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**METALS  
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# Distribution Function of Hubbard Quasiparticles in Two-Dimensional Systems with Inclusion of Dynamic Processes of Spin-Fluctuation Scattering

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Received July 30, 2008

**Abstract**—Spin-fluctuation scattering in an ensemble of strongly correlated electrons in CuO<sub>2</sub> planes of high-temperature superconductors is investigated. It is demonstrated that this process significantly modifies the distribution function of Hubbard quasiparticles. The influence of spin-fluctuation scattering mathematically manifests itself in the appearance of the correction to the strength operator in the numerator of the single-fermion Green's function dependent on the Matsubara frequency. This correction differently renormalizes the spectral intensity on different energy scales and determines the dependence of the Migdal discontinuity on the electron concentration in the system.

PACS numbers: 71.10.Fd, 71.10.Ay

DOI: 10.1134/S1063783409050011

## 1. INTRODUCTION

It is known that, in a free-fermion gas, the probability of occupation of the quantum state  $(\mathbf{k}, \sigma)$  is described by the Fermi–Dirac distribution function  $f_{\mathbf{k}, \sigma}^{(0)} = \{\exp[(\epsilon_{\mathbf{k}, \sigma} - \mu)/T] + 1\}^{-1}$ . In this expression,  $\epsilon_{\mathbf{k}, \sigma}$  is the energy of the single-particle state  $(\mathbf{k}, \sigma)$ ,  $\mathbf{k}$  is the quasi-momentum,  $\sigma$  is the spin moment projection (which takes on two values  $\sigma = \pm 1/2$ ),  $\mu$  is the chemical potential of the system, and  $T$  is the temperature in energy units. When fermions interact with each other, the physical properties of the system are discussed in terms of quasiparticle excitations. In this case, one of the key problems of the theory is the problem of the distribution function of Fermi quasiparticles [1–6]. Previously, it was demonstrated that, when the interaction between fermions is switched on, the volume of the Fermi sphere remains unchanged (the Luttinger theorem) [3] and the discontinuity in the distribution function on the Fermi surface (the Migdal discontinuity) is retained and depends on the interaction intensity [2].

Owing to the discovery of high-temperature superconductivity, investigations of properties of two-dimensional electron systems with strong correlations have acquired a special importance. It is believed that these models adequately describe the main features of the electronic structure of cuprate superconductors. The majority of works in this direction have been performed in the framework of the Hubbard model [7] or its reduced variant, which arises when constructing the effective Hamiltonian describing the low-energy range. Despite the relative simplicity, this model allows one to describe the main effects of strong intra-atomic interac-

tions, namely, the metal–insulator transition [8] in so-called Mott–Hubbard insulators and the nonphonon mechanisms of Cooper instability in high-temperature superconductors [9–11] (see the reviews [12, 13]).

In recent years, there have appeared many publications devoted to the study of normal and superconducting phases within the Hubbard model and its modifications. However, a number of fundamental problems remain unsolved up to now. In particular, the question as to the distribution function of quasiparticle excitations in the strong-correlation limit and the main factors determining its characteristics remains open. One of the obstacles to the correct calculation of the distribution function is a complexity of the inclusion of the spin dynamics in the presence of strong correlations. For the Hubbard model, this manifests itself in the problem associated with the description of spin-fluctuation scattering processes. In this respect, investigation of the influence of spin-fluctuation scattering on the characteristics of the distribution function of Fermi quasiparticles within the Hubbard model in the strong-correlation regime seems to be an important problem.

In this work, the distribution function of Hubbard quasiparticles  $f_{\mathbf{k}}$  was calculated using the diagram technique in the atomic representation for the Hubbard model at  $U = \infty$  within the one-loop approximation. This made it possible to investigate the influence of dynamic spin-fluctuation processes on the distribution function  $f_{\mathbf{k}}$ . It was shown that the spin-fluctuation scattering processes lead to qualitative changes in the distribution function  $f_{\mathbf{k}}$  as compared to the frequently used Hubbard I approximation.



