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Local structure of the charge ordered $La_{0.5}Ca_{0.5}MnO_3$ manganite

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Local lattice of the charge ordered $La_{0.5}Ca_{0.5}MnO_3$ has been studied by high k-resolution Mn K-edge extended x-ray absorption fine structure (EXAFS) measurements aiming to obtain the quantitative distortions of the MnO_6 octahedra and to explore how these distortions are associated with the charge ordering in the system. The measurements were made using fluorescence detection method to isolate the partial cross-section only due to transitions from the Mn 1s core states. We find that the MnO_6 octahedra are largely distorted at low temperature in the commensurate phase, the distortions get reduced at higher temperature while the system is in the incommensurate phase. The results show coexistence of two types of distortions related with the polaron ordering.

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Crystallographic features of the transitional state in $La_{1-x}Sr_xTiO_3$

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$LaTiO_3$ is one of the Mott insulators in 3d transition-metal oxides. When La is substituted by Sr, the insulator-to-metal (electronic phase) change occurs around x=0.05. The transitional state can be expected around this composition. In spite of previous works, the existence and crystallographic features of the transitional state have been unclear. Then we have examined crystallographic features of the transitional state in $La_{1-x}Sr_xTiO_3$ by transmission electron microscopy.
$La_{1-x}Sr_xTiO_3$ samples around x=0.05 were prepared by an arc-melting method in $Ar/20\%H_2$ atmosphere. Specimens for transmission-electron-microscopy observation were thin films obtained by Ar-ion thinning. The observation was mainly performed at room temperature by means of H-800 and H-9000 electron microscopes.
In electron diffraction patterns taken from $La_{0.95}Sr_{0.05}TiO_3$ specimens, there exist fundamental reflection spots at room temperature, which are forbidden for the *Pbnm* structure of the metallic phase in $0.05<x\leq0.4$. An extinction rule of the forbidden reflection spots indicates that the Jahn-Teller distortion of a TiO_6 octahedron is involved in the crystal structure of the transitional state. We then examined features of a microstructure in the specimen. In dark field images from the specimen, a number of spotty contrasts with a size of about 40Å were observed in each variant of the metallic *Pbnm* structure. This implies that regions with the static Jahn-Teller distortion is locally distributed in the metallic *Pbnm* matrix. In other words, the transitional state in $La_{1-x}Sr_xTiO_3$ can be understood to be characterized by electronic phase separation.

Keywords*: $La_{1-x}Sr_xTiO_3$, perovskite structure, transitional state, Jahn-Teller distortion, transmission electron microscopy.*

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High-resolution high energy X-ray diffraction studies of charge ordering in CMR manganites and nickelates

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High-resolution, high-energy, x-ray diffraction results are presented for the study of weak charge ordering phenomenon. Traditional high-resolution x-ray diffraction (E ≈ 10 keV) measurements are only sensitive to the near surface region, while bulk-sensitive neutron scattering studies suffer from relatively poor instrumental resolution and the need for relatively large sample sizes. X-rays, which are sensitive to the charge distribution in a solid, are an ideal tool for the study of weak superlattice reflections due to charge ordering. By utilizing x-rays in the 100 keV region the dramatic increase in the penetration depth allows for both bulk-sensitive and high- resolution measurements to be made. We will present the results taken on the high- energy, triple-axis diffractometer at ID15A, ESRF on both manganite and nickelate systems. The strontium doped La_2NiO_4 system is a prototypical system in the understanding of strong electron-phonon coupling, and the resultant effects on material properties. At doping levels of 1/3 and _commensurate charge modulations are observed indicating real-space charge stripes. We have measured the correlation lengths of these charge stripes using both 100 keV x-rays and 10 keV x-rays. In comparing our results we have observed that the charge stripes appear to be well correlated in the near-surface region with correlation lengths $\xi \approx 300$ Å. However, our bulk sensitive measurements show that the charge stripes appear in a possible stripe glass phase with a correlation length of only $\xi \approx 55$Å. This result agrees with previously published neutron scattering studies. Our measurements on the 3D charge ordering manganite system $Nd_{0.5}Sr_{0.5}MnO_3$ show that the charge ordering occurs in the bulk of the sample with correlation lengths $\xi > 700$Å in contrast to our nickelate results. Our results are the first comparison between the bulk and near surface region in these charge ordering systems.

