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ELECTRONIC PROPERTIES OF SOLIDS

The Electron Energy Spectrum and Superconducting Transition Temperature of Strongly Correlated Fermions with Three-Center Interactions

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Abstract—The renormalizations of the fermionic spectrum are considered within the framework of the *t–J** model taking into account three-center interactions ($H_{(3)}$) and magnetic fluctuations. Self-consistent spin dynamics equations for strongly correlated fermions with three-center interactions were obtained to calculate quasi-spin correlators. A numerical self-consistent solution to a system of ten equations was obtained to show that, in the nearest-neighbor approximation, simultaneously including $H_{(3)}$ and magnetic fluctuations at $n > n_1$ ($n_1 \approx 0.72$ for $2t/U = 0.25$) caused qualitative changes in the structure of the energy spectrum. A new Van Hove singularity is then induced in the density of states, and an additional maximum appears in the $T_c(n)$ concentration dependence of the temperature of the transition to the superconducting phase with order parameter symmetry of the $d_{x^2-y^2}$ type. © *2005 Pleiades Publishing, Inc.*

1. INTRODUCTION

It is commonly assumed [1–5] that strong electron correlation plays an important role in the mechanism of high-temperature superconductivity. One of the key models that includes strong electron correlation is the Hubbard model [6], which, in the simplest case, contains two energy parameters: the electron hopping integral between the nearest sites t and the Coulomb repulsion energy U between two electrons at one site with opposite spin moment projections (double occupancy). The inequality $U \gg |t|$ holds under strong electron correlation conditions.

At low electron concentrations, $n \ll 1$, this system is well described by Fermi liquid theory [7]. In the other limiting case of $n \longrightarrow 1$, we have the scenario of a Heisenberg antiferromagnet. At intermediate concentrations, $n < 1$, the problem of the ground state can only be described approximately.

At $U \gg t$ and $n < 1$, the Hubbard model is often considered in a truncated Hilbert space without double occupancy. The corresponding effective Hamiltonian contains not only terms that describe antiferromagnetic correlations between the spin moments of charge carriers but also three-center terms [8, 9]. Three-center interactions insignificantly influence the dispersion dependence of the spectrum of fermionic excitations [10, 11]. At the same time, their contribution becomes substantial in the superconducting phase. For the first time, this was shown in [12, 13]. In particular, the renormalization of the coupling constant when three-center terms are included [13] decreases the superconducting transition temperature by more than an order of magnitude [14].

The role played by magnetic fluctuations in superconducting pairing was studied in many works [3, 4, 15–17]. In recent years, magnetopolaron bound states have been introduced into the theory of the electronic structure of the CuO_2 plane [18].

We show in this work that magnetic fluctuations are capable of qualitatively renormalizing the electron energy spectrum and the density of states provided three-center interactions are taken into account. Such modifications substantially influence the concentration dependence of the superconducting transition temperature T_c. In this context, recent work [19] is noteworthy. In [19], the ideology of a substantial influence of three-center interactions and magnetic correlations was applied to describe the properties of *n*-type cuprates.

The present paper is organized as follows. The meaning of effective interactions in the *t–J** model is considered in Section 2. Section 3 contains self-consistency equations. Spin correlator calculations in the *t–J** model are described in Section 4. In what follows, the combined influence of three-center interactions and magnetic fluctuations is considered.

2. THE DOUBLE OCCUPANCY OPERATOR AND EFFECTIVE INTERACTIONS

The passage to the effective Hamiltonian in the atomic representation can be performed at $U \gg t$ and $n < 1$ either by canonical transformation [4] or using the operator form of perturbation theory [14, 20]. With an accuracy to terms proportional to t^2/U, we have

$$H_{\text{eff}} \equiv H_{t-J^*} = H_{t-J} + H_{(3)}, \tag{1}$$

where

$$H_{t-J} = \sum_{f\sigma}(\epsilon - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma} + \frac{1}{2}\sum_{fm\sigma} J_{fm}(X_f^{\sigma\bar{\sigma}} X_m^{\bar{\sigma}\sigma} - X_f^{\sigma\sigma} X_m^{\bar{\sigma}\bar{\sigma}}) \tag{2}$$

is the Hamiltonian of the t–J model [21] ($J_{fm} = 2t_{fm}^2/U$) and the three-center operator

$$H_{(3)} = \sum_{\substack{fmg\sigma \\ f \neq g}} \left(\frac{t_{fm} t_{mg}}{U}\right) \times \{X_f^{\sigma 0} X_m^{\bar{\sigma}\sigma} X_g^{0\bar{\sigma}} - X_f^{\sigma 0} X_m^{\bar{\sigma}\bar{\sigma}} X_g^{0\sigma}\} \tag{3}$$

takes into account the effect of correlated electron hoppings.

Let us elucidate the physical meaning of the terms proportional to t^2/U in the effective Hamiltonian. For this purpose, consider the operator $\hat{N}_2 = \sum_f X_f^{22}$ of the total number of doubly occupied sites. If $|\Psi_0\rangle$ is the ground state of the system described by the initial Hubbard Hamiltonian, the number of double occupancies is $N_2 = \langle\Psi_0|\hat{N}_2|\Psi_0\rangle$. The canonical transformation

$$H \longrightarrow H_{\text{eff}} = \exp(iS) H \exp(-iS)$$

changes the ground state function by the law

$$|\Psi_0\rangle \longrightarrow |\Psi_0\rangle = \exp(iS)|\Psi_0\rangle.$$

Therefore,

$$N_2 = \langle\Phi_0|\exp(iS)\hat{N}_2\exp(-iS)|\Phi_0\rangle.$$

It follows that the operator of double occupancies in the Hilbert space of the effective Hamiltonian is determined by the equation