In order to obtain the distribution function with allowance made for the dynamic and kinetic interactions in the system under consideration, it is necessary to calculate the mass operator and the correction  $\delta P_{0\sigma, 0\sigma}(k)$  to the strength operator in some approximation. In this case, the arising dependence of these quantities on the Matsubara frequencies leads to substantial renormalizations of the distribution function due to the influence of dynamic scattering processes. The magnitude of these renormalizations appears to be dependent on the quasiparticle energy. This circumstance is responsible for the qualitative modifications of the distribution function as compared to that obtained within the Hubbard I approximation.

### 3. ONE-LOOP APPROXIMATION FOR THE STRENGTH AND MASS OPERATORS

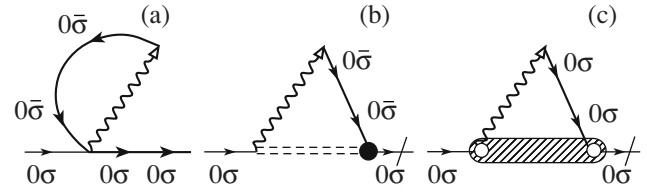
The first corrections to the distribution function due to the influence of spin-fluctuation scattering processes appear within the one-loop approximation. In the graphical form, the contributions to the quantities  $\Sigma_{0\sigma, 0\sigma}(k)$  and  $\delta P_{0\sigma, 0\sigma}(k)$  are determined by the diagrams shown in Fig. 1. These diagrams were constructed using the principle of topological continuity [15, 17] and the principle of dominance of Fermi-like Hubbard operators over Bose-like Hubbard operators. The latter principle means that, when writing the ordered thermodynamic average  $T_\tau$  of the product of an arbitrary number of Hubbard operators according to the Wick's theorem, the pairing begins with a Fermi-like operator, all other things being equal. Within the approximation under consideration, there is only one diagram for the mass operator, whereas the strength operator is characterized by two diagrams.

After assigning analytical expressions to graphical elements and introducing necessary summations, we obtain

$$\Sigma_{0\sigma, 0\sigma} = -\frac{T}{N} \sum_q t_q G_{0\bar{\sigma}, 0\bar{\sigma}}(q), \quad (9)$$

$$\begin{aligned} \delta P_{0\sigma, 0\sigma}(k) = & -\frac{T}{N} \sum_q t_q \{ G_{0\bar{\sigma}, 0\bar{\sigma}}(q) D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k-q) \\ & + G_{0\sigma, 0\sigma}(q) D_{\sigma\sigma, \sigma\sigma}^{(\text{irr})}(k-q) \}. \end{aligned} \quad (10)$$

Similar relationships for the mass and strength operators were previously derived using the generating functional method [16]. It should be noted that, since the mass operator depends neither on the frequency nor on the momentum, its inclusion is reduced to the renormalization of the chemical potential. However, the correction to the strength operator depends on the Matsubara frequency and the quasi-momentum, and its value in general is determined by the spin and charge fluctuations. The last statement is associated with the fact that



**Fig. 1.** One-loop diagrams for the (a) mass and (b, c) strength operators.

relationship (10) contains both the Fourier transform of the transverse quasi-spin Green's function

$$\begin{aligned} D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(f\tau; g\tau') &= -\langle T_\tau \tilde{X}_f^{\bar{\sigma}\sigma}(\tau) \tilde{X}_g^{\bar{\sigma}\sigma}(\tau') \rangle \\ &= \frac{T}{N} \sum_{\mathbf{k}, \omega_n} \exp\{i\mathbf{k}(\mathbf{R}_f - \mathbf{R}_g) - i\omega_n(\tau - \tau')\} D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k), \\ k &= (\mathbf{k}, \omega_n) \end{aligned} \quad (11)$$

and the Fourier transform of the irreducible longitudinal Green's function

$$\begin{aligned} D_{\sigma\sigma, \sigma\sigma}^{(\text{irr})}(f\tau; g\tau') &= -\langle T_\tau \Delta(\tilde{X}_f^{\sigma\sigma}(\tau)) \Delta(\tilde{X}_g^{\sigma\sigma}(\tau')) \rangle, \\ \Delta A &= A - \langle A \rangle. \end{aligned} \quad (12)$$