Keywords: *Stripes in a doped antiferromagnetic lattice, fluctuations in striped phases, CMR, High Energy X-ray scattering*.

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Crystallographic orientation mapping with electron back scattered diffraction technique in $(Bi,Pb)_2Sr_2Ca_2Cu_3O_{10+x}$ superconductor tapes

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It is believed that the grain boundaries act as the weak-link to limit the critical current density in the bulk high-T_c superconductors and the weak-link problem can be greatly reduced by elimination or minimization of the large-angle grain boundaries. It has been reported that the distribution of the current paths in $(Bi,Pb)_2Sr_2Ca_2Cu_3O_{10+x}$ (Bi2223) superconductor tapes presents a parabolic relationship in the transverse cross-section of the tapes and it was proposed to strongly depend on the local crystallographic orientation distribution of the Bi2223 oxides. However, the local crystallographic orientation distribution of $(Bi,Pb)_2Sr_2Ca_2Cu_3O_{10+x}$ crystals in three dimensions has not been experimentally determined yet. In present work, Electron Backscatter Diffraction technique was employed to map the crystallographic orientation distribution, determine the misorientation of grain boundaries and also map the misorientation distribution in Bi2223 superconductor tapes. The results indicate that the c-axes of almost Bi2223 grains were perpendicular to the rolling plan, while the 40% of a/b axes and 45% of [110] of Bi2223 grains were aligned along the rolling direction of the Bi2223 superconductor tapes after heavy mechanical deformation and heat treatment. From the map of the misorientation distribution, it can be observed that the low angle grain boundary are the main boundaries in Bi2223 superconductor tapes even though there were a number of 45° misorientation boundaries. The low angle boundaries distributed on the side zones of the EBSD measurement areas while the boundaries with 45° misorientation gathered in the middle zone of the measurement areas along the rolling direction. The understanding of the relationship between the local crystallographic orientation distribution, the boundary misorientation distribution and the fabrication parameters could be used to optimize the fabrication techniques, thus significantly increasing the critical current density.

Keywords*: Electron backscatter diffraction, local crystallographic orientation distribution and misorientation of grain boundaries.*

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Optical Anisotropic Properties of $La_{8-x}Sr_xCu_8O_{20}$

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In this work we present the optical properties of the oxygen-deficient perovskite cuprate $La_{8-x}Sr_xCu_8O_{20}$ (8820) with tetragonal crystal symmetry P4/mbm.
In this material transport and magnetic properties present an anomaly anisotropic behavior near a temperature $T^* \cong 150K$. These anomalies are particularly evident for doping near x=1.56 while they disappear for x=2.24. We measured the optical conductivity $\sigma(\omega)$ on two single crystal 8820 material with x=1.56 and x=2.24 from the far infrared (10meV) up to Ultra-Violet (3eV) for different temperatures and with polarized light along the crystal axes. $\sigma(\omega)$ shows an anisotropic behavior with a temperature dependence correlated to the observed anomalies in the transport properties.

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Polaron binding energy in A MnO_3 as a function of the A site ionic size by photoinduced IR absorption

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We observe broadening and a ~44% increase of the photoinduced midinfrared absorption polaron peak energy when La^{3+} is replaced with smaller Nd^{3+} in $AMnO_3$ (A=La,Nd). Due to the absence of any concurrent large frequency shifts of the observed PI phonon bleaching peaks and the Brillouin-zone-center internal perovskite phonon modes measured by Raman and infrared spectroscopy, the polaron peak energy shift is attributed to an increase of the electron phonon coupling constant with decreasing ionic radius $<r_A>$ on the perovskite A site. This indicates that the dynamical lattice effects strongly contribute to the electronic band narrowing with decreasing $<r_A>$ in giant magnetoresistance manganites.