$$\tilde{\hat{N}}_2 = \exp(iS)\hat{N}_2\exp(-iS).$$

Clearly, this conclusion remains valid when we pass to finite temperatures. Calculations with an accuracy quadratic in (t/U) give the effective operator of double occupancies in the form

$$\tilde{\hat{N}}_2 = -\sum_{fmg\sigma}\left(\frac{t_{fm}t_{mg}}{U^2}\right) \times \{X_f^{\sigma 0} X_m^{\bar{\sigma}\sigma} X_g^{0\bar{\sigma}} - X_f^{\sigma 0} X_m^{\bar{\sigma}\bar{\sigma}} X_g^{0\sigma}\} = -(H_{\text{exch}} + H_{(3)})/U, \tag{4}$$

where the exchange term H_{exch} is determined by the well-known equation

$$H_{\text{exch}} = \frac{1}{2}\sum_{fm\sigma} J_{fm}\{X_f^{\sigma\bar{\sigma}} X_m^{\bar{\sigma}\sigma} - X_f^{\sigma\sigma} X_m^{\bar{\sigma}\bar{\sigma}}\}. \tag{5}$$

It follows from these results that the Hamiltonian of the t–J^* model can be represented in the form

$$H_{t-J^*} = \sum_{f\sigma}(\epsilon - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma} - U\tilde{\hat{N}}_2. \tag{6}$$

We see that exchange and three-site interactions appear in H_{t-J^*} for the same reason determined by the presence of a finite number of double occupancies in the system.

3. SELF-CONSISTENCY EQUATIONS

The combined effects of magnetic correlations and three-center interactions on the renormalizations of the spectrum of fermionic excitations and the conditions of the existence of $d_{x^2-y^2}$ superconductivity will be studied using the irreducible Green functions constructed on Hubbard operators [22, 23].

When three-center interactions are taken into account, the first exact equation of motion for the anticommutator Green function is written in the form

$$\begin{aligned}(\omega - \varepsilon + \mu)\langle\langle X_f^{0\sigma}|X_g^{\sigma 0}\rangle\rangle_\omega &= \delta_{fg} N_{0\sigma} \\ &+ \sum_{m\sigma_1} t_{fm}\langle\langle(X_f^{\sigma_1\sigma} + \delta_{\sigma_1\sigma}X_f^{00})X_m^{0\sigma_1}|X_g^{\sigma 0}\rangle\rangle_\omega \\ &+ \sum_{m\sigma_1} J_{fm} 4\sigma_1\sigma\langle\langle X_f^{0\bar{\sigma}_1} X_m^{\bar{\sigma}\sigma_1}|X_g^{\sigma 0}\rangle\rangle_\omega \\ &+ \sum_{\substack{ml\sigma_1 \\ (m\neq l)}}\left(\frac{t_{fl}t_{mf}}{U}\right)4\sigma_1\sigma\langle\langle X_f^{0\sigma_1} X_l^{0\bar{\sigma}_1} X_m^{\bar{\sigma}0}|X_g^{\sigma 0}\rangle\rangle_\omega \\ &+ \sum_{\substack{ml\sigma_1 \\ (l\neq f)}}\left(\frac{t_{fm}t_{ml}}{U}\right) \\ &\times \langle\langle(X_m^{\sigma_1\bar{\sigma}_1} X_l^{0\sigma_1} - X_m^{\sigma_1\sigma_1} X_l^{0\bar{\sigma}_1})(X_f^{\bar{\sigma}_1\sigma} + \delta_{\sigma_1\bar{\sigma}}X_f^{00})|X_g^{\sigma 0}\rangle\rangle_\omega.\end{aligned} \tag{7}$$

In this equation, the terms that explicitly contain multipliers proportional to t^2/U originate from the inclusion of three-center interactions. The scheme of further calculations is quite usual for the method of irreducible Green functions [22, 23]. Equation (7) is linearized with the introduction of the anomalous function $\langle\langle X_f^{\bar{\sigma}0} | X_g^{\sigma 0}\rangle\rangle$. Next, the equation of motion for $\langle\langle X_f^{\bar{\sigma}0} | X_g^{\sigma 0}\rangle\rangle$ is constructed and linearization is repeated. The $\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'}\rangle$ means that appear in this scheme are approximated as [19]

$$\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'}\rangle = \frac{1}{4}n^2 + \eta(\sigma)\eta(\sigma')\langle S_f^z S_g^z\rangle, \qquad \eta(\sigma) = +1, -1, \quad \sigma = \uparrow, \downarrow. \tag{8}$$

Equation (8) is obtained from the exact equation

$$\langle X_f^{\sigma\sigma} X_g^{\sigma'\sigma'}\rangle = \frac{1}{4}n^2 + \frac{1}{2}\langle(\hat{n}_f - n)(\hat{n}_g - n)\rangle + \eta(\sigma)\eta(\sigma')\langle S_f^z S_g^z\rangle \tag{9}$$

by ignoring the correlator $\langle(\hat{n}_f - n)(\hat{n}_g - n)\rangle$. A similar approximation is used to represent the three-site mean in terms of quasi-spin correlators,

$$\langle(X_f^{00} + X_f^{\sigma\sigma})X_m^{\bar{\sigma}\bar{\sigma}}(X_g^{00} + X_g^{\sigma\sigma})\rangle = \frac{n}{2}\left(1 - \frac{n}{2}\right)^2 - \left(1 - \frac{n}{2}\right)(\langle S_f^z S_m^z\rangle + \langle S_m^z S_g^z\rangle) + \frac{n}{2}\langle S_f^z S_g^z\rangle. \tag{10}$$