In the paramagnetic phase, this Green's function with due regard for the condition of completeness of the basis set of single-site states  $X_f^{00} + X_f^{\sigma\sigma} + X_f^{\bar{\sigma}\bar{\sigma}} = 1$  and the operator identity  $X_f^{\sigma\sigma} = \hat{N}_f/2 + 2\sigma S_f^z$  ( $\sigma = \pm 1/2$ ) can be represented in the form

$$\begin{aligned} D_{\sigma\sigma, \sigma\sigma}^{(\text{irr})}(f\tau; g\tau') &= -\frac{1}{4} \langle T_\tau \Delta \tilde{N}_f(\tau) \Delta \tilde{N}_g(\tau') \rangle \\ &\quad - \langle T_\tau \tilde{S}_f^z(\tau) \tilde{S}_g^z(\tau') \rangle. \end{aligned} \quad (13)$$

In a strongly correlated system, the characteristic energies of charge fluctuations are higher than those of spin fluctuations. Therefore, the thermodynamic contribution of charge fluctuations is smaller than that of spin fluctuations. In this respect, hereafter, the irreducible Green's function will be calculated with allowance made only for the spin fluctuations. Taking into account the spherical symmetry of quasi-spin Green's functions in the paraphase, from expression (13), we obtain the relationship between the irreducible Green's function and the transverse quasi-spin Green's function in the form

$$D_{\sigma\sigma, \sigma\sigma}^{(\text{irr})}(f\tau; g\tau') = \frac{1}{2} D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(f\tau; g\tau'). \quad (14)$$

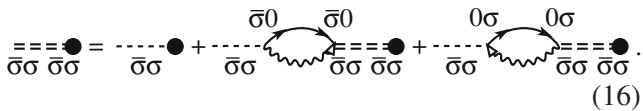
With due regard for this equality, the one-loop correction to the electronic strength operator in the paraphase can be written in the form

$$\delta P_{0\sigma, 0\sigma}(k) = -\frac{3T}{2N} \sum_q t_q D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k-q) G_{0\bar{\sigma}, 0\bar{\sigma}}(q). \quad (15)$$

The presence of the quasi-spin Green's function in this expression reflects the contribution of the spin degrees of freedom to the energy characteristic of the spectrum of Hubbard quasiparticles. Within the approximation under consideration, the spin-fluctuation scattering processes manifest themselves only through the correction to the strength operator. In order to determine finally their role, it is necessary to calculate the transverse quasi-spin Green's function in the same one-loop approximation. It should be noted that similar expressions for the Green's function (6) and the strength operator (15) were derived using the equations of motion for retarded Green's functions by Irkhin and Zarubin [18]. However, the used method for decoupling higher Green's function allowed the authors to take into account the spin-fluctuation dynamics only by introducing the averaged (over the Brillouin zone) spectral function of magnons with the spectrum  $\omega_k$  corresponding to spin excitations of the ferromagnetic type. In the framework of our approach, the spin dynamics is directly included through the spin Green's functions calculated in the paramagnetic phase.

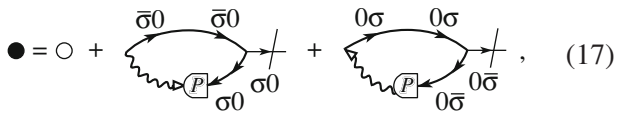
4. DYNAMIC MAGNETIC SUSCEPTIBILITY

The transverse spin Green's function  $D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k)$  is calculated by the same diagram technique as for the Hubbard operators. By designating this function as the double dashed line, the Dyson equation in the one-loop approximation can be written in the following graphical form:



(16)

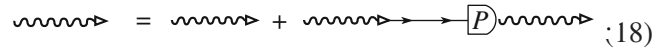
Here, the closed circle indicates the spin strength operator  $P_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(q)$ . Within the approximation under consideration, the contributions of this operator are determined by the graphs