Keywords*: giant magnetoresistance manganites, polarons, electron-phonon coupling, infrared spectroscopy*

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The surface impedance of Sr_2RuO_4

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The microwave surface impedance, $Z_s=R_s+iX_s$, of high-purity Sr_2RuO_4 single crystals with transition temperatures T_c=1.42-1.47 K has been measured at 10, 15 and 21 GHz using a hollow sapphire resonator technique. Above ~10 K, Z_s is well described by the classical skin effect with a strongly temperature dependent DC conductivity. Below 10 K, the quasiparticle relaxation rate $1/\tau$ becomes comparable with the microwave frequency, resulting in frequency dependent corrections to both the normal and superconducting state microwave properties. Below T_c, R_s decreases monotonically, while X_s initially increases and peaks at a frequency and purity dependent temperature. The data can be described by a two-fluid model with a Drude-like quasiparticle conductivity and a constant relaxation time $\tau \sim 10^{-11}$ s. The derived normal fraction $X_N(T)$ extrapolates almost linearly to a finite zero-temperature value, while the derived London penetration depth $\lambda \propto (1-X_N)^{-1/2}$ displays a quadratic temperature dependence at our lowest temperatures ~0.4K.

Keywords: *Surface Impedance, Sr_2RuO_4, London penetration depth*.

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Stripe conductivity in incommensurate charge ordered phase of $La_{1.775}Sr_{0.225}NiO_4$

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We present results from Raman light scattering (RLS) and optical conductivity measurements on a single crystal of $La_{1-x}Sr_xNiO_4$ with x=0.225, which was previously characterized by neutron[1] and x-ray[2] diffraction. The stripe order in this sample is incommensurate, and the hole density per Ni site along a stripe is significantly less than 1 (in contrast to x=1/3, where the density is exactly 1). The extra phonon peaks induced by stripe order can be understood in terms of the energies of phonons that occur at the charge-order wave vector, Q_c. We observe a strong Fano antiresonance in the optical conductivity at an energy well below the charge pseudo-gap, which is 0.105 eV at 10~K. From a careful analysis of the phonon spectra, we conclude that the energy of the antiresonance corresponds to Ni-O bond stretching motions along the stripes. It follows that the antiresonance, which results from electron-phonon coupling, provides strong evidence for finite conductivity along the stripes, at least at optical-phonon frequencies. Low-temperature RLS spectra in the x'y'-geometry reveal 2-magnon scattering bands at 739 and 1130cm^{-1}, frequencies remarkably similar to those[3,4] in $La_{5/3}Sr_{1/3}NiO_4$.

Keywords: *stripe ordering, Raman light scattering, optical conductivity measurements, $La_{1-x}Sr_xNiO_4$.*

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Role of polarons and stripes in the optical conductivity of $La_2NiO_{4.11}$

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In recent years, the Ln_2MO_4 (M = Cu, Ni) type oxide structure has attracted attention because it is the prototype of high-T_c superconducting cuprates which are derived from this structure. These compounds which are two-dimensional antiferromagnetics may be hole-doped by two methods: Sr-doping onto the La-site or insertion of additional oxygen atoms (O_i) between LaO layers. Alkaline earth element doping or introduction of interstitial oxygens confers to the materials electronic and magnetic properties that appear poorly. Even if these compounds are electric conductors, their low carrier concentration does not rank them as conventional metals. Here, the equivalent of the plasma edge stays in the near infrared. Another key point that makes a decisive difference with conventional metal is the incomplete screening. Charge carriers do interact and polar phonons are incompletely screened. As a result, the polaron concept is expected to replace the conventional metal concept. Another complication comes from the possible "phase separation" phenomena and the possible organization of charges and spins in "stripes". The direct or indirect indications about their formation are summarized in what follows in connection with other observations. Then, the temperature dependence of infrared reflectivity measurements in a $La_2NiO_{4.11}$ single crystal will be reported and analyzed in terms of optical conductivity. This spectral function, and its temperature dependence, will be shown to have little in common with conventional metals but rather to fit criteria expected for a polaronic conductor. The reflectivity will be fitted with a model allowing to discriminate between itinerant and trapped polarons.