The passage to the quasi-momentum representation yields a closed system of equations similar to the Gor'kov equations,

$$(E - \tilde{\varepsilon}_{\mathbf{k}} + \mu)\langle\langle X_{\mathbf{k}\sigma} | X_{\mathbf{k}\sigma}^+\rangle\rangle_E - \Delta_{\mathbf{k}}\langle\langle X_{-\mathbf{k}\bar{\sigma}}^+ | X_{\mathbf{k}\sigma}^+\rangle\rangle_E = 1 - \frac{n}{2}, \tag{11}$$

$$-(\Delta_{\mathbf{k}})^*\langle\langle X_{\mathbf{k}\sigma} | X_{\mathbf{k}\sigma}^+\rangle\rangle_E + (E + \tilde{\varepsilon}_{\mathbf{k}} - \mu)\langle\langle X_{-\mathbf{k}\bar{\sigma}}^+ | X_{\mathbf{k}\sigma}^+\rangle\rangle_E = 0,$$

where the renormalized spectrum of fermionic excitations is determined by the equation

$$\tilde{\varepsilon}_{\mathbf{k}} = \epsilon - \left(\frac{n^2}{16}\right)\frac{(1-n)}{(1-n/2)}J_0 + \left(1 - \frac{n}{2}\right)t_{\mathbf{k}} - \frac{n}{2}\left(1 - \frac{n}{2}\right)\frac{t_{\mathbf{k}}^2}{U} - \frac{1}{N}\sum_{\mathbf{q}}\left\{t_{\mathbf{q}} + \frac{n}{2}J_{\mathbf{k}-\mathbf{q}} + [(2-n)t_{\mathbf{k}} + (1-n)t_{\mathbf{q}}]\frac{t_{\mathbf{q}}}{U}\right\} \times \frac{K_{\mathbf{q}}}{1 - n/2} + \frac{1}{N}\sum_{\mathbf{q}}\left\{t_{\mathbf{k}-\mathbf{q}} + \frac{n}{2}J_{\mathbf{q}} + (2-n)\frac{t_{\mathbf{k}}t_{\mathbf{k}-\mathbf{q}}}{U} - \frac{n}{2}\frac{t_{\mathbf{k}-\mathbf{q}}^2}{U}\right\}\frac{C_{\mathbf{q}}}{1 - n/2}. \tag{12}$$

Here, $t_{\mathbf{q}}$ and $J_{\mathbf{q}}$ are the Fourier transforms of the hopping and exchange integrals, respectively. The renormalizations in spectrum (12) caused by three-center interactions are proportional to the ratio between the square of the hopping integral and the U parameter. The majority of them depend on the kinetic ($K_{\mathbf{q}} = \langle X_{\mathbf{q}\sigma}^+ X_{\mathbf{q}\sigma}\rangle$) and quasi-spin

$$C_{\mathbf{q}} = \sum_f \exp\{-i(\mathbf{R}_f - \mathbf{R}_m)\mathbf{q}\}\{\langle S_f^z S_m^z\rangle + \langle S_f^+ S_m^-\rangle\} \tag{13}$$

correlators. Solving (11) and applying the spectral theorem, we can find the kinetic correlator and the energy spectrum of the system

$$K_{\mathbf{q}} = \left(1 - \frac{n}{2}\right)\left(\frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{2E_{\mathbf{k}}} + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}f\left(\frac{E_{\mathbf{k}}}{T}\right)\right),$$

$$f(x) = (\exp x + 1)^{-1}, \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}, \tag{14}$$

$$\xi_{\mathbf{k}} = \tilde{\varepsilon}_{\mathbf{k}} - \mu,$$

and the self-consistency equation for the superconducting order parameter $\Delta_{\mathbf{k}}$,

$$\Delta_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{q}}\left\{2t_{\mathbf{q}} + \frac{n}{2}(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}}) + 4\left(1 - \frac{n}{2}\right)\frac{t_{\mathbf{k}}t_{\mathbf{q}}}{U} - n\frac{t_{\mathbf{q}}^2}{U}\right\}\frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{q}}}\tanh\left(\frac{E_{\mathbf{q}}}{2T}\right). \tag{15}$$

4. SPHERICALLY SYMMETRICAL CORRELATION FUNCTIONS

Let us find the equation for the quasi-spin correlator to obtain a closure to the self-consistency equations. We will use the ideology of the quantum spin liquid [24–26] and write the equations of motion for Bose Green functions describing the dynamics of the spin degrees of freedom. The first equation of motion has the form

$$\omega\langle\langle X_{j+l}^{\sigma\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega = -\sum_n t_{nl}L_{nl}^{\sigma\bar{\sigma}}(\omega) + 2\sum_n J_{ln}L_{ln}^z(\omega) + \langle\langle[X_{j+l}^{\sigma\bar{\sigma}}, H_{(3)}] | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega, \tag{16}$$

where $L_{nl}^{\sigma\bar{\sigma}}(\omega)$ and $L_{nl}^z(\omega)$ are antisymmetric with

respect to l and n,

$$L_{nl}^{\sigma\bar{\sigma}}(\omega) = \langle\langle X_{j+n}^{\sigma 0} X_{j+l}^{0\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega - [l \longleftrightarrow n],$$
$$L_{ln}^{z}(\omega) = \frac{1}{2}\langle\langle (X_{j+l}^{\sigma\sigma} - X_{j+l}^{\bar{\sigma}\bar{\sigma}}) X_{j+n}^{\sigma\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega - [l \longleftrightarrow n]. \quad (17)$$