(17)

where the open circle represents the zeroth-order contribution equal to  $N_{\bar{\sigma}} - N_{\sigma}$  and two diagrams after the open circle are one-loop corrections  $\delta P_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(q)$ . The

thick wavy line in formula (16) corresponds to the effective interaction satisfying the equation



(18)

In the graphical relationships (17) and (18), the symbol  $P$  in the open semicircle, as before, indicates the electronic strength operator  $P_{0\sigma, 0\sigma}(q)$ . By writing Eq. (16) in the analytical form, we obtain the following representation of the quasi-spin Green's function:

$$D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k) = \frac{P_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k)}{i\omega_m + 2\sigma h - \Sigma_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k)}. \quad (19)$$

Here, we took into account the explicit form of the quasi-spin bare propagator depicted by the thin dashed line:  $g_{\bar{\sigma}\sigma}(i\omega_m) = \{i\omega_m + 2\sigma h\}^{-1}$ . The spin mass operator  $\Sigma_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k)$  is determined by the contributions of two loops on the right-hand side of Eq. (16) and given by the expression

$$\Sigma_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k) = -\frac{T}{N} \sum_q t_q [(1 + t_q D_{0\sigma, 0\sigma}(q)) G_{\bar{\sigma}0, \bar{\sigma}0}(k-q) + (1 + t_q D_{0\bar{\sigma}, 0\bar{\sigma}}(q)) G_{0\sigma, 0\sigma}(k+q)]. \quad (20)$$

For the strength operator  $P_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k)$  determined by graphs (17), according to the rules of the diagram technique, we find

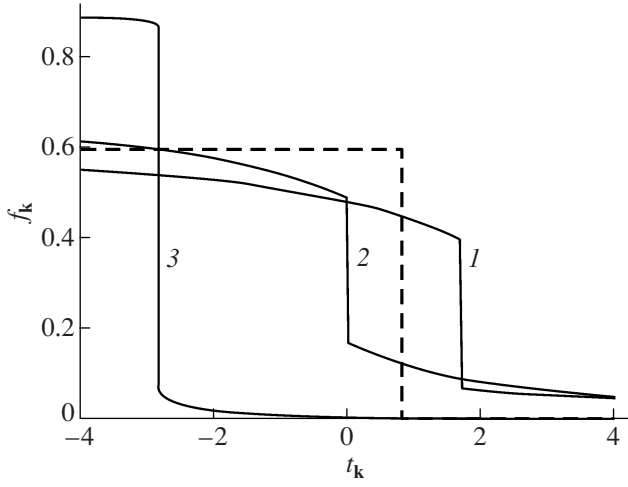
$$P_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(k) = (N_{\bar{\sigma}} - N_{\sigma}) + \frac{T}{N} \sum_q \{ t_{q+k} P_{0\sigma, 0\sigma}(q+k) - t_q P_{0\bar{\sigma}, 0\bar{\sigma}}(q) \} G_{0\sigma, 0\sigma}(q+k) G_{0\bar{\sigma}, 0\bar{\sigma}}(q). \quad (21)$$

The derived equations (19)–(21), together with Eqs. (6), (9), and (15), form a closed system of integral equations that makes it possible to investigate self-consistently the influence of spin-fluctuation processes on the thermodynamic characteristics of the Hubbard model. In particular, this system of equations allows one to study the renormalizations of the distribution function of Hubbard quasiparticles due to the spin-fluctuation scattering processes.

