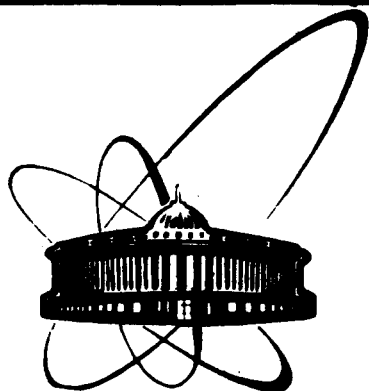


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ON d -WAVE PAIRING
IN THE SINGLE-BAND HUBBARD MODEL

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1. Introduction

Strong Coulomb correlations are now considered to play a very important role in forming the electron spectrum in oxide superconducting compounds (see, for example, ^{/1/}). Anderson was the first ^{/2/} to note the proximity of these compounds to the Mott-Hubbard system near the insulator-metal transition. He proposed the theory of superconductivity on the basis of the effective exchange Hamiltonian of the form ^{/3/}:

$$\mathcal{H} = t \sum_{\langle i,j \rangle, \sigma} (1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}) + J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j) \quad (1)$$

with $\langle i, j \rangle$ nearest neighbouring sites on a square lattice;
 $J = 4t^2/u$ is the antiferromagnetic coupling. The Hamiltonian (1) results from the Hubbard model when $u \gg t$ and acts in the subspace of singly occupied sites (i.e. in the lowest Hubbard subband). Anderson suggested that the exchange interaction on the 2D square lattice brings about a resonating valence bond state consisting of an ensemble of singlet electron pairs and giving rise to the superconductivity in the system. At the same time it was pointed out in ^{/4/} (see also ^{/5/}) that superconducting pairing may be caused by a kinematic interaction. This interaction is included immanently into the Hamiltonian (1) through operator factor $(1 - n_{i-\sigma})$ which restricts the phase space available for an electron motion.

In the present paper the role of exchange and kinematic interactions is considered and their contributions to a superconducting gap equation are investigated by the two-time Green function method on the basis of the Hamiltonian (1).

2. Green functions and gap equation

A very complicated problem, one encounters when treating an electron system on the basis of (1), is a relation between charge (boson) degrees of freedom and spin (fermion) ones. A coupling between these two classes of excitations is taken into account in ^{/3/}

in the simplest way by applying the mean-field approximation. This approach was elaborated in ^{/6,7/} by using a mixed boson-fermion (slave boson) technique ^{/8,9/}. However, in our opinion, the approximations employed in ^{/3,6,7/} ignore effects which may arise due to the kinematic interaction.

To avoid the difficulty just pointed out and to keep possible kinematic effects we choose an equivalent representation for the Hamiltonian (1) by using Hubbard operators ^{/10/}

$$X_i^{\sigma\sigma} = c_{i\sigma}^+ (1 - n_{i-\sigma}), \quad X_i^{\sigma\bar{\sigma}} = X_i^{\bar{\sigma}\sigma}, \quad X_i^{\bar{\sigma}\bar{\sigma}} = n_{i\sigma} (1 - n_{i-\sigma}),$$

$$X_i^{\bar{\sigma}\sigma} = c_{i\bar{\sigma}}^+ c_{i-\sigma}, \quad \text{etc.}$$

Then we have

$$\mathcal{H} = t \sum_{\langle ij \rangle \sigma} X_i^{\sigma\sigma} X_j^{\sigma\sigma} + \frac{1}{2} \sum_{\langle ij \rangle \sigma} (X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\bar{\sigma}} X_j^{\sigma\bar{\sigma}}) - \mu \sum_{i\sigma} X_i^{\sigma\sigma}, \quad (2)$$

where μ is the chemical potential and $\bar{\sigma} \equiv -\sigma$. The operators $X_i^{\sigma\sigma}$ ($X_i^{\bar{\sigma}\bar{\sigma}}$) correspond to creation (annihilation) of electrons in the lower Hubbard subband. Concerning the nature of commutation relations it should be noted that $X_i^{\sigma\sigma}$, $X_i^{\bar{\sigma}\bar{\sigma}}$ behave like fermion operators; while $X_i^{\sigma\bar{\sigma}}$, $X_i^{\bar{\sigma}\sigma}$ like boson ones.