Keywords: *Stripe, polarons, nickelate.*

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Anomalous magnetoresistance of borocarbide superconductor YNi_2B_2C

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We have carried out the measurements of the magnetoresistance (MR) of YNi_2B_2C single crystals (T_c = 15.3 K and H_{c2}(5.5 K) ~ 4.7 T) in a wide range of temperature and magnetic field, T_c+1 < T < T_c+145 K and 0 < H < 8 T. In the normal state, the in-plane magnetoresistance (MR), $\Delta\rho(H, T) = \rho(H, T) - \rho(0, T)$, changes from negative to positive as the temperature decreases. A pronounced sign-reversal is observed at T = 80 K with H = 4 T. A negative MR supports the presence of magnetically-related scattering and could signify considerable suppression of the spin fluctuations most likely associated with nearly magnetic metals in the presence of an external field. Such novel behavior reveals the possibility of pseudo-gap formation, which plays the role of unconventional superconducting mechanism, as indicated by the recent ^{11}B and ^{13}C NMR studies. Our results are also in quantitative agreement with the short-range magnetic moment dependence upon temperature and applied field.

Keywords: *Borocarbide Superconductor, Magnetoresistance, Pseudo-gap, Spin fluctuations.*

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Vortex pinning dependence of the critical current density in $YBa_2Cu_3O_{7-\delta}$ thin films

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We have studied the J-E characteristic in order to investigate the critical current density J_c behavior in high quality c-axis up $YBa_2Cu_3O_{7-\delta}$ thin film. J_c was measured for various magnetic field, temperature values, and θ (the angle between the magnetic field and the c-axis) using the standard four probe method. The sample was prepared by the laser ablation method and deposited onto $SrTiO_3$ substrate. In zero magnetic field the sample exhibit vanishing temperature at 90 K. To avoid the heating phenomena, the pulsed current technique was used. Our results show that the maximum of the critical current density was obtained for the configuration where the applied magnetic field is parallel to the ab planes. The angular dependence of the critical current density shows the existence of the intrinsic pinning between the CuO_2 layers for H parallel to the ab planes and the extrinsic pinning in the case where the magnetic field is parallel to the c axis.
A strong increase of the critical current density is observed when the flux lines are aligned similarly to the ab planes (θ = 90°), an other growth is also observed when the magnetic field is perpendicular to the ab planes (θ = 0°).
We have analyzed our results in the framework of the intrinsic flux pinning model proposed by Tachiki and Takahachi. This model reproduces well our results in a high magnetic field region (10 T). For the lower value of the field 0,3 T, the results disagreed with this model when θ approach 90°. The thermally activated flux motion plays a prominent role and can explain in large part the magnitude of the critical current density.

Keywords: *critical current density, flux lines, layers, intrinsic pinning, extrinsic pinning.*

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Interplay between transport, magnetic, and structural properties of Mn-perovskites with variable doping level

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Mn-perovskites of the type $RE_{1-x}D_xMnO_3$ (RE: rare earth, D: divalent dopant) exhibit a rich variety of phenomena like colossal negative magnetoresistance (CMR), orbital order, charge or-der and charge stripes. We focus on the negative magnetoresistivity and the Hall effect of man-ganites with intermediate doping ($x \approx 0.5$) and compare this to under- and overdoped materials ($x = 0.3$ and $x = 0.67$). The resulting carrier type, i. e. holes, electrons, or superpositions of both, depends on the band filling. The temperature variation of the carrier density (minimum at the Curie point) is related to the transition from polaron hopping to iterant-like transport upon ferro-magnetic spin alignment. We therefore describe the CMR effect in the paramagnetic-semicon-ducting regime (and tentatively in the disordered ferromagnetic phase) by the spin-dependent hopping model: the barrier for charge transport between regions of short-range ferromagnetic order is hereby controlled by their mutual spin-misorientation. For manganites in the strongly underdoped regime ($x < 0.15$) an additional mechanism for carrier localization˚is present: the Jahn-Teller distortions induced by Mn^{3+} form a regular pattern with preferential orientation of the electron orbitals. The transition from orbital disorder (high temperatures) to orbital order (low temperatures) weakens ferromagnetic correlations and enhances the resistivity by restricting the carrier movement to definite directions within the orbitally ordered network.