5. DISTRIBUTION FUNCTION OF HUBBARD QUASIPARTICLES

In order to solve the above system of integral equations, we introduce a number of simplifications. The first simplification is associated with the fact that, when calculating the spin Green's functions, the electron Green's functions are represented in the Hubbard I approximation. This circumstance allows us to perform the summation over the frequencies in Eqs. (20) and (21) in an explicit form. As a result, from relationships (20) and (21), the expressions for the mass and strength





**Fig. 2.** Distribution functions of Hubbard quasiparticles at different concentrations: (1)  $n = 0.8$ ,  $\bar{\mu} = 0.626$ ,  $\alpha = 2.2$ ; (2)  $n = 0.667$ ,  $\bar{\mu} = 5.2 \times 10^{-4}$ ,  $\alpha = 1.33$ ; and (3)  $n = 0.2$ ,  $\bar{\mu} = -2.51$ ,  $\alpha = 0.915$ . The dashed line indicates the distribution function  $f_{\mathbf{k}}$  calculated in the Hubbard I approximation at  $n = 0.8$ .

operators in the paramagnetic phase can be written in the form

$$\Sigma_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(\mathbf{k}, i\omega_m) = i\omega_m \frac{1}{N} \sum_{\mathbf{q}} \frac{(f_{\mathbf{q}-\mathbf{k}} - f_{\mathbf{q}})(t_{\mathbf{q}} + t_{\mathbf{q}-\mathbf{k}})}{i\omega_m - \xi_{\mathbf{q}} + \xi_{\mathbf{q}-\mathbf{k}}}, \quad (22)$$

$$P_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(\mathbf{k}, i\omega_m) = i\omega_m \frac{1}{N} \sum_{\mathbf{q}} \frac{f_{\mathbf{q}-\mathbf{k}} - f_{\mathbf{q}}}{i\omega_m - \xi_{\mathbf{q}} + \xi_{\mathbf{q}-\mathbf{k}}}. \quad (23)$$

According to the second simplification, the strength operator is calculated from formula (15) by replacing the dynamic susceptibility  $\chi(\mathbf{k}, i\omega_m)$  dependent on the quasi-momentum by the susceptibility averaged over the Brillouin zone; that is,

$$\chi(\mathbf{k}, i\omega_n) \longrightarrow \bar{\chi}(i\omega_n) = -\alpha \frac{3}{2N} \sum_{\mathbf{k}} D_{\bar{\sigma}\sigma, \bar{\sigma}\sigma}(\mathbf{k}, i\omega_n). \quad (24)$$

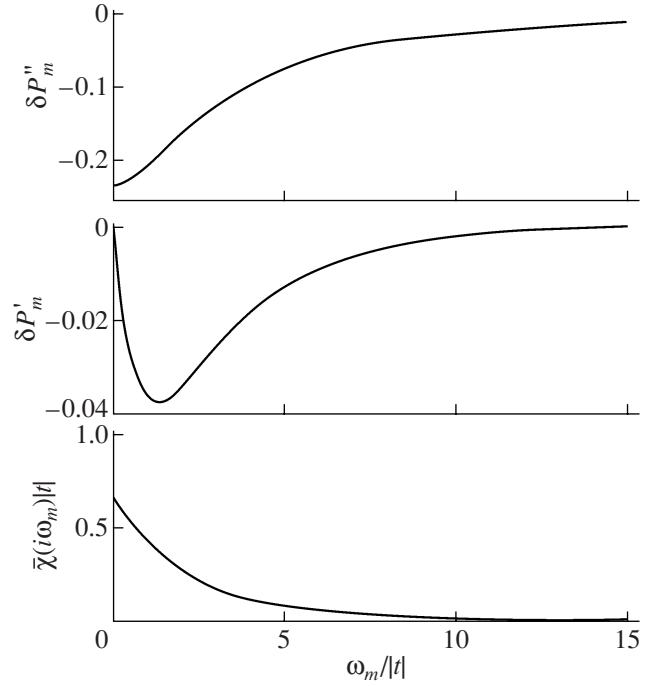
In this case, the correction coefficient  $\alpha$  is introduced into the right-hand side of Eq. (15) in order for the sum rule for the Matsubara susceptibility to be satisfied

$$\frac{T}{N} \sum_{\mathbf{k}, \omega_n} \chi(\mathbf{k}, i\omega_n) = T \sum_{\omega_n} \bar{\chi}(i\omega_n) = \frac{3n}{4}. \quad (25)$$

