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SUPERCONDUCTIVITY

Pseudogap Formation in Copper Oxide Superconductors with Inclusion of Spin and Charge Fluctuations

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Abstract—The influence of spin and charge fluctuations on the pseudogap formation in cuprate superconductors has been studied using the diagram technique for Hubbard operators. It has been shown that the joint inclusion of the spin and charge fluctuations leads to the formation of "shadow" bands with a strong modulation of the spectral intensity and to a decrease in the density of electronic states at the Fermi level.

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The presence of the pseudogap state [1], where a significant decrease in the density of electronic states in the vicinity of the Fermi level takes place, is one of nontrivial peculiarities of cuprate superconductors. Description of the pseudogap phase in some of the works is based on the models of strongly correlated electron systems. The key idea of this method is based on taking into account spin fluctuations [2–5]. In order to describe the pseudogap phase in [3], an assumption is made that a charge density wave is present in the system. This approach reveals the microscopic mechanism leading to the formation of shadow bands and to the modulation of spectral intensity at the Fermi contour. Despite the success of this approach, the origin of the spin density wave remains an open question. It seems relevant to develop an approach where the spin structure of a strongly correlated system remains homogeneous, and the pseudogap is induced due to pronounced fluctuations of the spin. In this work, we show that using a simple model of strongly correlated systems, namely, the t–t'–t'' model, makes it possible to relate electron degrees of freedom with spin ones and to find a renormalization of the electron energy structure, leading to the formation of the pseudogap phase.

The Hamiltonian in the t–t'–t'' model in the atomic representation can be written in the following form:

$$H = \sum_{j\sigma}(\varepsilon - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma}, \qquad (1)$$

where X_f^{pq} are Hubbard operators [6]: $X_f^{0\sigma}$ describes a transition of the ion at site f from the single electron state with spin projection $\sigma = \pm 1/2$ to a state without electrons, $X_f^{\sigma 0}$ describes the opposite process, $\bar{\sigma} = -\sigma$. The diagonal operator $X_f^{\sigma\sigma}$ is a projection operator for the single electron sector of Hilbert subspace corresponding to site f. The energy of the single-electron single-ion state is denoted as ε, μ is the chemical potential of the system, and t_{fm} is the electron hopping integral from site m to site f.

In order to obtain the equations describing the normal mode, we use in this work the graphical phase of perturbation theory for Matsubara Green's functions in the atomic representation. This approach is based on the diagram technique for Hubbard operators [7]. Earlier, it has been shown in [8], that in the one-loop approximation, the processes of scattering on spin and charge fluctuations can be represented by the force operator. The expression for the normal component of the force operator in the first Born approximation has the form

$$P_{0\uparrow,0\uparrow}(\mathbf{k}, i\omega_m) \equiv P_{11}(\mathbf{k}, i\omega_m) = \left(1 - \frac{n}{2}\right) + \frac{\chi_s \Omega_S t_{\mathbf{k}+\mathbf{Q}}}{i\omega_m + \mu - \left(1 - \frac{n}{2}\right)t_{\mathbf{k}+\mathbf{Q}}} + \frac{\chi_c \Omega_c t_{\mathbf{k}}}{i\omega_m + \mu - \left(1 - \frac{n}{2}\right)t_{\mathbf{k}}}, \qquad (2)$$

where ω_m is the Matsubara frequency, n is the concentration of electrons, T is the temperature, χ_s and χ_c are the static spin and charge susceptibilities respectively, $\Omega_s = 0.01|t|$ and $\Omega_c = 1.00|t|$ are weight coefficients characterizing the scale of excitations in spin and charge subsystems, $t_{\mathbf{k}}$ is the Fourier transform of the

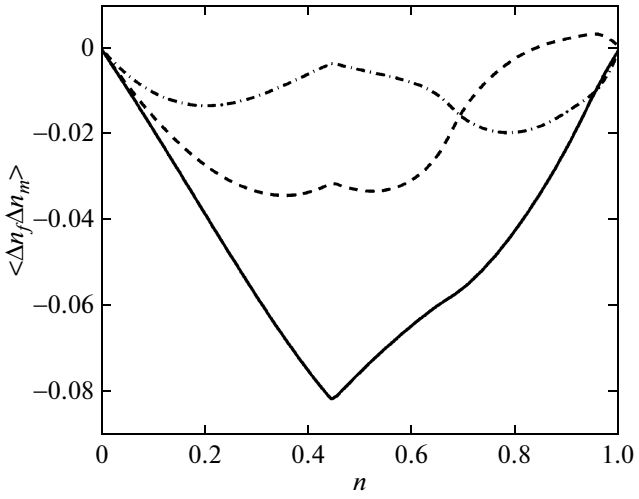

Fig. 1. Influence of long-range hops on the concentration dependence of the density–density correlator.

