Condensed Matter Physics, 2002, Vol. 5, No. 4(32), pp. 707–727

CONDENSED
MATTER
PHYSICS

Superconductivity in the t-J model

N.M.Plakida

Joint Institute for Nuclear Research, 141980 Dubna, Russia

Received September 2, 2002

A comparison of microscopic theories for superconductivity in the limit of strong electron correlations is presented. We consider the results for the two-dimensional t-J model obtained within a projection technique for the Green functions in terms of the Hubbard operators and a slave-fermion representation for the RVB state. It is argued that the latter approach resulting in an odd-symmetry p-wave pairing for fermions is inadequate.

Key words: *strong electron correlations, high-temperature superconductors, Green functions, slave fermions*

PACS: *74.20.-z, 74.20.Mn, 74.72.-h*

1. Introduction

A mechanism of high-temperature superconductivity in cuprates is still unresolved since strong electron correlations in copper-oxygen planes prevent us from applying the well established methods of band structure calculations developed for conventional metals. An important role of electron correlations in cuprates was initially stressed by Anderson [1] who suggested to consider them within the framework of the Hubbard model or the so-called t-J model which follows from the Hubbard model in the limit of strong correlations. To study these models, a lot of numerical work have been done [2,3] though the obtained results are still controversial. For instance, a robust d-wave pairing was observed for the t-J model [4], while a long-range order was not found in the original Hubbard model [5].

In analytical approaches, mostly a mean-field theory (MFA) was applied in the studies of the Hubbard or the t-J models. The resonating valence bond (RVB) state in the t-J model was proposed by Baskaran et al. [6] where superconductivity was obtained as a result of spin correlations induced by the superexchange interaction. Similar results were found by Cyrot [7] for a superconducting pairing mediated by superexchange interaction. To overcome the problem of strong correlations in the t-J model and nonfermionic commutation relations for the physical electron operators, a number of auxiliary field representations were proposed (see, e.g., [8–32]). However, in these methods, a spin-charge separation is usually assumed for spinon and holon fields which violates rigorous restrictions imposed by nonfermionic commutation relations as the “no double occupancy” constraint which may result in unphysical conclusions.

A reliable analytical approach to deal with strong correlations in the Hubbard or the t-J model is based on the Green function methods in terms of the Hubbard operators which rigorously preserve the non-fermionic commutation relations [33]. Here, we may mention our results based on the Mori-type projection technique for the Green functions [34–36] and the diagram technique calculations by Izyumov et al. [37,38]. These approaches enable one to go beyond MFA by taking into account self-energy corrections. For instance, a numerical solution of the Dyson equation in [36] revealed a non-Fermi-liquid behavior in the normal state at low doping and the d-wave superconductivity mediated by the exchange and spin-fluctuation pairing. In the recent paper [39] a microscopical theory of superconductivity in CuO_2 layer within the effective two-band p-d Hubbard model in the strong correlation limit was developed. It has been proved that the MFA for the Hubbard model results in the antiferromagnetic exchange d-wave pairing which is equivalent to the pairing observed in the t-J model in MFA.

In the present paper we compare the results for the t-J model obtained within the Green function method in terms of the Hubbard operators [34–36] and by applying the slave-fermion hard-boson representation [27] for the RVB state. It will be shown that the latter approach results in an odd-symmetry p-wave pairing for the spinless fermions as in the path-integral representation in [32] which contradicts the known numerical and analytical calculations. It casts doubts on the validity of spin-charge separation approach in studying the superconducting pairing in the t-J model.

In the next section we briefly present the results of the projection technique for the Green functions [36] for the t-J model. In section 3 superconducting pairing within the slave-fermion representation for the Hubbard operators is considered. Results and discussions are given in section 4. Concluding remarks are in section 5.

2. Green function method

2.1. Dyson equation for the t-J model

In the present section we consider the superconducting pairing in the t-J model by applying the Green function technique [34–36]. The t-J model in the standard notation [1,42] reads:

$$H_{t-J} = -t \sum_{i \neq j, \sigma} \tilde{a}^{+}_{i\sigma} \tilde{a}_{j\sigma} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j), \tag{1}$$

where $\tilde{a}^{+}_{i\sigma} = a^{+}_{i\sigma}(1 - n_{i-\sigma})$ are the projected operators for physical electrons, $n_i = \sum_\sigma \tilde{a}^{+}_{i\sigma} \tilde{a}_{i\sigma}$ is the number operator and $S^{\alpha}_i = (1/2) \sum_{s,s'} \tilde{a}^{+}_{is} \sigma^{\alpha}_{s,s'} \tilde{a}_{is'}$ are spin-1/2 operators. Here, t is the effective transfer integral and J is antiferromagnetic exchange energy for a pair of the nearest neighbor spins, $\langle ij \rangle$, $i > j$.

To take into account the projected character of electron operators on a rigorous basis we employ the Hubbard operator technique. The Hubbard operators (HO) are defined as $X_i^{\alpha\beta} = |i,\alpha\rangle\langle i,\beta|$ for three possible states $|i,\alpha\rangle$ at a lattice site i: for an empty site $|i,0\rangle$ and for a singly occupied site $|i,\sigma\rangle$ by an electron with the spin $\sigma/2$ ($\sigma = \pm 1,\ \bar{\sigma} = -\sigma$). They obey the completeness relation

$$X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} = 1, \tag{2}$$

which rigorously preserves the constraint of no double occupancy. The spin and density operators in equation (1) are expressed by HO as

$$S_i^{\sigma} = X_i^{\sigma\bar{\sigma}}, \qquad S_i^{z} = \frac{1}{2}\sum_{\sigma} \sigma X_i^{\sigma\sigma}, \qquad n_i = \sum_{\sigma} X_i^{\sigma\sigma}. \tag{3}$$

The HO obey the following multiplication rule $X_i^{\alpha\beta} X_i^{\gamma\delta} = \delta_{\beta\gamma} X_i^{\alpha\delta}$ and commutation relations

$$\left[X_i^{\alpha\beta}, X_j^{\gamma\delta}\right]_{\pm} = \delta_{ij}\left(\delta_{\beta\gamma} X_i^{\alpha\delta} \pm \delta_{\delta\alpha} X_i^{\gamma\beta}\right), \tag{4}$$

where the upper sign stands for the Fermi-like HO (as, e. g., $X_i^{0\sigma}$) and the lower sign stands for the Bose-like operators (as the spin and number operators in equation (3)).

By using the Hubbard operator representation, we write the Hamiltonian of the t-J model (1) in a more general form:

$$H_{t-J} = -\sum_{i\neq j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \mu \sum_{i\sigma} X_i^{\sigma\sigma} + \frac{1}{4}\sum_{i\neq j,\sigma} J_{ij}\left(X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}\right). \tag{5}$$

The electron hopping energy for the nearest neighbors, $t_{ij} = t$, and the second neighbors, $t_{ij} = t'$, on a 2D square lattice, and the exchange interaction $J_{ij} = J$ for the nearest neighbors[1] can be considered as independent parameters if, starting from a more realistic for copper oxides three-band p-d model [43], we reduce it to the t-J model [42]. In that case the parameters t, t' and J can be evaluated in terms of the original parameters of the p-d model (see, e.g., [44,45]). We also introduced the chemical potential μ which can be calculated from the equation for the average number of electrons

$$n = \langle n_i \rangle = \sum_{\sigma} \langle X_i^{\sigma\sigma} \rangle. \tag{6}$$

To discuss the superconducting pairing within the model (5), we introduce the Nambu notation for HO:

$$\Psi_{i\sigma} = \begin{pmatrix} X_i^{0\sigma} \\ X_i^{\bar{\sigma}0} \end{pmatrix}, \qquad \Psi_{i\sigma}^{+} = \left(X_i^{\sigma 0}\ X_i^{0\bar{\sigma}}\right),$$

and consider the matrix Green function (GF)

$$\hat{G}_{ij,\sigma}(t-t') = \langle\langle \Psi_{i\sigma}(t) | \Psi_{j\sigma}^{+}(t') \rangle\rangle = \begin{pmatrix} G_{ij\sigma}^{11} & G_{ij\sigma}^{12} \\ G_{ij\sigma}^{21} & G_{ij\sigma}^{22} \end{pmatrix}, \tag{7}$$

[1] Sometimes a coefficient (1/2) instead of (1/4) is written in the last sum in equation (5) that results in two times larger values of contributions given by the exchange energy J (see, e.g., [34]).

where Zubarev's notation for the anticommutator GF is used [46].

By differentiating the GF (7) over the time t we get for the Fourier component the following equation

$$\omega \hat{G}_{ij\sigma}(\omega) = \delta_{ij}\hat{Q}_{\sigma} + \langle\langle \hat{Z}_{i\sigma} | \Psi_{j\sigma} \rangle\rangle_{\omega} \, , \tag{8}$$

where

$$\hat{Z}_{i\sigma} = [\Psi_{i\sigma}, H], \qquad \hat{Q}_{\sigma} = \begin{pmatrix} Q_{\sigma} & 0 \\ 0 & Q_{\bar{\sigma}} \end{pmatrix}, \qquad Q_{\sigma} = \langle X_i^{00} + X_i^{\sigma\sigma} \rangle.$$

Since we consider a spin-singlet state, the correlation function $Q_{\sigma} = Q = 1 - n/2$ depends only on the average number of electrons (6).