The $[l \longleftrightarrow n]$ symbol in the right-hand sides of Eqs. (17) stands for the terms obtained from the preceding terms by the exchange of the indices l and n. The last term in (16) results in the appearance of Green functions containing the product of three Hubbard operators. If two Hubbard operators have equal site indices, then, thanks to the algebra of Hubbard operators, such a higher Green function reduces to a lower one. However, if all site indices are different, the reduction to a lower Green function is performed following the uncoupling scheme

$$\langle\langle X_m^{\bar{\sigma}\bar{\sigma}} X_n^{\sigma 0} X_l^{0\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega \longrightarrow \langle X_m^{\bar{\sigma}\bar{\sigma}}\rangle \langle\langle X_n^{\sigma 0} X_l^{0\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega,$$
$$\langle\langle X_m^{\sigma\bar{\sigma}} X_l^{\sigma 0} X_n^{0\sigma} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega \longrightarrow \langle X_l^{\sigma 0} X_n^{0\sigma}\rangle \langle\langle X_m^{\sigma\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega. \quad (18)$$

After the Fourier transform, (16) takes the form

$$\omega G_q^{\sigma\bar{\sigma}}(\omega) = \frac{1}{N}\sum_k \left(-t_k + \frac{n}{2}\frac{t_k^2}{U}\right) L_{k,q-k}^{\sigma\bar{\sigma}}(\omega) + 2\frac{1}{N}\sum_k J_k L_{q-k,k}^{z}(\omega), \quad (19)$$

where we introduced the Fourier transforms of the corresponding Green functions,

$$\langle\langle X_{j+l}^{\sigma\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega = \frac{1}{N}\sum_q e^{iql} G_q^{\sigma\bar{\sigma}}(\omega),$$
$$L_{nl}^{\alpha}(\omega) = \frac{1}{N^2}\sum_{qp} e^{iqn+ipl} L_{qp}^{\alpha}(\omega), \quad \alpha = \{\sigma, \bar{\sigma}, z\}. \quad (20)$$

The higher Green functions $L_{nl}^{\sigma\bar{\sigma}}(\omega)$ and $L_{ln}^{z}(\omega)$ are calculated using a similar procedure. We omit cumbersome intermediate calculations and only give the final result.

The equation for the $L_{qp}^{\sigma\bar{\sigma}}(\omega)$ Green function can be written in the form

$$\omega L_{q,p}^{\sigma\bar{\sigma}}(\omega) = 2(K_q - K_p) + G_{q+p}^{\sigma\bar{\sigma}}(\omega)\left\{\frac{2}{U}\frac{1}{N}\sum_k t_k\left[t_q\left(K_k + \frac{2}{3}C_{k+q}\right) - t_p\left(K_k + \frac{2}{3}C_{k+p}\right)\right] + \frac{2}{U}t_q t_p (K_q - K_p) + \frac{n}{2}(J_0 + J_{q+p})(K_q - K_p) + \left(n\frac{t_q + t_p}{U} - 2\right)(t_p K_p - t_q K_q)\right\}$$
$$+ M_{q,p}^{\sigma\bar{\sigma}}(\omega)\left\{\left(1 - \frac{n}{2}\right)\left(t_p - t_q + \frac{n}{2}\frac{t_q^2 - t_p^2}{U}\right) + \frac{1}{N}\sum_k \frac{t_k}{U}\left[t_q\left(K_k - \frac{2}{3}C_{k+q}\right) - t_p\left(K_k - \frac{2}{3}C_{k+p}\right)\right] + \frac{1}{2}\frac{1}{N}\sum_k J_k (K_{k+p} - K_{k+q})\right\}$$
$$+ \left[\frac{n}{2}\left(1 - \frac{n}{2}\right)(t_p - t_q) + t_q K_q - t_p K_p\right] \times \frac{1}{U}\frac{1}{N}\sum_k t_k M_{q+p-k,k}^{\sigma\bar{\sigma}}(\omega) + (K_q - K_p) \times \frac{1}{N}\sum_k M_{q+p-k,k}^{\sigma\bar{\sigma}}(\omega)\left[\frac{t_k t_{q+p-k}}{U} - \frac{1}{2}J_{p-k}\right]$$
$$+ \frac{1}{U}\frac{1}{N}\sum_k t_k M_{q+p-k,k}^{\sigma\bar{\sigma}}(\omega)\frac{1}{N} \times \sum_{k_1} t_{k_1}\left[\frac{2}{3}C_{q+k_1} - \frac{2}{3}C_{p+k_1} + K_{q+k_1-k} - K_{p+k_1-k}\right], \quad (21)$$

where $M_q^{\sigma\bar{\sigma}}(\omega)$ is the Fourier transform of the higher Green function symmetrical with respect to the n and l indices,

$$M_{nl}^{\sigma\bar{\sigma}}(\omega) = \langle\langle X_{j+n}^{\sigma 0} X_{j+l}^{0\bar{\sigma}} | X_j^{\bar{\sigma}\sigma}\rangle\rangle_\omega + [n \longleftrightarrow l].$$

This equation can be simplified using the approximation applied in [25] to study the t–J model. As the contributions of the $M_{n,l}^{\sigma\bar{\sigma}}(\omega)$ functions to (21) are negligibly small if $n \neq l$ and

$$M_{l,l}^{\sigma\bar{\sigma}}(\omega) = 2G_n^{\sigma\bar{\sigma}}(\omega)$$

at $n = l$, we obtain the approximate equation

$$M_{n,l}^{\sigma\bar{\sigma}}(\omega) = 2\delta_{nl} G_n^{\sigma\bar{\sigma}}(\omega).$$

In the quasi-momentum representation, this equation is written as

$$M_{qp}^{\sigma\bar{\sigma}}(\omega) = 2G_{q+p}^{\sigma\bar{\sigma}}(\omega). \quad (22)$$