hopping integral, and $\mathbf{Q} = (\pi, \pi)$. The use of the static spin susceptibility is based on the well-known experimental fact [9] that the magnetic susceptibility has a sharp maximum at the point of the antiferromagnetic instability $\mathbf{Q} = (\pi, \pi)$. That is why for spin susceptibility we chose the model [10, 11]

$$\chi_s = \frac{3n}{2\pi\omega_s C(\xi)}, \quad \omega_s = 0.2|t_1|, \quad \xi = 3,$$
$$C(\xi) = \frac{1}{N}\sum_{\mathbf{q}} \frac{1}{1+\xi^2(1+\gamma_{1\mathbf{q}})}. \tag{3}$$

The value of static spin susceptibility χ_c corresponds to the dynamic charge susceptibility at zero frequency averaged over Brillouin zone. The dynamic charge susceptibility was found by taking a Fourier transform of two-time temperature Green's function

$$\chi_{CF}(\mathbf{k}, \omega) = -\frac{1}{4}\langle\langle N_{\mathbf{k}\sigma}|N_{\mathbf{k}}\rangle\rangle_\omega. \tag{4}$$

Using equations of motion in a usual manner [12], we find

$$\langle\langle N_{\mathbf{k}\sigma}|N_{\mathbf{k}}\rangle\rangle_\omega = \frac{\frac{2}{N}\sum_{\mathbf{q}}(t_{\mathbf{k}-\mathbf{q}} - t_{\mathbf{q}})K_{\mathbf{q}}}{\omega^2 - \left(1-\frac{n}{2}\right)\frac{1}{N}\sum_{\mathbf{q}} t_{\mathbf{q}}(t_{\mathbf{q}} - t_{\mathbf{k}+\mathbf{q}})}, \tag{5}$$

where $K_{\mathbf{q}}$ is Fourier transform of kinetic correlator. The performed calculations showed that charge susceptibility has a maximum at zero value of quasi-momentum. Density–density correlator is one of the quantities, which can characterize the contribution of charge fluctuations to the energy structure of system under consideration. Using the spectral theorem [13] and also using Eqs. (4) and (5) we find the correlator

$$\langle \Delta n_f \Delta n_m\rangle = \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}(f-m)}\langle N_{\mathbf{k}}\rangle$$
$$= \frac{2}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}(f-m)}\frac{(1+2f_{\mathrm{B}}(E_{\mathbf{k}}))}{E_{\mathbf{k}}}\Bigg((\gamma_{1\mathbf{k}}-1)\frac{1}{N}\sum_{\mathbf{p}} 4t_1\gamma_{1\mathbf{p}}K_{\mathbf{p}} \tag{6}$$
$$+ (\gamma_{2\mathbf{k}}-1)\frac{1}{N}\sum_{\mathbf{p}} 4t_2\gamma_{2\mathbf{p}}K_{\mathbf{p}} + (\gamma_{3\mathbf{k}}-1)\frac{1}{N}\sum_{\mathbf{p}} 4t_3\gamma_{3\mathbf{p}}K_{\mathbf{p}}\Bigg).$$

The energy spectrum of Bose excitations, which is present in this expression,

$$E_{\mathbf{k}} = \sqrt{\left(1-\frac{n}{2}\right)(4t_1^2(1-\gamma_{1\mathbf{k}})) + 4t_2^2(1-\gamma_{2\mathbf{k}}) + 4t_3^2(1-\gamma_{2\mathbf{k}})} \tag{7}$$

is gapless, and it has a linear in quasi-momentum dependence in the region of small $\mathbf{k}$, $f_{\mathrm{B}}(x) = 1/[\exp((x-\mu)/T) - 1]$ is Bose–Einstein distribution function, $\gamma_{1\mathbf{k}}$, $\gamma_{2\mathbf{k}}$, $\gamma_{3\mathbf{k}}$ are invariants of a simple square lattice

$$\gamma_{1\mathbf{k}} = \frac{1}{2}(\cos k_x + \cos k_y),$$
$$\gamma_{2\mathbf{k}} = \cos k_x \cos k_y, \tag{8}$$
$$\gamma_{3\mathbf{k}} = \frac{1}{2}(\cos 2k_x + \cos 2k_y).$$

We show in Fig. 1 dependences of density–density correlators on concentration, calculated taking into account hops in three coordinate spheres $t_2 = -0.65|t|$, $t_3 = -0.4|t|$, $T = 0.01|t|$, $t \equiv t_1$. The solid, dashed and dash-dotted lines correspond to dependences of correlator at the first, second and third coordination spheres correspondingly. It can be seen that the absolute value of this correlator can be as high as 0.08 (for the nearest neighbors). The performed calculations make it possible to conclude that taking into account scattering processes on charge fluctuations plays an important role in description of the energy structure of a strongly correlated electron system. In the figure one can also see that a kink at concentration value $n = 0.44$ is present in all the curves, which is related with the change in the topology of the Fermi surface at a given doping. A similar kink was observed earlier in the studies of the energy structure of the t–J^* model [14], and the relation with the change in topology was established in [15]. Using Eq. (2) and Green's function

$$D_{11}(\mathbf{k}, i\omega_m) = \frac{P_{11}(\mathbf{k}, i\omega_m)}{i\omega_m + \mu - t_{\mathbf{k}}P_{11}(\mathbf{k}, i\omega_m)}, \tag{9}$$