Now, we project the many-particle GF in (8) on the original single-electron GF

$$\langle\langle \hat{Z}_{i\sigma} | \Psi_{j\sigma}^{+} \rangle\rangle = \sum_{l} \hat{E}_{il\sigma} \langle\langle \Psi_{l\sigma} | \Psi_{j\sigma}^{+} \rangle\rangle + \langle\langle \hat{Z}_{i\sigma}^{(\mathrm{irr})} | \Psi_{j\sigma}^{+} \rangle\rangle, \tag{9}$$

where the irreducible (irr) part of the many-particle operator $\hat{Z}_{i\sigma}$ is defined by the equation

$$\langle \{ \hat{Z}_{i\sigma}^{(\mathrm{irr})}, \Psi_{j\sigma}^{+} \} \rangle = \langle \{ \hat{Z}_{i\sigma} - \sum_{l} \hat{E}_{il\sigma} \Psi_{l\sigma}, \, \Psi_{j\sigma}^{+} \} \rangle = 0,$$

which results in the definition of the frequency matrix

$$\hat{E}_{ij\sigma} = \langle \{ [\Psi_{i\sigma}, H], \Psi_{j\sigma}^{+} \} \rangle \, Q^{-1}. \tag{10}$$

Now, we can introduce the zero-order GF in the generalized MFA which is given by the frequency matrix (10)

$$\hat{G}_{ij\sigma}^{0}(\omega) = Q \{ \omega \hat{\tau}_0 \delta_{ij} - \hat{E}_{ij\sigma} \}^{-1}. \tag{11}$$

To derive the Dyson equation for the single-electron GF (7) we write down an equation of motion for the irreducible part of the GF in (9) with respect to the second time t' for the right-hand side operator $\Psi_{j\sigma}^{+}(t')$. Then, performing the same projection procedure as in equation (9) we obtain the Dyson equation for the GF in the form

$$\hat{G}_{ij\sigma}(\omega) = \hat{G}_{ij\sigma}^{0}(\omega) + \sum_{kl} \hat{G}_{ik\sigma}^{0}(\omega) \, \hat{\Sigma}_{kl\sigma}(\omega) \, \hat{G}_{lj\sigma}(\omega), \tag{12}$$

where the self-energy operator $\hat{\Sigma}_{kl\sigma}(\omega)$ is defined by the equation

$$\hat{T}_{ij\sigma}(\omega) = \hat{\Sigma}_{ij\sigma}(\omega) + \sum_{kl} \hat{\Sigma}_{ik\sigma}(\omega) \, \hat{G}_{kl\sigma}^{0}(\omega) \, \hat{T}_{lj\sigma}(\omega). \tag{13}$$

Here, the scattering matrix is given by

$$\hat{T}_{ij\sigma}(\omega) = Q^{-1} \langle\langle \hat{Z}_{i\sigma}^{(\mathrm{irr})} | \hat{Z}_{j\sigma}^{(\mathrm{irr})^{+}} \rangle\rangle_{\omega} \, Q^{-1}. \tag{14}$$

From equation (13) it follows that the self-energy operator is given by the irreducible part of the scattering matrix (14) that has no parts connected by the single zero-order GF (11):

$$\hat{\Sigma}_{ij\sigma}(\omega) = Q^{-1} \langle\langle \hat{Z}^{(\mathrm{irr})}_{i\sigma} | \hat{Z}^{(\mathrm{irr})^+}_{j\sigma} \rangle\rangle^{(\mathrm{irr})}_{\omega} \, Q^{-1}. \tag{15}$$

Equations (11), (12) and (15) give an exact representation for the single-electron GF (7). However, to solve the self-consistent system of equations, one has to introduce an approximation for the many-particle GF in the self-energy matrix (15) which describes inelastic scattering of electrons on spin and charge fluctuations.

2.2. Self-consistent equations

Here, we derive a self-consistent system of equations in MFA. To calculate the frequency matrix (10) we use the equation of motion for the HO:

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} + \mu\right) X_i^{0\sigma} = -\sum_{l,\sigma'} t_{il} B_{i\sigma\sigma'} X_l^{0\sigma'} + \frac{1}{2}\sum_{l,\sigma'} J_{il}(B_{l\sigma\sigma'} - \delta_{\sigma\sigma'}) X_i^{0\sigma'}, \tag{16}$$

where we introduced the operator

$$B_{i\sigma\sigma'} = (X_i^{00} + X_i^{\sigma\sigma})\delta_{\sigma'\sigma} + X_i^{\bar{\sigma}\sigma}\delta_{\sigma'\bar{\sigma}} = (1 - \frac{1}{2}n_i + \sigma S_i^z)\delta_{\sigma'\sigma} + S_i^{\bar{\sigma}}\delta_{\sigma'\bar{\sigma}}\,. \tag{17}$$

The Bose-like operator (17) describes electron scattering on spin and charge fluctuations caused by the kinematic interaction (the first term in (16)) and by the exchange spin-spin interaction (the second term in (16)).

By performing commutations in (10) we get the following for the normal and for the anomalous parts of the frequency matrix:

$$\begin{aligned} E^{11}_{ij\sigma} &= -\mu\delta_{ij} + \delta_{ij}\sum_l \{t_{il}\langle X_i^{\sigma 0} X_l^{0\sigma}\rangle/Q + \frac{1}{2}J_{il}(Q - 1 + \chi^{cs}_{il}/Q)\} \\ &\quad - t_{ij}(Q + \chi^{cs}_{ij}/Q) - \frac{1}{2}J_{ij}\langle X_j^{\sigma 0} X_i^{0\sigma}\rangle/Q, \end{aligned} \tag{18}$$

$$\begin{aligned} E^{12}_{ij\sigma} &= \Delta_{ij\sigma} = \delta_{ij}\sum_l t_{il}\langle X_i^{0\bar{\sigma}} X_l^{0\sigma} - X_i^{0\sigma} X_l^{0\bar{\sigma}}\rangle/Q \\ &\quad - \frac{1}{2}J_{ij}\langle X_i^{0\bar{\sigma}} X_j^{0\sigma} - X_i^{0\sigma} X_j^{0\bar{\sigma}}\rangle/Q. \end{aligned} \tag{19}$$

Here, in the calculation of the correlation function for the normal component of the frequency matrix:

$$\begin{aligned} \sum_{\sigma'}\langle B_{i\sigma\sigma'} B_{j\sigma'\sigma}\rangle &= \langle (1 - \frac{1}{2}n_i + \sigma S_i^z)(1 - \frac{1}{2}n_j + \sigma S_j^z) + S_i^{\sigma} S_j^{\bar{\sigma}}\rangle \\ &= \langle (1 - \frac{1}{2}n_i)(1 - \frac{1}{2}n_j)\rangle + \langle \mathbf{S}_i \mathbf{S}_j\rangle = Q^2 + \chi^{cs}_{ij}, \end{aligned}$$

we introduce the charge- and spin-fluctuation correlation functions

$$\chi^{cs}_{ij} = \frac{1}{4}\langle \delta n_i \delta n_j\rangle + \langle \mathbf{S_i}\mathbf{S_j}\rangle,$$

with $\delta n_i = n_i - \langle n_i \rangle$. Further, we neglect the charge fluctuations, $\langle \delta n_i \delta n_j \rangle \simeq 0$, but take into account spin correlations given by spin correlation functions for the nearest (χ_{1s}) and for the next-nearest (χ_{2s}) neighbor lattice sites:

$$\chi_{1s} = \langle \mathbf{S}_i \mathbf{S}_{i+a_1} \rangle, \quad \chi_{2s} = \langle \mathbf{S}_i \mathbf{S}_{i+a_2} \rangle, \tag{20}$$

where $a_1 = (\pm a_x, \pm a_y)$ and $a_2 = \pm(a_x \pm a_y)$. In a paramagnetic state assumed here they depend only on the distance between the lattice sites.

In the $\mathbf{k}$-representation for the GF

$$G_\sigma^{\alpha\beta}(\mathbf{k},\omega) = \sum_j G_{oj\sigma}^{\alpha\beta}(\omega)\, \mathrm{e}^{-\mathrm{i}\mathbf{kj}},$$

we get for the zero-order GF (11):

$$\begin{aligned} \hat{G}_\sigma^{(0)}(\mathbf{k},\omega) &= Q\,\{\omega\hat{\tau}_0 - (\varepsilon_{\mathbf{k}} - \tilde{\mu})\hat{\tau}_3 - \Delta_{\mathbf{k}}^\sigma \hat{\tau}_1\}^{-1} \\ &= Q\,\frac{\omega\hat{\tau}_0 + (\varepsilon_{\mathbf{k}} - \tilde{\mu})\hat{\tau}_3 + \Delta_{\mathbf{k}}^\sigma \hat{\tau}_1}{\omega^2 - (\varepsilon_{\mathbf{k}} - \tilde{\mu})^2 - |\Delta_{\mathbf{k}}^\sigma|^2}, \end{aligned} \tag{21}$$

where $\hat{\tau}_0,\ \hat{\tau}_1,\ \hat{\tau}_3$ are the Pauli matrices. The quasiparticle energy $\varepsilon_{\mathbf{k}}$ and the renormalized chemical potential $\tilde{\mu} = \mu - \delta\mu$ in the MFA are defined by the frequency matrix (18)

$$\varepsilon_{\mathbf{k}} = -\tilde{t}(\mathbf{k}) - \frac{2J}{N}\sum_{\mathbf{q}} \gamma(\mathbf{k}-\mathbf{q}) N_{\mathbf{q}\sigma}, \tag{22}$$

$$\delta\mu = \frac{1}{N}\sum_{\mathbf{q}} t(\mathbf{q}) N_{\mathbf{q}\sigma} - 2J(n/2 - \chi_{1s}/Q), \tag{23}$$

where

$$J(\mathbf{q}) = 4J\gamma(\mathbf{q}), \qquad t(\mathbf{k}) = 4t\gamma(\mathbf{k}) + 4t'\gamma'(\mathbf{k})$$

with

$$\gamma(\mathbf{k}) = (1/2)(\cos a_x q_x + \cos a_y q_y), \qquad \gamma'(\mathbf{k}) = \cos a_x q_x \cos a_y q_y\,,$$

while the renormalized hopping integral is given by

$$\tilde{t}(\mathbf{k}) = 4t\,\gamma(\mathbf{k})\,Q\,(1 + \chi_{1s}/Q^2) + 4t'\,\gamma'(\mathbf{k})\,Q\,(1 + \chi_{2s}/Q^2). \tag{24}$$