Equation (21) then takes the form that explicitly relates the higher Green function under consideration to the lower functions,

$$\begin{aligned}\omega L_{k,q-k}^{\sigma\bar{\sigma}}(\omega) &= 2(K_k - K_{q-k}) \\ &+ G_q^{\sigma\bar{\sigma}}(\omega)\Bigg[(t_k - t_{q-k})\Bigg(n - 2 + \frac{4}{U}\frac{1}{N}\sum_{k_1} K_{k_1} t_{k_1}\Bigg) \\ &+ n\Bigg(1 - \frac{n}{2}\Bigg)\frac{t_k^2 - t_{q-k}^2}{U} \\ &+ (K_k - K_{q-k})\Bigg(\frac{2t_k t_{q-k}}{U} + n\frac{J_0 + J_q}{2} + J_q\Bigg) \\ &+ (t_{q-k}K_{q-k} - t_k K_k)\Bigg(-2 + n\frac{t_k + t_{q-k}}{U}\Bigg)\Bigg].\end{aligned} \quad (23)$$

Applying approximation (22) to the Fourier transform of the third Green function $L_{q,k}^z(\omega)$ defined by (20) yields

$$\begin{aligned}\omega L_{q-k,k}^z(\omega) &= \frac{4}{3}(C_{q-k} - C_k) + \frac{4}{3}G_q^{\sigma\bar{\sigma}}(\omega) \\ &\times \frac{1}{N}\sum_{k_1} J_{k_1}(\tilde{C}_{q-k+k_1} - \tilde{C}_{k-k_1}) \\ &+ \frac{4}{3}G_q^{\sigma\bar{\sigma}}(\omega)[J_q\tilde{C}_{q-k} - J_{q-k}\tilde{C}_{q-k} - J_q\tilde{C}_k + J_k\tilde{C}_k] \\ &+ G_q^{\sigma\bar{\sigma}}(\omega)\Bigg[\frac{n}{2}(J_{q-k} - J_k) + \frac{2}{U}\frac{1}{N} \\ &\times \sum_{k_1} t_{k_1}(t_{k-k_1}K_{k-k_1} - t_{q-k-k_1}K_{q-k-k_1})\Bigg],\end{aligned} \quad (24)$$

where $\tilde{C}_q = \alpha C_q + (1 - \alpha)3n/4$. As in [24–26], we here introduced the vertex correction α according to the equation

$$\tilde{C}_{nl} = (\alpha(1 - \delta_{nl}) + \delta_{nl})C_{nl}.$$

This procedure allows the errors of uncoupling to be corrected by imposing the requirement of the fulfillment of the corresponding sum rules. In our problem, the sum rule role is played by the condition $C_{ll} = 3n/4$. Note that all terms in the last two rows of (24) appear because of the interaction $H_{(3)}$.

The system of three equations, (19), (23), and (24), allows us to find the quasi-spin correlator. To simplify the final analytic equations, we use the small parameters of the system $\lambda = 2|t|/U \ll 1$ and $\delta = (1 - n) \ll 1$ (below, we only consider the region of low hole doping). It is easy to see that $K_p = (1 - n/2)f(\varepsilon_p) \longrightarrow 1/2$ as $n \longrightarrow 1$, and all terms related to the kinematics of the problem are therefore canceled in (23) and (24). The remaining three rows of (24) describe spin correlations in the Heisenberg limit [24, 26]. Clearly, all terms related to kinematics are proportional to either the concentration of holes $\delta = 1 - n$ or kinematic correlators K_f ($f \neq 0$), which are also proportional to $(1 - n)$. These two parameters have equal orders of smallness at the characteristic λ value $\lambda = 0.25$ and the concentration of electrons $n > 0.75$. Calculations show that, in the region of low doping, the kinematic correlators K_f ($f \neq 0$) are much smaller than λ and magnetic correlators C_f (at $f \neq 0$).

The above considerations allow us to simplify equations by retaining terms of order δ, $\lambda\delta$, and λ^2 only and ignoring all terms of order $\lambda^2\delta$. The Green function $G_q^{\sigma\bar{\sigma}}(\omega)$ found from (19), (23), and (24) then takes the eventual form

$$\begin{aligned}C_q^{\sigma\bar{\sigma}}(\omega) &= \frac{A_q(\omega)}{\omega^2 - \omega^2(q)}, \\ A_q(\omega) &= \frac{1}{N}\sum_k\Bigg[\Bigg(-2t_k + \frac{n}{U}t_k^2\Bigg)(K_k - K_{q-k}) \\ &+ \frac{8}{3}J_k(C_{q-k} - C_k)\Bigg],\end{aligned} \quad (25)$$

where the spectrum of magnetic excitations $\omega(q)$ is determined by the equation

$$\begin{aligned}\omega^2(q) &= \frac{1}{N}\sum_k\Bigg[t_k(t_k - t_{q-k})\Bigg((2 - n)\Bigg(1 - n\frac{t_k}{U}\Bigg) \\ &+ 2nK_k\frac{t_k + t_{q-k}}{U} - \frac{4}{U}\frac{1}{N}\sum_{k_1} t_{k_1}K_{k_1}\Bigg) \\ &+ 2t_k(t_{q-k}K_{q-k} - t_k K_k) - t_k(K_k - K_{q-k}) \\ &\times\Bigg(\frac{2t_k t_{q-k}}{U} + n\frac{J_0 + J_q}{2} + J_q\Bigg) \\ &+ \frac{8}{3}J_k\frac{1}{N}\sum_{k_1} J_{k_1}(\tilde{C}_{q-k+k_1} - \tilde{C}_{k-k_1}) \\ &+ \frac{8}{3}J_k(J_q\tilde{C}_{q-k} - J_{q-k}\tilde{C}_{q-k} - J_q\tilde{C}_k + J_k\tilde{C}_k)\Bigg].\end{aligned} \quad (26)$$

Only the last two rows of (26) remain in the limit $n \longrightarrow 1$, which corresponds to the spectrum of magnons in the Heisenberg model [24, 26].

Applying the spectral theorem in the usual way leads to self-consistent equations for magnetic correlators. By numerically solving these equations, we can calculate correlator values. After this, spectrum renormalizations caused by magnetic fluctuations and their influence on the superconducting transition temperature are determined.