With allowance made for approximation (24), the correction to the electronic strength operator  $\delta P_{0\sigma, 0\sigma}(\mathbf{k}, i\omega_n)$  takes the form

$$\delta P_{0\sigma, 0\sigma}(i\omega_n) = \frac{T}{N} \sum_{\mathbf{q}, m} \frac{t_{\mathbf{q}} \bar{\chi}(i\omega_{n-m})}{i\omega_m - \xi_{\mathbf{q}}}. \quad (26)$$

In order to close the system of self-consistent equations, it is necessary to add the following equation for



**Fig. 3.** Dependences of the real and imaginary parts of the mass operator and the dynamic susceptibility on the Matsubara frequency at the concentration  $n = 0.8$ .

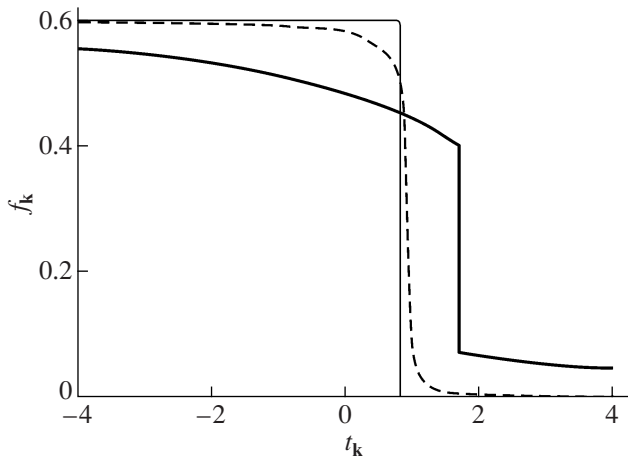
the determination of the renormalized chemical potential ( $\bar{\mu} = \mu - \Sigma_{0\sigma, 0\sigma}$ ):

$$n/2 = \frac{1}{N} \sum_{\mathbf{k}} f_{\mathbf{k}},$$

where  $f_{\mathbf{k}}$  is the above-defined distribution function (7) of Hubbard quasiparticles. The spin index is omitted because we consider the paramagnetic phase.

The results of the solution to the system of self-consistent integral equations for  $\mu$ ,  $\alpha$ ,  $\bar{\chi}(i\omega_m)$ , and  $\delta P_{0\sigma, 0\sigma}(i\omega_m)$  are presented in Figs. 2 and 3. The calculations were carried out using the nearest neighbor approximation when  $t_{\mathbf{k}} = -2|t|(\cos(k_x) + \cos(k_y))$ . The chemical potentials are given in units of  $|t|$ . The temperature was taken to be  $T = 5$  K.

For a clear illustration of the spin-fluctuation effects, the distribution function  $f_{\mathbf{k}}$  of Hubbard quasiparticles according to the calculation within the Hubbard I approximation at the concentration  $n = 0.8$  is depicted by the dashed line in Fig. 2. It can be seen from this figure that, in the case under consideration, the distribution function  $f_{\mathbf{k}}$  has the form of a conventional Fermi step decreased by the well-known renormalizing factor  $1 - n/2$ . Solid line 1 in the same figure shows the distribution function  $f_{\mathbf{k}}$  calculated with allowance made for the spin-fluctuation scattering processes at the same concentration  $n = 0.8$ . A comparison of two dependences demonstrates that there are three



**Fig. 4.** Distribution functions of Hubbard fermions according to the calculations in the static approximation. Thin solid and dashed lines correspond to  $\bar{\chi}(0) = 0.74|t|$  and  $80|t|$ , respectively. For comparison, the thick solid line indicates the distribution function  $f_k$  calculated using the dynamic susceptibility at the same parameters  $n = 0.8$  and  $T = 5$  K.

fundamental differences between them. First, the inclusion of the dynamic spin-fluctuation processes leads to a finite probability of occupation of states above the Fermi momentum  $k_F$  defined as the quasi-momentum at which the distribution function  $f_k$  has a discontinuity with a finite value  $Z$ . Second, in the energy range lower than the chemical potential, there arises a strong renormalization of the distribution function, which depends on the deviation of the quasiparticle energy from the chemical potential. Third, the position of the discontinuity in the distribution function changes substantially due to the one-loop corrections to the mass operator.