The average number of electrons in equations (22), (23) in the $\mathbf{k}$-representation is written in the form:

$$n_{\mathbf{k},\sigma} = \langle X_{\mathbf{k}}^{\sigma 0} X_{\mathbf{k}}^{0\sigma} \rangle = Q N_{\mathbf{k}\sigma}.$$

It should be pointed out that the renormalization of the hopping parameter (24) caused by the spin correlation functions (20) is essential at low doping when short-range antiferromagnetic correlations are strong. For instance, for the hole doping $\delta = 1 - n \simeq 0.05$ and $Q = (1+\delta)/2 \simeq 0.53$ the correlation functions are estimated as [36]: $\chi_{1s} \simeq -0.3$, $\chi_{2s} \simeq 0.2$, which results in complete suppression of the nearest neighbors hopping, while the next-neighbor hopping is quite large:

$$t_{\text{eff}} = t\, Q[1 + \chi_{1s}/Q^2] \simeq 0, \qquad t'_{\text{eff}} = t'\, Q[1 + \chi_{2s}/Q^2] \simeq 0.9t'.$$

For a large doping, the antiferromagnetic correlations are suppressed and the nearest neighbor hopping prevails: $t_{\text{eff}}/t'_{\text{eff}} \simeq t/t' \gg 1$.

The superconducting gap $\Delta_{\mathbf{k}}^{\sigma}$ in equation (21) is defined by the anomalous component of the frequency matrix (19):

$$\Delta_{\mathbf{k}}^{\sigma} = \frac{2}{NQ} \sum_{\mathbf{q}} \left[\, t(\mathbf{q}) - \frac{1}{2} J(\mathbf{k}-\mathbf{q}) \right] \langle X_{-\mathbf{q}}^{0\bar{\sigma}} X_{\mathbf{q}}^{0\sigma} \rangle, \tag{25}$$

There are two contributions in equation (25) given by the $\mathbf{k}$-independent kinematic interaction $t(\mathbf{q})$ and the exchange interaction $J(\mathbf{k}-\mathbf{q})$. The kinematic interaction gives no contribution to the d-wave pairing in MFA, equation (25) (see [34]), and we disregard it in the subsequent equations.[2] The anomalous correlation function in equation (25) can be easily calculated from the anomalous part of the GF (21):

$$\langle X_{-\mathbf{q}}^{0\bar{\sigma}} X_{\mathbf{q}}^{0\sigma} \rangle = -Q \, \frac{\Delta_{\mathbf{q}}^{\sigma}}{2E_{\mathbf{q}}} \tanh \frac{E_{\mathbf{q}}}{2T}, \tag{26}$$

which results in the BCS-type equation for the gap function:

$$\Delta_{\mathbf{k}}^{\sigma} = \frac{1}{N} \sum_{\mathbf{q}} J(\mathbf{k}-\mathbf{q}) \frac{\Delta_{\mathbf{q}}^{\sigma}}{2E_{\mathbf{q}}} \tanh \frac{E_{\mathbf{q}}}{2T}, \tag{27}$$

where $E_k = [\,(\varepsilon_{\mathbf{k}} - \tilde{\mu})^2 + |\Delta_{\mathbf{k}}^{\sigma}|^2\,]^{1/2}$ is the quasiparticle energy in the superconducting state. As was proved in [39], the retardation effects for the exchange interaction are negligible and therefore there is no restriction in integrating over the energy in equation (27). It means that all electrons in the conduction band participate in the superconducting pairing contrary to the BCS equation for the electron-phonon model where the energy integration and pairing are restricted to a narrow energy shell of the order of the phonon energy close to the Fermi energy.

The equation (27) is identical to the results in MFA of the diagram technique [37], while the gap equation obtained in [40] has an additional factor $Q = (1 - n/2)$ which is spurious. This factor appears if we apply a simple decoupling procedure in the equation of motion (16) for GF instead of the projection technique given by equation (10). Writing the bosonic operators in the exchange interaction as a product of two fermionic operators: $X_i^{\bar{\sigma}\sigma} = X_i^{\bar{\sigma}0} X_i^{0\sigma}$ and performing a decoupling of the fermionic operators:

$$\langle\langle X_l^{\bar{\sigma}0} X_l^{0\sigma} X_i^{0\bar{\sigma}} - X_l^{\bar{\sigma}0} X_l^{0\bar{\sigma}} X_i^{0\sigma} | X_j^{\sigma0} \rangle\rangle_{\omega} \simeq \langle X_l^{0\sigma} X_i^{0\bar{\sigma}} - X_l^{0\bar{\sigma}} X_i^{0\sigma} \rangle \, \langle\langle X_l^{\bar{\sigma}0} | X_j^{\sigma0} \rangle\rangle_{\omega}\,, \tag{28}$$

[2]Superconducting pairing mediated by the kinematic interaction was first proposed by Zaitsev and Ivanov [47].

we obtain the same equation (27) for the gap function but with the additional Q-factor at the right hand side. In the decoupling we miss the normalization factor for the correlation functions in the denominator of the frequency matrix, equation (10), which cancels out with Q in the numerator of the corresponding GF (21) and therefore there is no Q-factor in equation (27). So, a rigorous way to apply MFA with a proper account of the projected character of HO is to use the projection technique as discussed above.

The self-energy contribution (15) in the second order of the kinematic interaction is considered in [36] while it is omitted in [37]. As discussed in [36,39], it mediates the spin-fluctuation pairing and results in finite life-time effects for the quasiparticle spectrum giving rise to an incoherent contribution to the single-particle density of states. Here, we shall not further discuss these self-energy effects since to compare the GF approach with the slave-fermion technique it will be sufficient to consider only MFA for the gap equation (27).

3. Slave-fermion approach

3.1. Slave-fermion representation

A number of auxiliary field representations have been proposed so far (see, e.g., [8–32]). In the slave-boson method [8–10] the projected electron operator is expressed as a product of auxiliary Bose field for charge degree of freedom (holon) and Fermi field for spin degree of freedom (spinon). The main problem in this approach is the so-called constraint imposed by the projected character of electronic operators in the t-J model which prohibits double occupancy of any lattice site. To treat the constraint, a site-dependent Lagrange multiplier is introduced. However, to solve the problem the MFA is usually applied and the Lagrange multiplier is taken to be independent of the lattice site, so the local constraint is replaced by a global one with uncontrollable consequences. In the slave-fermion method, the charge degree of freedom is represented by spinless fermion operators, while to describe the spin degree of freedom the Bose field (Schwinger bosons [13–22] or spin operators [23–27]) is used. The Schwinger boson representation though being physically meaningful for the Heisenberg model [11,12] gives poor results for the doped case: the antiferromagnetic ground state persists up to a very high doping and it does not reproduce the large Fermi surface as in the slave-boson method. In the slave fermion and in the spin operator representation, the magnetic properties of the model are described in a more reliable way (see, e.g., [25,29,31]).

Below, we consider the slave-fermion hard-core boson representation proposed in [27] and later employed in [28–31] to investigate different physical properties of cuprates within the t-J model. It has some advantages since the constraint of no double occupancy can be fulfilled without introducing the Lagrange multiplier. To decouple the charge and spin degrees of freedom for physical electrons, the HO in the theory [27] is represented as a product of a spinless fermion h_i^+ for the charge degree of freedom (holon) and a hard-core boson $b_{i\sigma}$ for the spin degree of freedom (spinon):

$$X_i^{0\sigma} = h_i^+ \, b_{i\sigma} \,, \qquad X_i^{\sigma 0} = h_i \, b_{i\sigma}^+ \,, \tag{29}$$

which have the following commutation relations:

$$h_i^+ h_j + h_j h_i^+ = \delta_{i,j} \,, \qquad b_{i\sigma} b_{j\sigma}^+ - b_{j\sigma}^+ b_{i\sigma} = \delta_{i,j}(1 - 2b_{i\sigma}^+ b_{i\sigma}).$$

The hard-core bosons are Pauli operators which commute on different lattice sites and anticommute on the same lattice site prohibiting double occupancy. The Pauli operators can be also represented by the spin-lowering S_i^- and spin-raising S_i^+ operators for spin-1/2:

$$b_{i\uparrow}^+ = S_i^+ = b_{i\downarrow} \,, \quad b_{i\downarrow}^+ = S_i^- = b_{i\uparrow} \,, \qquad \text{or} \qquad b_{i\sigma}^+ = S_i^\sigma \,, \quad b_{i\sigma} = S_i^{\bar\sigma} \,.$$

The on-site electron local constraint

$$\sum_\sigma X_i^{\sigma 0} X_i^{0\sigma} = \sum_\sigma X_i^{\sigma\sigma} = h_i h_i^+ \sum_\sigma b_{i\sigma}^+ \, b_{i\sigma} = h_i h_i^+ = 1 - h_i^+ h_i \leqslant 1 \tag{30}$$

is satisfied here since, for the Pauli operators at any lattice site, we have the equation

$$\sum_\sigma b_{i\sigma}^+ \, b_{i\sigma} = S_i^+ S_i^- + S_i^- S_i^+ = 1, \tag{31}$$

and the spinless holon number $n_i^{(\mathrm{h})} = h_i^+ h_i$ can be equal to 1 or 0.