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Keywords*: colossal negative magnetoresistivity, orbital order, Hall effect.*

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Extended $d_{x^2-y^2}$-wave gap anisotropy in high-T_c superconductors

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Several experiments evidenced a remarkable structure in the **k**-dependence of the *d*-wave superconducting order parameter of underdoped high-T_c cuprates near a node. Here, it is pointed out that deviations from a simple *d*-wave superconducting spectrum induce corrections to the superconducting DOS and the low-T asymptotic behavior of various electronic properties in the superconducting state at intermediate energies. Such corrections depend on the theoretical scheme employed to describe the deviations.

Keywords*: d-wave superconductivity, unconventional models, electronic properties.*

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Stability of d-wave superconductivity in the t-J model

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We investigate the stability of the d-wave superconductivity in the t—J model by using a recently developed technique which allows to apply statistically few Lanczos steps to a given wavefunction even for large system size. Our statistical Lanczos algorithm has been extensively tested on a small 18-site cluster where many ea;act Lanczos steps are possible. In this case, at doping $\delta \sim 10\%$ the BCS wavefunction represents a very good initial state to achieve extremely accurate energies and correlation functions with few Lanczos iterations. For large size ($L \sim 100$) the behavior looks similar, i.e. the d-wave order parameter p_d is weakly affected by a couple of Lanczos iterations in the low-doping region ($\delta \sim 10\%$), whereas the energy is remarkably lowered. By contrast, at large doping Pd iS strongly suppressed, suggesting that also for large size a couple of Lanczos steps are really effective for this correlation function. These results strongly support the existence of off-diagonal long-range d-wave superconducting order in the two-dimensional t—J model in the low-doping region.

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Pairing, crossover and inhomogeneous superconductivity in the attractive Hubbard model

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The one- and two-dimensional attractive Hubbard model in the presence of magnetic field *h* are studied in a wide range of coupling strength *U*, temperature and band filling *n* by using of the generalized self-consistent field (GSCF) approach with renormalized chemical potential. Pairing, the smooth crossover from the BCS regime into the Bose condensation state and the inhomogeneous superconductivity with the non-uniform order parameter are investigated. The excitation spectrum, the momentum distribution function and thermodynamic properties, including the number of double occupied sites, the kinetic energy, and the chemical potential, are calculated. The numerical calculations are found in a good numerical agreement with the Bethe-ansatz results and quantum Monte-Carlo calculations in a wide range of system parameters *U*, *n* and *h*. The GSCF theory correctly displays the separation of the energy gap from the order parameter (crossover) as *n* or *U* decrease. The number of double occupied sites and the bound electron pairs n_{pair} are calculated and we found a simple relationship between the order parameter and n_{pair}, valid for the arbitrary *U* and all *n*. The developed GSCF approach in magnetic field suggests a smooth transition into the inhomogeneous superconducting state.

Keywords: *phase diagram, crossover, inhomogeneous superconductivity, BCS-BC crossover, magnetic transitions.*

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Electronic theory for electron-doped cuprate superconductors: *d*-wave superconductivity and the phase diagram

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Using as a model the 2D-Hubbard Hamiltonian we calculate various basic properties of electron-doped cuprate superconductors like $Nd_{2-x}Ce_xCuO_4$ (NCCO)and $Pr_{2-x}Ce_xCuO_4$ (PCCO) for a spin-fluctuation-induced pairing mechanism. Most importantly we find a narrow range of superconductivity and like for hole-doped cuprates $d_{x^2-y^2}$ – symmetry for the superconducting order parameter [1]. Recently, phase sensitive measurements [2] indeed found $d_{x^2-y^2}$ –wave symmetry in optimally doped NCCO and PCCO. The superconducting transition temperatures $T_c(x)$ for various electron doping concentrations x are calculated to be much smaller than for hole-doped cuprates due to a different energy dispersion and a flat band well below the Fermi level. We also discuss the possible occurrence of a normal-state pseudogap and the effect of lattice disorder, which may sensitively distort the symmetry $d_{x^2-y^2}$ via electron-phonon interaction.