As the concentration decreases, the fraction of electrons occupying states with  $k > k_F$  initially increases, reaches a maximum at  $n = 0.667$  (Fig. 2, curve 2), and then decreases. It is evident that, at concentrations considerably lower than unity, the efficiency of the spin-fluctuation scattering processes should be low and, correspondingly, the distribution function  $f_k$  should differ little from the Fermi step. As can be seen from the presented dependences, this regularity actually occurs.

The frequency dependences of the strength operator  $\delta P_{0\sigma,0\sigma}(i\omega_m) = \delta P'_m + i\delta P''_m$  and the dynamic Matsubara susceptibility  $\bar{\chi}(i\omega_m)$  at the concentration  $n = 0.8$  are plotted in Fig. 3. The strength operator and the susceptibility correspond to the odd and even Matsubara frequencies, respectively. It should be noted that the real part  $\delta P'_m$  of the mass operator is a symmetric function of the Matsubara frequency, whereas the imaginary part  $\delta P''_m$  of the mass operator is an antisymmetric function of the Matsubara frequency. It can be seen from Fig. 3 that, on a scale of the band width  $W \approx 4|t|$ , the renormalizations of the strength operator due to the

inclusion of the one-loop corrections ( $\delta P'_m$ ) are very significant and they are responsible for the substantial modification of the distribution function  $f_k$ .

As can be seen from Fig. 3, the contribution to the dynamic Matsubara susceptibility  $\bar{\chi}(i\omega_m)$  at high temperatures is made only by frequencies with small numbers  $m$ . In this case, it is possible to use the so-called high-temperature limit when  $\bar{\chi}(i\omega_m) \equiv \delta_{m0}\bar{\chi}(0)$ . This corresponds to the static approximation. The results of the calculations performed within this approximation are presented in Fig. 4 by the solid and dashed lines representing the distribution functions  $f_k$  at small and large values of the susceptibility  $\bar{\chi}(0)$ , respectively. It can be seen from Fig. 4 that, in the low-temperature range ( $T = 5$  K), the static approximation at the small value of the susceptibility in actual fact does not lead to the difference between the distribution function  $f_k$  and the Fermi step and corresponds to the simplest Hubbard I approximation with  $Z = 1 - n/2$ . For larger values of the susceptibility  $\bar{\chi}(0)$ , the distribution function is characterized by a strong smearing that should be observed at high temperatures. However, in this case, the temperature is low and the smearing is completely associated with the scattering processes.

Therefore, when the efficiency of the spin-fluctuation scattering processes is high, the use of the static approximation can lead to an incorrect result (manifesting itself in a strong smearing of the distribution function) and the disappearance of the Migdal discontinuity. However, the inclusion of the dynamic effects of spin-fluctuation scattering retains the Migdal discontinuity and brings the distribution function into the form characteristic of the Landau theory of Fermi liquids.

## 6. CONCLUSIONS

It should be emphasized that, as follows from the results obtained, the spin-fluctuation scattering processes for electron systems in the strong-correlation regime substantially affect the distribution function of Hubbard quasiparticles. It is evident that this influence is not the only manifestation of the spin-fluctuation processes. These processes are mathematically taken into account through the strength operator in the numerator of the single-fermion Green's function. This means that the processes under consideration should significantly affect the spectral intensities and, hence, the characteristics of the pseudogap behavior of strongly correlated electron systems. The proposed method for including the spin-fluctuation scattering processes makes it possible to solve the above problems. However, this is beyond the scope of the present work.

## ACKNOWLEDGMENTS

This study was supported by the Russian Foundation for Basic Research (project no. 06-02-16100) and per-

formed within the framework of the Program of the Branch of General Physics and Astronomy of the Russian Academy of Sciences and the Integration Project of the Siberian Branch of the Russian Academy of Sciences.

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