However, the spin-charge separation imposed by the representation (29) results in extra degrees of freedom: a spin 1/2 is assigned to any lattice site including an empty site, while in the HO representation, equation (2), we have only 3 states: an empty state and a filled state with spin $\pm 1/2$. To cure this defect one should introduce a projection operator to exclude the unphysical states [27][3]. Otherwise the commutation relations for the original HO, equation (4), and their representation, equation (29), will give different results. For instance, for the physical electrons which are described by HO we have

$$\begin{aligned} &\{X_i^{0\sigma}, \, X_i^{\sigma 0}\} = X_i^{00} + X_i^{\sigma\sigma} = 1 - X_i^{\bar\sigma\bar\sigma}, \\ &\sum_\sigma \langle \{X_i^{0\sigma}, \, X_i^{\sigma 0}\}\rangle = 2 - \langle n_i \rangle = 1 + \delta, \end{aligned} \tag{32}$$

where the hole doping concentration $\delta = 1 - n$. If we use the representation (29) then we can write the commutation relations as

$$\begin{aligned} &\{X_i^{0\sigma}, \, X_i^{\sigma 0}\} = \{h_i^+ \, b_{i\sigma} \,, h_i \, b_{i\sigma}^+\} = h_i^+ \, h_i + (1 - 2\, h_i^+ \, h_i) b_{i\sigma}^+ b_{i\sigma} \,, \\ &\sum_\sigma \{h_i^+ \, b_{i\sigma} \,, h_i \, b_{i\sigma}^+\} = 1, \end{aligned} \tag{33}$$

where we have used equation (31). For the average value in equation (33) we get, respectively,

$$\textstyle\sum_\sigma \langle \{h_i^+ \, b_{i\sigma} \,, h_i \, b_{i\sigma}^+\}\rangle = 1, \tag{34}$$

[3]The same applies to other slave-fermion spin operator representations as in [23–26].

which contradicts the rigorous result for HO, equation (32). For the average number of electrons in the representation (29) by using the definition (6) we can write

$$n = \langle n_i \rangle = \sum_{\sigma} \langle X_i^{\sigma 0} X_i^{0\sigma} \rangle = \sum_{\sigma} \langle h_i b_{i\sigma}^{+} h_i^{+} b_{i\sigma} \rangle = \langle h_i h_i^{+} \rangle = 1 - \delta, \tag{35}$$

which coincides with the definition (6) if we take the definition $X_i^{00} = h_i^{+} h_i$ for the hole number operator. However, this definition is not unique. For instance, we can write: $X_i^{00} = X_i^{0\sigma} X_i^{\sigma 0} = X_i^{0\bar{\sigma}} X_i^{\bar{\sigma} 0}$, which results in the equation: $X_i^{00} = (1/2) h_i^{+} h_i$ if we use the representation (29) and the condition(31). Thus, the double counting of empty sites results in a controversial equation for an average number of electrons which is therefore valid only with accuracy of $\pm\delta$.

3.2. Mean-field approximation

Let us consider the resonating valence bond (RVB) state in the original Hamiltonian (5) as proposed by Baskaran et al. [6]. To this end we should write the Bose-like spin operators in the exchange energy in H_{t-J} (5) as a product of two single-particle Fermi-like operators: $X_i^{\sigma\bar{\sigma}} = X_i^{\sigma 0} X_i^{0\bar{\sigma}}$ and introduce the singlet operators

$$b_{ij}^{\uparrow} \equiv b_{ij} = \frac{1}{\sqrt{2}} (X_i^{0+} X_j^{0-} - X_i^{0-} X_j^{0+}). \tag{36}$$

Then, using MFA for the singlet operators in the exchange interaction of the t-J model, we get the RVB effective Hamiltonian:

$$\begin{aligned} H_J &= \frac{1}{2} \sum_{i \neq j} J_{ij} \left(X_i^{+-} X_j^{-+} - X_i^{++} X_j^{--} \right) = -\frac{1}{2} \sum_{i \neq j} J_{ij}\, b_{ij}^{+} b_{ij} \\ &\simeq -\frac{1}{2} \sum_{i \neq j} J_{ij} \left(B_{ij}^{+} b_{ij} + b_{ij}^{+} B_{ij} - |B_{ij}|^2 \right), \end{aligned} \tag{37}$$

where we introduced the RVB order parameter:

$$B_{ij}^{(\uparrow)} \equiv B_{ij} = \langle b_{ij} \rangle = \frac{1}{\sqrt{2}} \langle X_i^{0+} X_j^{0-} - X_i^{0-} X_j^{0+} \rangle. \tag{38}$$

Here, we should point out that MFA in equation (37) employs a decoupling of the Hubbard operators on the same lattice site:

$$X_i^{+-} X_j^{-+} = X_i^{+0} X_i^{0-} X_j^{-0} X_j^{0+} \;\Rightarrow\; \langle X_i^{+0} X_j^{-0} \rangle\, X_j^{0+} X_i^{0-}, \tag{39}$$

which is not unique and results in an uncontrollable approximation since the Hubbard operators obey the multiplication rule: $X_i^{\alpha\beta} X_i^{\beta\gamma} = X_i^{\alpha\gamma}$, and any intermediate state β can be used in the decoupling.

To obtain a self-consistent equation for the order parameter, we assume a spin-charge separation as is usually done in the slave-particle methods by applying a decoupling of spinon and holon degrees of freedom introduced in equation (29):

$$\begin{aligned} B_{ij} &= \frac{1}{\sqrt{2}} \langle h_i^+ \, b_{i\uparrow} \, h_j^+ \, b_{j\downarrow} - h_i^+ \, b_{i\downarrow} \, h_j^+ \, b_{j\uparrow} \rangle \\ &\simeq \langle h_i^+ \, h_j^+ \rangle \, \frac{1}{\sqrt{2}} \, \langle b_{i\uparrow} \, b_{j\downarrow} - b_{i\downarrow} \, b_{j\uparrow} \rangle \equiv \langle h_i^+ \, h_j^+ \rangle \, \varphi_{ij} \, , \qquad (40) \\ b_{ij} &= \frac{1}{\sqrt{2}} (h_i^+ \, b_{i\uparrow} \, h_j^+ \, b_{j\downarrow} - h_i^+ \, b_{i\downarrow} \, h_j^+ \, b_{j\uparrow}) \simeq \, h_i^+ \, h_j^+ \varphi_{ij} \, . \qquad (41) \end{aligned}$$

Within these approximations we obtain the effective Hamiltonian for holons

$$\begin{aligned} H_h \;\simeq\; & -\sum_{i\neq j} \tilde{t}_{ij} \, h_i \, h_j^+ \; - \mu \sum_i \, h_i \, h_i^+ \\ & - \frac{1}{2} \sum_{i\neq j} \tilde{J}_{ij} \, (\langle h_j \, h_i \rangle \, h_i^+ \, h_j^+ + h_j \, h_i \langle h_i^+ \, h_j^+ \rangle - |\langle h_i^+ \, h_j^+ \rangle|^2) \, , \qquad (42) \end{aligned}$$

where the effective hopping parameter and the exchange energy are given by

$$\begin{aligned} \tilde{t}_{ij} &= t_{ij} \, \langle b_{i\uparrow}^+ \, b_{j\uparrow} + b_{i\downarrow}^+ \, b_{j\downarrow} \rangle = t_{ij} \, \langle S_i^+ \, S_j^- + S_i^- \, S_j^+ \rangle, \\ \tilde{J}_{ij} &= J_{ij} \, |\varphi_{ij}|^2 = J_{ij} \, \frac{1}{2} \, |\langle b_{i\uparrow} \, b_{j\downarrow} - b_{i\downarrow} \, b_{j\uparrow} \rangle|^2 \, . \qquad (43) \end{aligned}$$

To obtain a phase diagram for the RVB order parameter $B_{ij} = F_{ij}^+ \, \varphi_{ij}$ as a function of temperature T and hole doping δ one should solve a self-consistent system of equations for the both order parameters, holon F_{ij} and spinon φ_{ij} ones. Here we consider only the equations for the holon order parameter by suggesting that there exists a region of $(T, \, \delta)$ where the spinon order parameter is nonzero.