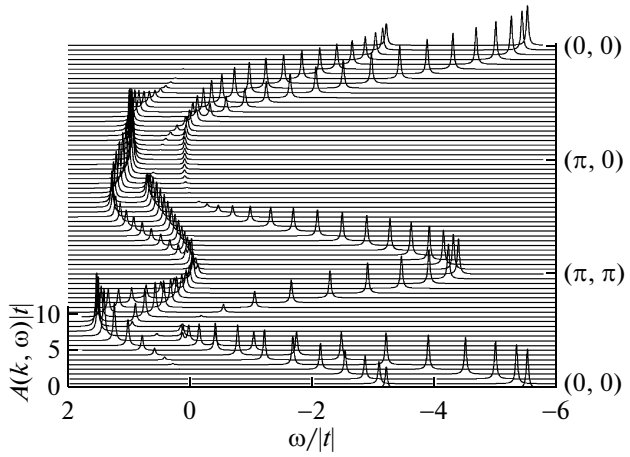

Fig. 2. Modulation of the spectral intensity in the pseudogap phase with due regard for the spin and charge fluctuations. The parameters are taken as follows: $t' = -0.65|t|$, $t'' = -0.4|t|$, $n = 0.95$, and $T = 0.01|t|$.

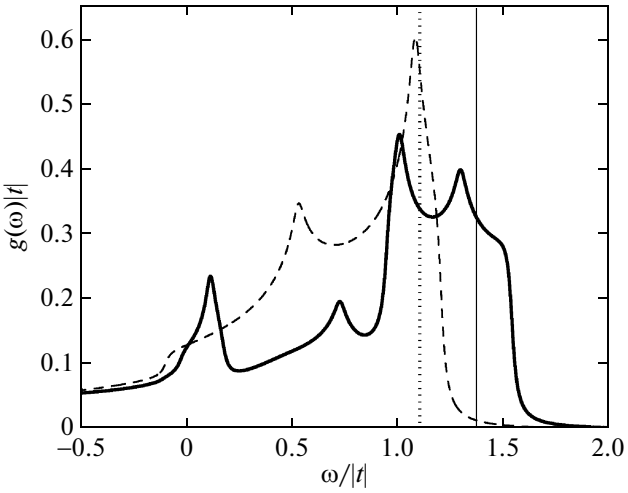

Fig. 3. Density of states calculated in the Hubbard-I approximation (dashed line) and also calculated taking into account the spin and charge fluctuations (thick solid line). Comparing the density at the intersection point of the dotted and dashed lines and the density at the intersection point of the thin and thick lines, one can see that the inclusion of the fluctuations leads to a strong decrease in the density of states in the vicinity of the Fermi level.

and having performed analytic continuation $i\omega_m \longrightarrow \omega + i\delta$, we can calculate the electronic spectral intensity

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi}\mathrm{Im}D_{11}(\mathbf{k}, \omega). \quad (10)$$

The inclusion of the scattering processes leads to the fact that electron Green's function (9) acquires a tripolar structure, and, consequently, the equation determining the spectrum becomes cubic. We show the dependence of spectral intensity on the wave vector along the main directions in Brillouin zone and on the energy of excitations in Fig. 2. One can see that the inclusion of the fluctuation processes in spin and charge subsystems leads to splitting of the main band and the formation of the so-called shadow bands. One of these bands corresponds to scattering processes on spin fluctuations and another corresponds to scattering on charge fluctuations. One can also see from this figure that a considerable modulation of spectral intensity is present in different points in Brillouin zone.

The influence of spin and charge fluctuations on the density of electronic states for electron concentration $n = 0.95$ is shown in Fig. 3. Dashed line shows the density of states obtained in the simplest Hubbard-I approximation disregarding fluctuation processes completely. In this case the chemical potential depicted by a vertical dotted line lies in the region of large density of states. Taking into account the above mentioned fluctuation processes leads to inhomogeneous in charge carrier concentration renormalization of the density of states. One can see that broadening of the band takes place in the high-energy region and the profile of the curve of density of states becomes more complex. An important peculiarity of renormalization is related with the fact that a significant decrease in the density of states takes place in the vicinity of the chemical potential, depicted in the figure by a solid vertical line. This fact is related with the formation of pseudogap phase, when modulation of the spectral intensity at the Fermi contour is caused by hybridization of the main band and two shadow bands (spin fluctuation band and charge band).

In conclusion we wish to note that the formation of pseudogap state in the frame of developed approach is induced both by spin and by charge fluctuations. The hybridization of the main band with two shadow bands is related with this fact, and it constitutes the main difference of our approach from the conventional one, when taking into account spin fluctuation processes leads to hybridization of the main band with one shadow band only. In our case we obtain a more complex pattern of spectral intensity redistribution along the Fermi contour, which correlates well with experimental data for pseudogap state of the normal phase of cuprate superconductors.

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