5. THE SPECTRUM AND DENSITY OF STATES OF FERMIONIC EXCITATIONS IN THE t–J^* MODEL

It is well known [3–5] that high-temperature superconductivity conditions are to a substantial extent determined by the special features of the energy spectrum of Fermi quasi-particles. These features can be responsible for the singular behavior of the density of states of charge carriers. Bearing this in mind, let us first comparatively analyze the renormalizations of the energy spectrum caused by simultaneous magnetic fluctuation and three-center interaction effects.

Numerical calculations were performed in the nearest-neighbor approximation (the influence of long-range hoppings is in part discussed in the concluding section). Generally, a system of ten self-consistent transcendental equations was solved. This system determined ten values: three magnetic and five kinetic correlators, the chemical potential, and the vertex renormalization α. For convenience of comparing the results, we first give the fermionic energy spectrum of the t–J model without the inclusion of magnetic correlators,

$$\tilde{\varepsilon}_H(\mathbf{k}) = -4|t|\left[1 - \frac{n}{2} + \frac{\lambda K_1}{1-n/2}\right]\gamma_1(\mathbf{k}),$$
$$\gamma_1(\mathbf{k}) = \frac{1}{2}(\cos(k_x a) + \cos(k_y a)), \tag{27}$$

where a is the distance between square lattice sites.

If three-center interactions are included (the t–J^* model), the quasi-momentum dependence of the energy spectrum $\tilde{\varepsilon}_{tJ^*}(\mathbf{k})$ is described by a linear superposition of three invariants for a square lattice. If magnetic fluctuations are ignored, the fermionic spectrum is determined by the equation

$$\tilde{\varepsilon}'_{tJ^*}(\mathbf{k}) = -4|t|\left[1 - \frac{n}{2} + \frac{(4-3n/2)\lambda K_1}{1-n/2}\right]\gamma_1(\mathbf{k})$$
$$-|t|\lambda n\left(1-\frac{n}{2}\right)[2\gamma_2(\mathbf{k}) + \gamma_3(\mathbf{k})]. \tag{28}$$

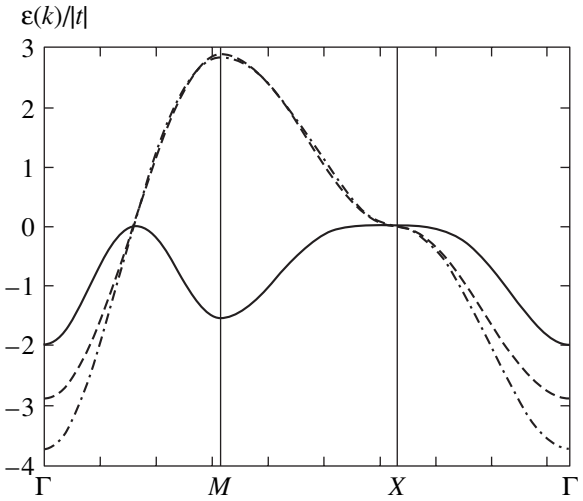

Fig. 1. Spectrum of fermionic excitations in the Hubbard model for various approximations under strong electron correlation conditions.

The appearance of two new invariants compared with (27),

$$\gamma_2(\mathbf{k}) = \cos(k_x a)\cos(k_y a),$$
$$\gamma_3(\mathbf{k}) = \frac{1}{2}(\cos(2k_x a) + \cos(2k_y a)), \tag{29}$$

formally corresponds to the presence of effective hoppings between sites of distant coordination spheres in the system. The physical origin of such hoppings is fairly simple to explain if the operator structure of three-center interactions is taken into account.

The self-consistent calculations of the kinetic correlator for spectrum (28) at $n = 0.92$ give $K_1 = 0.0628$. The corresponding calculated dispersion dependence of excitation energy is shown by the dot-and-dash line in Fig. 1. The dispersion dependences are given with the standard denotations of the distinguished Brillouin zone points, $\Gamma = (0, 0)$, $X = (\pi, 0)$, and $M = (\pi, \pi)$. A comparison of the dot-and-dash line with the dashed line corresponding to spectrum (27) shows that, quantitatively, spectrum renormalizations are insignificant under these conditions. This conclusion fully corresponds to the results reported in [10, 11].

A quite different result is obtained if not only three-center interactions but also magnetic correlations are included. The equation for the energy spectrum then takes the form

$$\tilde{\varepsilon}_{tJ^*}(\mathbf{k}) = -4|t|\left[1 - \frac{n}{2} + \frac{(4-3n/2)\lambda K_1 + C_1}{1-n/2}\right]\gamma_1(\mathbf{k})$$
$$-2|t|\lambda\left[n\left(1-\frac{n}{2}\right) - 4C_1 + \frac{nC_2}{1-n/2}\right]\gamma_2(\mathbf{k}) \tag{30}$$
$$-|t|\lambda\left[n\left(1-\frac{n}{2}\right) - 4C_1 + \frac{nC_3}{1-n/2}\right]\gamma_3(\mathbf{k}),$$