Introducing $\mathbf{k}$-vector representation for the correlation functions:

$$F_{ij} = \langle h_i \, h_j \rangle = \frac{1}{N} \sum_{\mathbf{k}} \, \mathrm{e}^{\mathrm{i}(\mathbf{k}(\mathbf{i}-\mathbf{j}))} \, F(\mathbf{k}) = \frac{\mathrm{i}}{N} \sum_{\mathbf{k}} \, \sin(\mathbf{k}(\mathbf{i}-\mathbf{j})) \, \langle h_{\mathbf{k}} \, h_{-\mathbf{k}} \rangle, \qquad (44)$$

$$\begin{aligned} \varphi_{ij} &= \frac{1}{\sqrt{2}} \, \langle b_{i\uparrow} \, b_{j\downarrow} - b_{i\downarrow} \, b_{j\uparrow} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \, \mathrm{e}^{\mathrm{i}(\mathbf{k}(\mathbf{i}-\mathbf{j}))} \, \varphi(\mathbf{k}) \\ &= \frac{2\mathrm{i}}{N} \sum_{\mathbf{k}} \, \sin(\mathbf{k}(\mathbf{i}-\mathbf{j})) \frac{1}{\sqrt{2}} \, \langle b_{\mathbf{k}\uparrow} \, b_{-\mathbf{k}\downarrow} \rangle, \qquad (45) \end{aligned}$$

the Hamiltonian (42) can be written in $\mathbf{k}$-space as

$$H_h = \sum_{\mathbf{k}} \, (\varepsilon(\mathbf{k}) - \mu_h) \, h_{\mathbf{k}}^+ \, h_{\mathbf{k}} \; - \frac{1}{2} \sum_{\mathbf{k}} \, \{\Delta(\mathbf{k}) \, h_{-\mathbf{k}}^+ \, h_{\mathbf{k}}^+ + \Delta^+(\mathbf{k}) \, h_{\mathbf{k}} \, h_{-\mathbf{k}}\}, \qquad (46)$$

where the chemical potential for holons $\mu_h = -\mu$ and the holon spectrum $\varepsilon(\mathbf{k})$ according to equation (43) is written in the form (cf. equation (24)):

$$\varepsilon(\mathbf{k}) = \tilde{t}(\mathbf{k}) = 4t \, \gamma(\mathbf{k}) \, 2\langle S_i^+ \, S_{i+a_1}^- \rangle \; + 4t' \, \gamma'(\mathbf{k}) \, 2\langle S_i^+ \, S_{i+a_2}^- \rangle, \qquad (47)$$

Here, we assumed that the spin correlation functions have s-wave symmetry, e.i., $\chi_{i,i\pm a_x} = \chi_{i,i\pm a_y}$. We also introduced the holon gap function defined by the equation

$$\Delta(\mathbf{k}) = -\Delta(-\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{q}} \tilde{J}(\mathbf{k}-\mathbf{q})\, \langle h_{\mathbf{q}}\, h_{-\mathbf{q}} \rangle. \tag{48}$$

In equations (47), (48) we used a notation $\varepsilon(\mathbf{k})$, $\Delta(\mathbf{k})$ for the holon spectrum and the holon gap to distinguish them from those of physical electrons in section 2.2.

The normal and the anomalous correlation functions can be easily calculated for the BCS-type Hamiltonian (46):

$$\langle h^{+}_{\mathbf{q}}\, h_{\mathbf{q}} \rangle = \frac{1}{2}\left(1 - \frac{\varepsilon(\mathbf{q}) - \mu_h}{E(\mathbf{q})} \tanh\frac{E(\mathbf{q})}{2T}\right), \tag{49}$$

$$F(\mathbf{q}) = \langle h_{\mathbf{q}}\, h_{-\mathbf{q}} \rangle = \frac{\Delta(\mathbf{q})}{2E(\mathbf{q})} \tanh\frac{E(\mathbf{q})}{2T}, \tag{50}$$

where the quasiparticle spectrum $E(\mathbf{k}) = [(\varepsilon(\mathbf{k}) - \mu_h)^2 + |\Delta(\mathbf{k})|^2]^{1/2}$. From these equations there follow the self-consistent equations for the gap function and the average number of holes δ which defines the holon chemical potential μ_h:

$$\Delta(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{q}} \tilde{J}(\mathbf{k}-\mathbf{q})\, \frac{\Delta(\mathbf{q})}{2E(\mathbf{q})} \tanh\frac{E(\mathbf{q})}{2T}, \tag{51}$$

$$\delta = \frac{1}{N}\sum_{\mathbf{q}} \langle h^{+}_{\mathbf{q}}\, h_{\mathbf{q}} \rangle = \frac{1}{N}\sum_{\mathbf{q}} \frac{1}{2}\left(1 - \frac{\varepsilon(\mathbf{q}) - \mu_h}{E(\mathbf{q})}\right) \tanh\frac{E(\mathbf{q})}{2T}. \tag{52}$$

These equations are identical to the results obtained in [32] where the path-integral representation for the t-J model was applied and an effective BCS-type Hamiltonian analogous to equation (46) was derived. Starting from the MFA for RVB order parameter as in equation (37), the authors introduced MFA for the spinon auxiliary field that resulted in the spin-charge separation as in our equation (41). Therefore, we have proved that the results of the path-integral representation for the t-J employed in [32] are equivalent to the MFA for the slave fermion – hard-core boson approach considered in this section.

3.3. Holon Green functions

To avoid uncontrollable approximation caused by the decoupling of the Hubbard operators on the same lattice site in equation (39) used in MFA for RVB state in the Hamiltonian (37), in the present section we consider a projection technique for the holon GF for the spinon-holon model. By using the spinless fermion hard-core boson representation (29) we write the Hamiltonian of the t-J model (5) as follows:

$$\begin{aligned} H_{t_J} &= -\sum_{i\neq j} t_{ij}\, h_i\, h^{+}_j\, (S^{+}_i\, S^{-}_j + S^{-}_i\, S^{+}_j) - \mu \sum_i h_i\, h^{+}_i \\ &\quad - \frac{1}{4}\sum_{i\neq j} J_{ij}\; h_i\, h_j\, h^{+}_j\, h^{+}_i\; (S^{+}_i\, S^{-}_j - S^{-}_i\, S^{+}_j)(S^{+}_j\, S^{-}_i - S^{-}_j\, S^{+}_i). \end{aligned} \tag{53}$$

To obtain an equation for the holon GF, we apply the projection technique described in section 2.1. By introducing the matrix GF for holon operators:

$$\hat{G}^h_{ij}(t-t') = \begin{pmatrix} \langle\langle h_i(t)|h_j^+(t')\rangle\rangle & \langle\langle h_i(t)|h_j(t')\rangle\rangle \\ \langle\langle h_i^+(t)|h_j^+(t')\rangle\rangle & \langle\langle h_i^+(t)|h_j(t')\rangle\rangle \end{pmatrix},$$

we can obtain an equation of motion for the GF as discussed in section 2.1 (see equations (8)–(11)). For the zero-order GF in MFA we get the following result:

$$\hat{G}^{(h,0)}(\mathbf{k},\omega) = \frac{\omega\hat{\tau}_0 + (\tilde{\varepsilon}(\mathbf{k}) - \mu_h)\hat{\tau}_3 + \tilde{\Delta}(\mathbf{k})\hat{\tau}_1}{\omega^2 - (\tilde{\varepsilon}(\mathbf{k}) - \mu_h)^2 - |\tilde{\Delta}(\mathbf{k})|^2}, \tag{54}$$

where the holon dispersion and the gap function are given by the equations:

$$\tilde{\varepsilon}(\mathbf{k}) = \tilde{t}(\mathbf{k}) - \frac{1}{N}\sum_{\mathbf{q}} \{\tilde{J}'(\mathbf{k}-\mathbf{q}) - \tilde{J}'(0)\} \langle h^+_{\mathbf{q}}\, h_{\mathbf{q}}\rangle, \tag{55}$$

$$\tilde{\Delta}(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{q}} \tilde{J}'(\mathbf{k}-\mathbf{q}) \langle h_{\mathbf{q}}\, h_{-\mathbf{q}}\rangle. \tag{56}$$

In comparison with MFA for RVB state considered previously, in the GF approach we obtain additional renormalization for the holon dispersion, equation (47), while the gap equation has the same form, equation (48), but with a different renormalized exchange interaction:

$$\tilde{J}'_{ij} = J_{ij}\,\frac{1}{2}\langle|S_i^+\, S_j^- - S_i^-\, S_j^+|^2\rangle = J_{ij}\,(\frac{1}{4} - \langle S_i^z\, S_j^z\rangle). \tag{57}$$

By using an equation of motion method instead of MFA for RVB state, we managed to take into account spinon correlations in the effective holon interaction (57) and obtained a simple formula for it by using the identities: $S_i^+\, S_i^+ = 0$, $S_i^-\, S_i^+ = (1/2) - S_i^z$ in the last equation. From equation (57) we get the following estimation for the effective exchange energy for the nearest neighbors: $\tilde{J}' \simeq (0.5 - 0.25)\, J$ if we assume the AFM Neél phase: $\langle S_i^z\, S_j^z\rangle = -1/4$ or completely neglect AFM correlations: $\langle S_i^z\, S_j^z\rangle = 0$.

4. Results and discussion

4.1. Spectral density

Spectral density for physical electron excitations in the lower Hubbard subband within the t-J model which is defined by the equation

$$A_\sigma(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\langle X^{0\sigma}_{\mathbf{k}} \mid X^{\sigma 0}_{\mathbf{k}}\rangle\rangle_{\omega+\mathrm{i}\epsilon}, \tag{58}$$

satisfies the sum rule:

$$\sum_\sigma \int\limits_{-\infty}^{+\infty} \mathrm{d}\omega\, A_\sigma(\mathbf{k},\omega) = \sum_\sigma \langle\{X_i^{0\sigma},\, X_i^{\sigma 0}\}\rangle = 2\,Q = 1 + \delta. \tag{59}$$

In the MFA for the GF in terms of the HO, equation (21), we get:

$$A_\sigma(\mathbf{k},\omega) = Q\, u_{\mathbf{k}}\, \delta(\omega - E_{\mathbf{k}}) \;+ Q\, v_{\mathbf{k}}\, \delta(\omega + E_{\mathbf{k}}), \tag{60}$$

where

$$u_{\mathbf{k}} = \frac{1}{2}\left(1 + \frac{(\varepsilon_{\mathbf{k}} - \tilde{\mu})}{E_{\mathbf{k}}}\right), \qquad v_{\mathbf{k}} = \frac{1}{2}\left(1 - \frac{(\varepsilon_{\mathbf{k}} - \tilde{\mu})}{E_{\mathbf{k}}}\right). \tag{61}$$

In MFA, the spectral density (60) satisfies the sum rule (59) but it has no incoherent background which appears if one takes into account the self-energy corrections as shown in [36].