Keywords: *high-temperature superconductivity, spin-fluctuation-induced pairing mechanism, electron-doped cuprates.*

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Collective-mode contribution to the superfluid density depletion in d-wave superconductors

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The role of the collective modes in determing the low-temperature properties of a d-wave superconductor is an intriguing issue both from the theoretical and the experimental point of view. Recent measurements in cuprate superconductors seem to indicate that other excitations besides the quasiparticles may be responsible for the depletion of the superfluid density at finite temperature. We analyze the effect of phase-fluctuations of the superconducting order parameter on the superfluid density at low temperature, discussing the problem of the derivation of a phase-only effective action and the peculiar role of dissipation in a d-wave superconductor.

Keywords: *Superfluid density; phase fluctuations; d-wave superconductors.*

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Exact ground-state properties and phase transitions within one-dimensional Hubbard model in magnetic field

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The ground-state phase diagram and the critical behavior of the one-dimensional Hubbard model, both attractive and repulsive, are investigated numerically in the entire parameter space of electron concentration n, interaction strength U and magnetic field h. The magnetic ground-state properties, including the spin and charge susceptibilities, and the spin and charge energy gaps are calculated as functions of U, h and n. It is found that the spin (magnetic) susceptibility at half-filling changes discontinuously as U_0 and is enhanced by electron repulsion in comparison with that of the non-interacting case. The compressibility decreases with n at $U < 0$ and shows non-monotonous behavior with dramatic increase while $U > 0$. The critical behavior near the onset of magnetization and magnetic saturation is also analyzed. Our numerical results are in full agreement with calculated analytical expressions at strong magnetic field near the saturation, empty band filling, strong and weak interaction limits, the previous numerical studies for $h = 0$ and provide a solid ground for the evaluation of the different self-consistent theories.

Keywords: *Hubbard model; exact solution; superconductivity; magnetic transitions; phase diagram.*

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Autolocalization of electrons and structure of crystals

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It has been shown by us earlier [1,2] that autolocalization of electrons caused by electron-phonon interaction changes essentially structure of the crystal electronic bands. In certain conditions, in particular, at temperature lower than some critical one some band states of electrons turn out to be forbidden. Simultaneously macroscopic number of electrons can appear in autolocalized states. At such conditions the electronic density structure in the crystal differs essentially from one predicted by the band theory. As a consequence the observable structure of the crystal lattice will not correspond to structure used in band calculations. If some part of valence electrons is autolocalized then localized and delocalized electrons turn out to belong to the same band with corresponding symmetry of the Bloch wave function amplitudes (which form wave packets of autolocalized electrons). Therefore, autolocalization of valence electrons apparently changes the crystal symmetry only by freezing normal lattice vibrations participating in the autolocalization with generation of generally incommensurate structure. Autolocalization of electrons from the conduction band can essentially change the elementary cell structure by redistribution of the electronic density inside the elementary cell.

Keywords: *autolocalization, electron-phonon coupling, crystal symmetry*.

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Stripe stability in doped antiferromagnets

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In the framework of the t-J we construct localized spin polaron states for some different original hole arrangements in different spin backgrounds. According to the so-called string picture we assume that local destruction in the magnetic structure caused by hole motion tends to localize holes and acts on them as a kind of well potential. Previously, after considering processes that give rise to tunneling between holes, this method turned out to be very efficient for description of spectral properties and hole binding in weakly doped antiferromagnets. This time, we apply it to the case of the hole concentration 1/8 for which stripes are observed. We consider several possible configurations, which represent:

1. holes homogeneously distributed in the antiferromagnetic background,
2. hole pairs (which correspond to spin bipolarons) homogeneously distributed in the antiferromagnetic background,
3. hole pairs which form the stripe structure in the perfect antiferromagnetic background,
4. and eventually holes in stripes which separate antiferromagnetic domains with alternating direction of the staggered magnetization.

Spin polarons are constructed by means of some computer algebra. It turns out that lowest eigenenergy has a state that represents a single hole polaron in the case 4. The calculation demonstrates how the hole uses antiferromagnetic bonds, which must form at the border between antiphase antiferromagnetic domains to lower the energy. Binding of holes in stripes is disfavored. Bipolarons that form stripes in the perfect antiferromagnetic background have higher energy than homogeneously distributed holes.

Keywords: *theory, stripe stability, t-J model.*

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