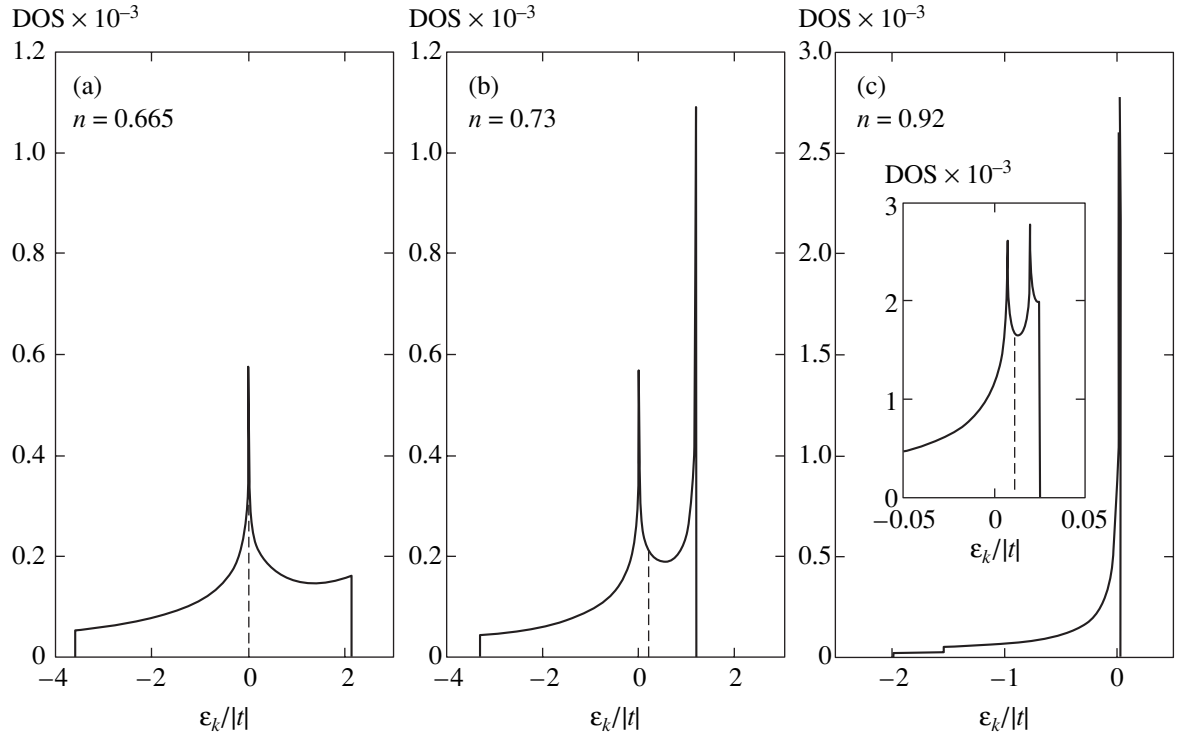

Fig. 2. Evolution of the density of fermionic states in the t–J* model depending on the concentration n. The structure of the density of states at $n = 0.92$ (two closely spaced peaks) is shown in the inset in Fig. 2c on a smaller scale. The vertical dashed line corresponds to the chemical potential position.

where C_2 and C_3 are the magnetic correlators for the second and third coordination sphere, respectively [26]. The self-consistent calculations performed with this energy spectrum for $n = 0.92$ give the correlator values $C_1 = -0.2639$, $C_2 = 0.1347$, $C_3 = 0.1115$, and $K_1 = 0.0037$. The corresponding quasi-momentum dependence of the energy spectrum is shown by the solid line in Fig. 1. The principal feature that qualitatively distinguishes this spectrum from the two previous ones is the presence of a minimum at the M Brillouin zone point. This minimum only appears at $n > n_1$. The n_1 value depends on the model parameters. According to the self-consistent calculations for spectrum (30) with $\lambda = 0.25$, $n_1 \approx 0.72$.

To describe the renormalizations of the spectrum mentioned above, let us consider the evolution of the density of states as n varies. The density of states calculated self-consistently for $n = 0.665$ is shown in Fig. 2a. As $n < n_1$, there is only one well-known Van Hove singularity corresponding to the Brillouin zone saddle points X. It is present in all the spectra considered above at all concentrations n. The states with the energies corresponding to this Van Hove singularity are populated at $n \approx 0.66$. This is why the theoretical concentration dependences $T_c(n)$ contain maxima at $n \approx 0.66$ (see Fig. 3). The structure of the density of states at $n > n_1$ is shown in Fig. 2b. The second Van Hove singularity then appears close to the top of the zone. It is formed when the spectral curve has a minimum at the M Brillouin zone points provided $n = n_1$ (at $n < n_1$, the kinetic and spin correlator values are such that dispersion dependence (30) has a maximum rather than a minimum at the M Brillouin zone points). Just the appearance of the local minimum at $n \approx n_1$ induces the new logarithmic singularity of the density of states. This Van Hove singularity is retained as the concentration increases up to $n = 1$. At $n \approx n_1$, the two singularities are spaced fairly far apart on the energy scale. The distance between them, however, decreases as n increases because the top of the zone lowers. The structure of the density of states shown in Fig. 2c corresponds to the concentration at which T_c is maximum (see solid curve in Fig. 3). The distance between the peaks of the density of states is then commensurate with the critical temperature T_c. In addition, the chemical potential and temperature then have values at which the contribution to thermodynamics is determined by all states in the vicinity of the top of the zone. To conclude this section, note again that the new peak of the density of states in the nearest-neighbor approximation only appears when both spin correlations and three-center interactions are included simultaneously.

6. THE CONCENTRATION DEPENDENCE OF THE SUPERCONDUCTING TRANSITION TEMPERATURE

Clearly, the special features of the energy spectrum mentioned above should manifest themselves in many

t–J* model characteristics. By way of example, let us consider the concentration dependence of the transition temperature to the superconducting state with the order parameter of $d_{x^2-y^2}$-type symmetry.

The superconducting state can be formed if integral equation (15) has a nontrivial solution $\Delta_{\mathbf{k}} \neq 0$. The kernel of this equation is the sum of four terms. The first term, which is proportional to $2t_{\mathbf{q}}$, corresponds to the kinematic mechanism of pairing [2]. The origin of the second kernel term is both exchange and three-center interactions. Exchange interaction gives the contribution proportional to $(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})$, and three-center interaction introduces a correction proportional to $(-1 + n/2)(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})$, which tends to suppress superconductivity. Because of the superposition of these contributions, the coefficient of the term proportional to $(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})$ equals the renormalization factor $n/2$ [13] rather than one as in the t–J model. Precisely this renormalization of the coupling constant in the t–J* model substantially suppresses T_c [14].