In the spinon-holon representation (29), the spectral density, as follows from equation (34), does not obey the sum rule (59):

$$\begin{aligned}
\sum_\sigma \int\limits_{-\infty}^{+\infty} \mathrm{d}\omega\, A_\sigma^{(\mathrm{sh})}(\mathbf{k},\omega) \;&=\; \sum_{(\mathbf{i}-\mathbf{j})} \mathrm{e}^{-\mathrm{i}(\mathbf{k}(\mathbf{i}-\mathbf{j}))} \int\limits_{-\infty}^{+\infty} \mathrm{d}\omega \left\{-\frac{1}{\pi}\mathrm{Im}\langle\langle h_i^+ \, b_{i\sigma} \,| h_j \, b_{j\sigma}^+ \rangle\rangle_{\omega+\mathrm{i}\epsilon}\right\} \\
&=\; \sum_\sigma \langle \{ h_i^+ \, b_{i\sigma} \,, h_i \, b_{i\sigma}^+ \}\rangle = 1.
\end{aligned} \tag{62}$$

MFA for the spinon-holon GF in equation (62) results in the spin-charge separation which defines the spectral density (62) as a convolution of the anticommutator holon and the commutator spinon GF [28]:

$$\begin{aligned}
A_\sigma^{(\mathrm{sh})}(\mathbf{k},\omega) \;&=\; \frac{1}{N}\sum_q \frac{1}{2\pi^2} \int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty} \mathrm{d}\omega_1 \mathrm{d}\omega_2 \frac{\tanh(\omega_1/2T) + \coth(\omega_2/2T)}{\omega - \omega_1 - \omega_2} \\
&\times \mathrm{Im}\langle\langle h_{\mathbf{q}}^+ | h_{\mathbf{q}} \rangle\rangle_{\omega_1} \; \mathrm{Im}\langle\langle S_{\mathbf{k}-\mathbf{q}}^{\bar\sigma} | S_{\mathbf{k}-\mathbf{q}}^{\sigma} \rangle\rangle_{\omega_2} \, .
\end{aligned} \tag{63}$$

In this representation, the spectral density of physical electron excitations is given by a superposition of the spectral density for spinless fermion (holon) excitations and a background produced by spin excitations [28]. In MFA, the holon spectral density in the paired state below T_c is defined by the GF (54):

$$A^{(\mathrm{h})}(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\langle h_{\mathbf{k}}^+ \mid h_{\mathbf{k}} \rangle\rangle_{\omega+\mathrm{i}\epsilon} = \tilde{u}_{\mathbf{k}}\, \delta(\omega + \tilde{E}(\mathbf{k})) + \tilde{v}_{\mathbf{k}}\, \delta(\omega - \tilde{E}(\mathbf{k})), \tag{64}$$

where the quasiparticle energy $\tilde{E}(\mathbf{k}) = [(\tilde{\varepsilon}(\mathbf{k}) - \mu_h)^2 + |\tilde{\Delta}(\mathbf{k})|^2]^{1/2}$ and $\tilde{u}_{\mathbf{k}}$, $\tilde{v}_{\mathbf{k}}$ are given by equation (61) but with quasiparticle energies for holons. The spectral density of electron excitations is measured in the angle-resolved photoemission (ARPES) experiments which provide information concerning the symmetry of the gap function. As discussed below, the symmetry of superconducting gap function $\Delta_{\mathbf{k}}$ defined by equation (27) appears to be d-wave, while the holon gap function $\Delta(\mathbf{k})$ in equation (51) has an odd symmetry of the p-type as in the triplet pairing. This p-wave gap symmetry has never been observed in ARPES experiments in cuprates.

4.2. Gap symmetry

For the models with strong electron correlations, the s-wave component of superconducting gap should be strongly suppressed due to the on-site Coulomb correlations. For the t-J model it follows from the constraint of no double occupancy on a single site given by the identity:

$$\langle \hat{c}_{i,\sigma}\hat{c}_{i,-\sigma}\rangle = \frac{1}{N}\sum_{\mathbf{k}}\langle \hat{c}_{\mathbf{k},\sigma}\hat{c}_{-\mathbf{k},-\sigma}\rangle = 0, \tag{65}$$

for the physical electron operators $\hat{c}_{i,\sigma} = c_{i,\sigma}(1 - n_{i,-\sigma})$. Since the anomalous correlation function $\langle \hat{c}_{k,\sigma}\hat{c}_{-k,-\sigma}\rangle$ is proportional to the gap function $\Delta(\mathbf{k})$, equation (65) imposes a certain constraint on the symmetry of the gap function. In particular, for the solution (26) in MFA equation (65) reads [34,35]:

$$\langle X_i^{0\sigma}X_i^{0\bar{\sigma}}\rangle = \frac{1}{N}\sum_{\mathbf{q}}\langle X_{\mathbf{q}}^{0\sigma}X_{-\mathbf{q}}^{0\bar{\sigma}}\rangle = \frac{Q}{N}\sum_{\mathbf{q}}\frac{\Delta_{\mathbf{q}}^{\sigma}}{2E_{\mathbf{q}}}\tanh\frac{E_{\mathbf{q}}}{2T} = 0. \tag{66}$$

For a tetragonal lattice, the Fermi surface (FS) is invariant under the C_4-axis rotation in the $\mathbf{k}$-space and, therefore, to satisfy the condition (66) for $E_{\mathbf{q}} > 0$, the gap function $\Delta_{\mathbf{q}}^{\sigma}$ should change its sign along the FS. It means that the symmetric s-wave solution, $\Delta_s(k_x,k_y) \propto (\cos q_x + \cos q_y)$, does not fit equation (66), while the d-wave solution with B_{1g} or B_{2g} symmetry, $\Delta_d(k_x,k_y) = -\Delta_d(k_y,k_x)$, satisfies the condition (66). In general, equation (66) should be considered as a constraint on the symmetry of the gap function in the superconducting phase and the solutions which violate this constraint should be disregarded.

Now we consider the symmetry of the spinon and the holon order parameters. The condition (65) for the RVB order parameter reads

$$B_{ii} = \frac{1}{N}\sum_{\mathbf{k}} B(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{k},\mathbf{q}} \varphi(\mathbf{k}-\mathbf{q})\, F^{+}(\mathbf{q}) = 0, \tag{67}$$

which also imposes a constraint on the symmetry of the spinon and holon order parameters. Since the symmetry of the holon pairing order parameter, equation (44), for spinless fermions is odd, being imposed by their anticommutation relations, it results in the odd symmetry of the gap $\Delta(\mathbf{k})$ in equation (48). For a tetragonal lattice, the symmetry is given by the odd two-dimensional irreducible representation E_u which can be modelled by the function: $\Delta(\mathbf{k}) \propto \eta_p^{\pm}(\mathbf{k}) = (\sin k_x \pm \sin k_y)$ as in the p-wave triplet pairing. The same holds for the spinon order parameter in equation (45), $\varphi(\mathbf{k}) \propto \eta_p^{\pm}(\mathbf{k})$.

The RVB order parameter $B_{ij} = \langle b_{ij}\rangle = \varphi_{ij}F_{ij}^{+}$ as a product of two antisymmetric order parameters with E_u symmetry has either A (s-wave) or B_{1g} (d-wave) symmetry. Namely, if we adopt only the nearest neighbor pairing for both the order parameters:

$$\begin{aligned}\varphi_{ij} &= \varphi_{i,i+a_x}\{(\delta_{j,i+a_x} - \delta_{j,i-a_x}) \pm (\delta_{j,i+a_y} - \delta_{j,i-a_y})\},\\ F_{ij}^{+} &= F_{i,i+a_x}^{+}\{(\delta_{j,i+a_x} - \delta_{j,i-a_x}) \pm (\delta_{j,i+a_y} - \delta_{j,i-a_y})\},\end{aligned} \tag{68}$$

then, for the Fourier transform of the RVB order parameter, we get

$$B(\mathbf{k}) = \sum_{\mathbf{q}} \varphi(\mathbf{k}-\mathbf{q})\, F^{+}(\mathbf{q}) = 2b \sum_{\mathbf{q}} \{\sin(k_x - q_x) \pm \sin(k_y - q_y)\}\, \{\sin q_x \pm \sin q_y\}$$
$$= -b\,(\cos k_x \pm \cos k_y), \tag{69}$$

where $b = \varphi_{i,i+a_x}\, F^{+}_{i,i+a_x}$ and the sign + (−) in the last line corresponds to the same (different) signs in the first line. The solution (69) satisfies the condition (67) for both the s- and d-wave symmetry: $\sum_{\mathbf{k}} B(\mathbf{k}) \propto \sum_{\mathbf{k}} (\cos k_x \pm \cos k_y) = 0$.

