is detected along (0,0) to $(0,\pi)$ direction.

Keywords: spin (charge) density wave, pseudogap, spin (charge) susceptibility.

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Single-particle spectral weight in the antiferromagnetic stripe phase

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Recent angle-resolved photoemission (ARPES) studies of $La_{2x}Sr_xCuO_4$ (LSCO) provide a new piece of information on the evolution of the electronic structure in cuprate systems with doping. Using the spin polaron approach based on the string picture we study the motion of a single mobile hole in the stripe phase of the doped antiferromagnet. The holes within the stripes are taken to be static, the undoped antiferromagnetic domains between hole stripes are assumed to have alternating staggered magnetization, as is suggested by neutron scattering experiments. The system is described by the t-t'-t"-J model with realistic parameters and we compute the single particle spectral density. Theoretical spectra and results of measurements performed at the hole concentration 1/8 show reasonable agreement. In both cases we observe, along the directions $(0,0) \rightarrow (\pi,0)$ and $(0,0) \rightarrow (0 \pi)$, the 'splitting' of the spectrum and formation of new low energy states around $(\pi, 0)$. This splitting is much less pronounced in the direction $(0,\pi) \to (\pi,\pi)$. The spectra along the direction $(\pi, 0) \rightarrow (\pi, \pi)$ are very broad. That prevents assignment of a band for some range of \mathbf{k} points in that direction. Finally, the spectra along the direction $(0,0) \rightarrow (\pi,\pi)$ are very broad and it is also practically impossible to distinguish any sharp band.

Keywords: theory, stripes, angle-resolved photoemission, t-t'-t"-J model.

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Recent photoemission (ARPES) experiments on cuprate superconductors provide important guidelines for a theory of electronic excitations in the stripe phase. Using a cluster perturbation theory, where short-distance effects are accounted for by exact cluster diagonalization and long-distance effects by perturbation (in the hopping), we calculate the single-particle Green's function for a striped \tjm model. The data obtained quantitatively reproduce salient (ARPES-) features and may serve to rule out "bond-centered" in favor of "site-centered" stripes.

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