As is well known, (15) reduces to a transcendental equation in the nearest-neighbor approximation. In what follows, we only consider superconducting phases with order parameter of $d_{x^2-y^2}$ symmetry. Its quasi-momentum dependence has the form $\Delta(\mathbf{k}) = \Delta_0(\cos k_x a - \cos k_y a)$. The equation determining the temperature of the superconducting transition then takes the form

$$1 = \frac{n}{2}\frac{J}{N}\sum_{\mathbf{q}}\frac{(\cos q_x a - \cos q_y a)^2}{\tilde{\varepsilon}_{\mathbf{q}} - \mu}\tanh\left(\frac{\tilde{\varepsilon}_{\mathbf{q}} - \mu}{2T_c}\right). \quad (31)$$

We see that, for $d_{x^2-y^2}$ symmetry, the first, third, and fourth terms of the kernel of (15) make no contribution. Three-center interactions therefore manifest themselves only by renormalizing the coupling constant and modifying the spectrum of fermionic excitations.

The solid curve shown in Fig. 3 was obtained by numerically solving (31). To better visualize the effects under consideration, we plotted the concentration dependence of the critical temperature T_c for spectrum (27) of the t–J model (dashed line) and the $T_c(n)$ dependence for the t–J* model without taking magnetic correlations into account [14] (dot-and-dash line) in the same figure. We see that simultaneously including three-center interactions and magnetic correlations changes the $T_c(n)$ dependence qualitatively, namely, a second maximum appears in the low doping region, which corresponds to a substantial increase in the number of electrons participating in Cooper pairing. Figure 2c shows that this increase is related to a considerable growth of the density of fermionic states in the vicinity of the Fermi level and to effective broadening of the energy region that makes the major contribution to the integration. The second $T_c(n)$ maximum at $n = 0.92$ is much higher than the first one ($n = 0.66$) because of a much larger number of electrons in the vicinity of the chemical potential and a large increase in the effective coupling constant value caused by its dependence on n.

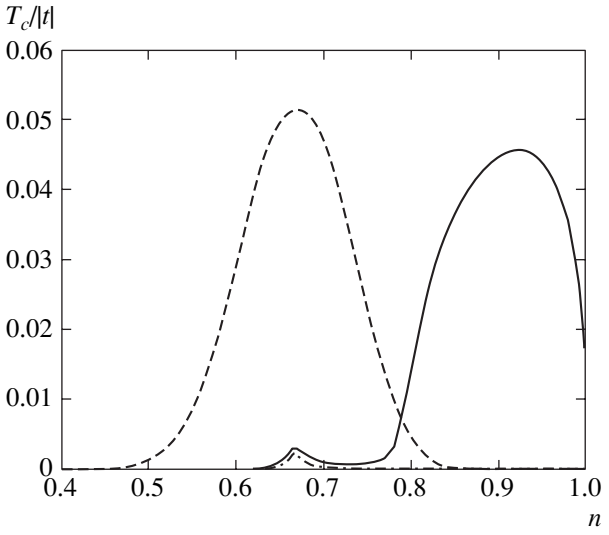

Fig. 3. Concentration dependences of the critical temperature for various approximations.

7. CONCLUSIONS

The results presented above show that joint three-center interaction and magnetic correlation effects play an important role in the t–J* model. A new Van Hove singularity is then induced in the density of states of Fermi quasi-particles at high energies. As this singularity appears at low hole concentrations, the suggestion can be made of the magnetopolaron nature of the induction of the new Van Hove singularity. This suggestion correlates with recent results obtained in studies of the electronic structure of a strongly correlated spin-fermion liquid with invoking an extended basis set for including magnetopolaron states [27]. The second argument in favor of this hypothesis is the structure of $H_{(3)}$, which relates electron hopping to the spin dynamics of neighboring sites. It is clear in view of these considerations why the inclusion of $H_{(3)}$ without taking magnetic correlations into account did not cause substantial changes in the electron energy spectrum and the density of states of fermionic excitations.

Changes in the energy spectrum were considered for the example of the concentration dependence of the superconducting transition temperature. Clearly, such qualitative changes in the density of fermionic states should also result in other noticeable changes in the thermodynamic properties of the system. We also think it important that the reproduction of energy spectrum parameters, for instance, from the angular resolution photoemission spectra (ARPES) requires taking into account the renormalizations described above. Note that, although our analysis was limited to the use of the nearest-neighbor approximation, long-range hoppings

were effectively included. This circumstance should substantially influence the values of the parameters being reproduced.

Including the kinetic energy of long-range hoppings (t' and t'') into the Hamiltonian can strengthen as well as suppress the new Van Hove singularity in the region of low hole concentrations. The corresponding calculations are a separate problem; they must include new magnetic correlators between sites from more distant coordination spheres (up to the ninth sphere inclusive). Solving the self-consistent problem for the values of these correlators is beyond the scope of the present work. As concerns the influence of long-range hoppings on the conditions of superconducting phase existence, changes in the kernel of the integral equation should primarily be taken into account [28]. The renormalizations of effective hoppings considered in this work can then also influence the concentration dependence $T_c(n)$. Note one more subtlety. Formally, the effect of three-center interactions related to inducing hoppings between sites from distant coordination spheres can be modeled by going beyond the scope of the nearest-neighbor approximation but without taking $H_{(3)}$ into account. However, we then lose the second effect of $H_{(3)}$, essential to superconductivity, which is related to the renormalization of the effective coupling constant [13] and responsible for the dependence of T_c on n just such as is shown in Fig. 3.

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