However, the explicit solution for the holon order parameter (50) shows its more complicated $\mathbf{k}$-dependence which proves that the frequently used model for the nearest neighbor pairing, equations (68), is inadequate. For the solution (50), the condition (67) for the RVB order parameter reads:

$$\sum_{\mathbf{k},\mathbf{q}} \varphi(\mathbf{k}-\mathbf{q})\, F^{+}(\mathbf{q}) = \sum_{\mathbf{k},\mathbf{q}} \varphi(\mathbf{k}-\mathbf{q})\, \frac{\Delta^{+}(\mathbf{q})}{2E(\mathbf{q})} \tanh\frac{E(\mathbf{q})}{2T} = 0, \tag{70}$$

which also imposes a requirement on the symmetry of the singlet (RVB) order parameter which should have only the d-wave symmetry, $B(k_x, k_y) = -B(k_y, k_x)$, to satisfy this condition.

It is interesting to compare the results for the gap equation derived in MFA for the t-J model and that one for the Hubbard model. By applying the projection technique for the GF for the Hubbard model, one can get the following equation for the gap function (see, e.g., [39]):

$$\Delta_{ij\sigma} \propto \langle X_i^{02} N_j \rangle = \langle c_{i\downarrow} c_{i\uparrow} N_j \rangle, \tag{71}$$

where we have used the identity for the Hubbard operators, $X_i^{02} = X_i^{0\downarrow} X_i^{\downarrow 2} = c_{i\downarrow} c_{i\uparrow}$. From equation (71) it follows that the pairing occurs on one lattice site but in the different Hubbard subbands. By using the equation of motion for the GF $\langle\langle X_i^{02}(t) | N_j(t') \rangle\rangle$, the anomalous correlation function $\langle X_i^{02} N_j \rangle$ can be calculated without any decoupling that results in the same gap equation as in the MFA for the t-J model [39]): $\Delta_{ij\sigma} = J_{ij}\, \langle X_i^{0\sigma} X_j^{0\bar{\sigma}} \rangle / Q$ where we have used the notation of the present paper. Therefore, the symmetry constraint considered above is also applicable to the gap solutions obtained in the Hubbard model.

4.3. Superconducting T_c

In the present section we compare the pairing temperature T_c defined by the gap equation for physical electrons (27) and that one for holons, equation (51). We study T_c as a function of a corresponding chemical potential $\nu = \mu/W$ for a given value of the pairing interaction $\lambda = J/W$ where all energies are measured in units of the renormalized half bandwidth for pairing fermions $W = 4\,\tilde{t}$:

$$e(\mathbf{k}) = \frac{\varepsilon(\mathbf{k})}{W} = \gamma(\mathbf{k}) + \tau\gamma^{'}(\mathbf{k}), \qquad \tau = \frac{t'_{\text{eff}}}{t_{\text{eff}}}, \qquad d(\mathbf{k}) = \frac{\Delta(\mathbf{k})}{W}. \tag{72}$$

The gap equations (27), (51) (or (56)) can be written in the form

$$d(\mathbf{k}) = \frac{4\lambda}{N}\sum_{\mathbf{q}} \frac{\gamma(\mathbf{k}-\mathbf{q})\, d(\mathbf{q})}{2[(e(\mathbf{q})-\nu)^2 + d(\mathbf{q})]^{1/2}} \tanh\frac{[(e(\mathbf{q})-\nu)^2 + d(\mathbf{q})]^{1/2}}{2T}, \tag{73}$$

Let us consider $T_c(\nu)$ for different pairing symmetry, $d(\mathbf{k}) = d_\alpha\, \eta_\alpha(\mathbf{k})$:

$$\begin{aligned} &s\text{-wave:} \quad && \eta_s(\mathbf{k}) = (\cos k_x + \cos k_y), \\ &d\text{-wave:} \quad && \eta_d(\mathbf{k}) = (\cos k_x - \cos k_y), \\ &p\text{-wave:} \quad && \eta_p^{\pm}(\mathbf{k}) = (\sin k_x \pm \sin k_y). \end{aligned} \tag{74}$$

By integrating equation (73) with the corresponding symmetry parameter $\eta_\alpha(\mathbf{k})$ we obtain equation (73) for $T = T_c$ in the same form for any symmetry:

$$\begin{aligned} \frac{1}{\lambda} &= \frac{1}{N}\sum_{\mathbf{k}} (\eta_\alpha(\mathbf{k}))^2 \frac{1}{2(e(\mathbf{k})-\nu)} \tanh\frac{e(\mathbf{k})-\nu}{2T_c^{(\alpha)}} \\ &= \frac{1}{2}\int_{-1}^{+1} \frac{\mathrm{d}\epsilon}{\epsilon-\nu} N_\alpha(\epsilon) \tanh\frac{\epsilon-\nu}{2T_c^{(\alpha)}}\,, \end{aligned} \tag{75}$$

if we introduce an effective density of state (DOS) for the corresponding symmetry, $\alpha = s, d, p$:

$$N_\alpha(\epsilon) = \frac{1}{N}\sum_{\mathbf{k}} (\eta_\alpha(\mathbf{k}))^2\, \delta(\epsilon - e(\mathbf{k}))\,, \tag{76}$$

which is normalized

$$\int_{-1}^{+1} \mathrm{d}\epsilon\, N_\alpha(\epsilon) = 1, \quad \text{since} \quad \frac{1}{N}\sum_{\mathbf{k}} (\eta_\alpha(\mathbf{k}))^2 = 1.$$

The results of calculation of the effective DOS, equation (76), for different symmetry $\alpha = s, d, p$ is presented in figure 1 for $t' = 0$. From this dependence it is easy to draw a conclusion that the $T_c(\nu)$ function will follow the dependence $N_\alpha(\nu)$ for a corresponding symmetry since the effective coupling constant $V \simeq \lambda N_\alpha(\nu)$ reaches its maximum value at the maximum value of $N_\alpha(\nu)$. In the logarithmic approximation a solution for $T_c(\mu)$, equation (75), can be written in the conventional BCS form:

$$T_c \simeq \sqrt{\mu(W-\mu)}\exp(-1/V), \quad V \simeq J\, N_\mu\,, \tag{77}$$

but with the prefactor proportional to the Fermi energy, $\mu = E_F$ which can result in high-T_c. The highest $T_c(\nu)$ appears for the d-wave pairing and the lowest $T_c(\nu)$ – for the p- wave pairing since in the former case the van Hove singularity gives a strong contribution for DOS ($[\eta_d(\mathbf{k} = (\pm\pi, \mathbf{0}))]^2 = 4$), while in the latter case it is completely suppressed ($[\eta_p(\mathbf{k} = (\pm\pi, \mathbf{0}))] = 0$). This estimation can be checked by a direct numerical solution of equation (75) (see, e.g. [35,36] and [48] for p-wave symmetry).

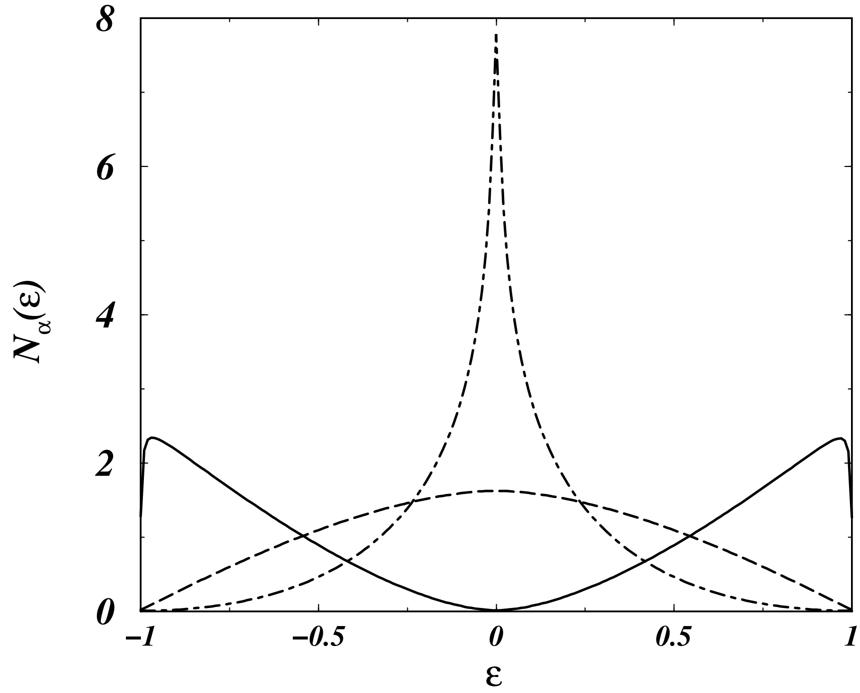

Figure 1. Effective density of states (76) for s (solid line,) d (dot-dashed line) and p (dashed line) symmetry.

5. Conclusion

In the present paper we consider a superconducting pairing mediated by the exchange interaction which is generic for the system with strong electron correlations such as cuprates. The mechanism of the exchange pairing is the lowering of kinetic energy of electron pairs due to their coherent hopping between different Hubbard subbands. Since the excitation energy of this hopping is much larger than the Fermi energy the retardation effects in the exchange interaction are negligible [39] which results in the pairing of all electrons (holes) in the conduction band and a high-T_c proportional to the Fermi energy, equation (77).

To obtain the estimation for the superconducting T_c it is tempting to use a mean-field approximation for the exchange interaction within the t-J model. However, meaningful physical results can be obtained only if one takes into account strong electron correlations on a rigorous basis which is provided by the Hubbard operator (HO) technique. Any auxiliary field representations applied within MFA inevitably violate rigorous commutation relations for HO which may result in unphysical conclusions. In the present paper we have proved this by comparing the results for superconducting gap equation derived within the slave fermion – hard-core boson representation, equation (29), and HO technique for the Green functions (section 2.1). In the former method, the projected character of physical electron operators is neglected that results in a double counting of empty states and in violation of the sum rule, equation (62). The spin-charge separation which occurs in

MFA, equations (40), (41), results in separate equations for two order parameters for spinons and holons instead of one equation for physical electrons as in the GF method. The gap equation (51) for spinless fermions has only antisymmetric solutions which results in an unphysical p-wave gap for the quasiparticle excitations in superconducting state never observed in ARPES experiments and much lower T_c than for the d-wave pairing given by equation (27) for physical electrons.

The obtained results within MFA for the spinless fermion – hard-core bosons in section 2 appear to be identical to the path-integral representation for the t-J model employed in [32]. Therefore, the latter results have the same flaws as discussed above which casts doubts on the approaches based on the idea of spin-charge separation treated in MFA which results in violation of the local constraint. Violation of the local constraint in the two-band Hubbard model may also lead to unphysical results, as shown in [49].

References

1. Anderson P.W. // Science, 1987, vol. 235, p. 1196–1198; Anderson P.W. The Theory of Superconductivity in the High-T_c Cuprates. Princeton, New Jersey, Princeton University Press, 1997.
2. For a review see: Scalapino D.J. // Phys. Reports, 1995, vol. 250, p. 329–365; arXiv: cond-mat/9908287.
3. Dagotto E. // Rev. Mod. Phys., 1994, vol. 66, No. 3, p. 763–840.
4. Sorella S., Martins G.B., Becca F., Gazza C., Capriotti L., Parola A., Dagotto E. // Phys. Rev. Lett., 2002, vol. 88, p. 117002.
5. Huang Z.B., Lin H.Q., Gubernatis J.E. // Phys. Rev. B, 2001, vol. 64, p. 205101.
6. Baskaran B., Zou Z., Anderson P.W. // Solid State Comm., 1987, vol. 63, No. 11, p. 973–976.
7. Cyrot M. // Solid State Comm., 1987, vol. 62, No. 12, p. 821–823; Solid State Comm., 1987, vol. 63, No. 11, p. 1015–1018.
8. Ruckenstein A.E., Hischfeld P.J., Appel J. // Phys. Rev. B, 1987, vol. 36, No. 1, p. 857–860.
9. Kotliar G., Liu J. // Phys. Rev. B, 1998, vol. 38, No. 7, p. 5142–5145.
10. Suzumura Y., Hasegawa Y., Fukuyama H. // Jour. Phys. Soc. Jpn., 1988, vol. 57, No. 2. p. 401–404.
11. Arovas D.P., Auerbach A. // Phys. Rev. B, 1988, vol. 38, No. 1. p. 316–332.
12. Auerbach A., Arovas D.P. // Phys. Rev. Lett., 1988, vol. 61, No. 5, p. 617–620.
13. Yoshioka D. // Jour. Phys. Soc. Jpn., 1989, vol. 58, No. 1, p. 32–35.
14. Yoshioka D. // Jour. Phys. Soc. Jpn., 1989, vol. 58, No. 5, p. 1516–1519.
15. Sarker S., Jayaprakash C., Krishnamurthy H.R., Ma M. // Phys. Rev. B, 1989, vol. 40, No. 7, p. 5028–5035.
16. Flensberg K., Hedegård P., Pedersen M.B. // Phys. Rev. B, 1989, vol. 40, No. 1, p. 850–853.
17. Hedegård P., Pedersen M.B. // Phys. Rev. B, 1990, vol. 42, No. 16, p. 10035–10040.
18. Hedegård P., Pedersen M.B. // Phys. Rev. B, 1991, vol. 43, No. 13, p. 11504–11507.
19. Kane C.L., Lee P.A., Ng T.K., Chakraborty B., Read N. // Phys. Rev. B, 1990, vol. 41, No. 4, p. 2653–2656.

20. Chakraborty B., Read N., Kane C.L., Lee P.A. // Phys. Rev. B, 1990, vol. 42, No. 7, p. 4819–4822.
21. Li Y.M., Sheng D.N., Su Z.B., Yu Lu. // Phys. Rev. B, 1992, vol. 45, No. 10, p. 5428–5437.
22. Khaliullin G., Horsch P. // Phys. Rev. B, 1993, vol. 47, No. 1, p. 463–469.
23. Khaliullin G. // JETP Lett., 1990, vol. 52, p. 389–393.
24. Richard J.L., Yushankhai V.Yu. // Phys. Rev. B, 1993, vol. 47, No. 2, p. 1103–1106.
25. Wang Y.R., Wu J., Franz M. // Phys. Rev. B, 1993, vol. 47, No. 18, p. 12140–12152.
26. Wang Y.R., Rice M.J. // Phys. Rev. B, 1994, vol. 49, No. 6, p. 4360–4363.
27. Shiping Feng, Su Z.B., Yu Lu. // Phys. Rev. B, 1994, vol. 49, No. 4, p. 2368–2384.
28. Shiping Feng, Song Y. // Phys. Rev. B, 1997, vol. 55, No. 1, p. 642–646.
29. Shiping Feng, Huang Z. // Phys. Rev. B, 1998, vol. 57, No. 17, p. 10328–10331.
30. Xianglin Ke, Feng Yuan, Shiping Feng. // Phys. Rev. B, 2000, vol. 62, No. 1, p. 134–137.
31. Feng Yuan, Shiping Feng, Zhao-Bin Su, Yu Lu. // Phys. Rev. B, 2001, vol. 64, p. 224505.
32. Kochetov E., Mierzejewski M. // Phys. Rev. B, 2000, vol. 61, No. 2, 1580–1583.
33. Izyumov Yu.A. // Physics Uspekhi, 1997, vol. 40, No. 5, p. 445-476 (in Russian: Uspekhi Fiz. Nauk, 1997, vol. 167, No. 5, p. 465–497).
34. Plakida N.M., Yushankhai V.Yu., Stasyuk I.V. // Physica C, 1989, vol. 160, p. 80–88.
35. Yushankhai V.Yu., Plakida N.M., Kalinay P. // Physica C, 1991, vol. 174, p. 401–408.
36. Plakida N.M., Oudovenko V.S. // Phys. Rev. B, 1999, vol. 59, No. 18, p. 11949–11961.
37. Izyumov Yu.A., Letfulov B.M. // J. Phys.: Condens. Matter, 1991, vol. 3, p. 5373–5391.
38. Izyumov Yu.A., Letfulov B.M. // Int. J. Mod. Phys. B, 1992, vol. 6, p. 321.
39. Plakida N.M., Anton L., Adam S., Adam Gh. // Exchange and spin-fluctuation superconducting pairing in cuprates. Preprint of the Joint Institute for Nuclear Research, E-17-2001-59, Dubna, 2001 p. 24; arXiv: cond-mat/0104234.
40. Onufrieva F., Petit S., Sidis Y. // Phys. Rev. B, 1996, vol. 54, No. 17, p. 12464–12487.
41. Plakida N.M, Hayn R., Richard J.-L. // Phys. Rev. B, 1995, vol. 51, No. 23, p. 16599–16607.
42. Zhang F.C., Rice T.M. // Phys. Rev. B, 1988, vol. 37, No. 7, p. 3759–3761.
43. Emery V.J. // Phys. Rev. Lett., 1987, vol. 58, No. 26, p. 2794–2797; Varma C.M., Schmitt-Rink S., Abrahams E. // Solid State Commun., 1987, vol. 62, No. 10, p. 681–685.
44. Feiner L.F., Jefferson J.H., Raimondi R. // Phys. Rev. B, 1996, vol. 53, No. 13, p. 8751–8773; Raimondi R., Jefferson J.H., Feiner L.F. // Phys. Rev. B, 1996, vol. 53, No. 13, p. 8774–8788.
45. Yushankhai V.Yu., Oudovenko V.S., Hayn R. // Phys. Rev. B, 1997, vol. 55, No. 23, p. 15562–15575.
46. Zubarev D.N. // Sov. Phys. Usp., 1960, vol. 3, p. 320.
47. Zaitsev R.O., Ivanov V.A. // Fiz. Tver. Tela, 1987, vol. 29, No. 8, p. 2554–2556; ibid., No. 10, p. 3111 (in Russian); Int. J. Mod. Phys. B, 1988, vol. 5, p. 153; Phisica C, 1988, vol. 153–155, p. 1295–1296.
48. Kuz'min E.V., Baklanov I.O. // JETP, 1999, vol. 89, No. 2, p. 349–357.
49. Zhang L., Jain J.K., Emery V.J. // Phys. Rev. B, 1993, vol. 47, No. 6, p. 3368–3373.

Надпровідність в t-J моделі

М.М.Плакіда

Об'єднаний інститут ядерних досліджень, Росія, 141980 м. Дубна

Отримано 2 вересня 2002р.

Представлено порівняння мікроскопічних теорій для надпровідності в границі сильних електронних кореляцій. Ми розглядаємо результати для двовимірної t-J моделі, отриманої в рамках методу проектування для функцій Гріна на мові операторів Габбарда, а також представленні допоміжних ферміонів для стану резонуючих валентних зв'язків. Стверджується, що останнє наближення, яке приводить до непарної симетрії p-хвильового спарювання для ферміонів є непридатним.

Ключові слова: *сильні електронні кореляції, високотемпературні надпровідники, функції Гріна, допоміжні ферміони*

PACS: *74.20.-z, 74.20.Mn, 74.72.-h*