Now to take account of pairing let us introduce two-component Nambu operators

$$X_i^{\sigma} = \begin{pmatrix} X_i^{\sigma\sigma} \\ X_i^{\bar{\sigma}\bar{\sigma}} \end{pmatrix}, \quad X_i^{\bar{\sigma}} = \begin{pmatrix} X_i^{\bar{\sigma}\bar{\sigma}} \\ X_i^{\sigma\sigma} \end{pmatrix} \quad (3)$$

and define the two-time (anticommutator) matrix Green function

$$G_{ij}^{\sigma}(t-t') = \ll X_i^{\sigma}(t) | X_j^{\bar{\sigma}}(t') \gg =$$

$$= \begin{pmatrix} \langle\langle X_i^{0\sigma}(t) | X_j^{+\sigma\bar{0}}(t') \rangle\rangle & \langle\langle X_i^{0\sigma}(t) | X_j^{0\bar{0}}(t') \rangle\rangle \\ \langle\langle X_i^{+\sigma\bar{0}}(t) | X_j^{+\sigma\bar{0}}(t') \rangle\rangle & \langle\langle X_i^{+\sigma\bar{0}}(t) | X_j^{0\bar{0}}(t') \rangle\rangle \end{pmatrix} \quad (4)$$

with normal diagonal matrix elements and anomalous nondiagonal ones. The Fourier transform of it is given by

$$G_{ij}^{\sigma}(t-t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega G_{ij}^{\sigma}(\omega) e^{-i\omega(t-t')} \quad (5)$$

To obtain a quasiparticle spectrum of the system, we employ the method of the irreducible Green functions developed in ^{11,12}. According to this method the equation of motion for a dynamical variable $X_i^{\sigma}(t)$ is written as a sum of a regular linear in $X_l^{\sigma}(t)$ part due to time averaged forces and an irregular part $\mathcal{F}_i^{\sigma}(t)$ due to inelastic quasiparticle scattering

$$i \frac{d}{dt} X_i^{\sigma}(t) = [X_i^{\sigma}, \mathcal{H}] = \sum_l A_{il}^{\sigma} X_l^{\sigma}(t) + \mathcal{F}_i^{\sigma}(t). \quad (6)$$

Here the irreducible part $\mathcal{F}_i^{\sigma}(t)$ of the operator $X_i^{\sigma}(t)$ is defined as an orthogonal one to the linear term $\sum A_{il}^{\sigma} X_l^{\sigma}(t)$ by the equation

$$\langle \{ \mathcal{F}_i^{\sigma}, X_l^{\sigma} \} \rangle = 0. \quad (7)$$

Simultaneously this equation determines the coefficients A_{il}^{σ} , as it will be shown below (see eq.(10)).

After the Fourier transformation (5) we obtain the following equation for the Green function

$$\omega G_{ij}^{\sigma}(\omega) = \langle \{ X_i^{\sigma}, X_j^{+\sigma} \} \rangle + \sum_l A_{il}^{\sigma} G_{lj}^{\sigma}(\omega) + \langle\langle \mathcal{F}_i^{\sigma} | X_j^{+\sigma} \rangle\rangle_{\omega}.$$

(8)

To derive an equation for the irreducible Green function $\langle\langle \tilde{X}_i^\sigma(t) / \tilde{X}_j^\sigma(t') \rangle\rangle$ entering into (8), we differentiate it with respect to the second time t' :

$$-i \frac{d}{dt'} \langle\langle \tilde{X}_i^\sigma(t) / \tilde{X}_j^\sigma(t') \rangle\rangle = \sum_e \tilde{A}_{je}^* \langle\langle \tilde{X}_i^\sigma(t) / \tilde{X}_e^\sigma(t') \rangle\rangle + \langle\langle \tilde{X}_i^\sigma(t) / \tilde{X}_j^\sigma(t') \rangle\rangle, \quad (9)$$

where we have used eqs. (6) and (7). As it is easy to check that the irreducible Green functions $\langle\langle \tilde{X}_i^\sigma / \tilde{X}_j^\sigma \rangle\rangle_\omega$ is proportional to the scattering matrix $\langle\langle \tilde{X}_i^\sigma / \tilde{X}_j^\sigma \rangle\rangle_\omega$. This matrix defines all the inelastic scattering processes of quasiparticles and is proportional to the second and higher order in \tilde{t} and $\tilde{\mathcal{I}}$ interaction terms.

In the present paper we derive a renormalized quasiparticle spectrum only to the lowest order in interactions, keeping in (6) and (8) the linear terms, and ignore the finite life-time effects described by the irreducible Green functions (9). This approximation can be called the generalized Hartree-Fock-Bogolubov approximation allowing to take into account effects of superconducting pairing. Sometimes it is also called the moment-conserving approximation since in this approach the first two moments of the spectral density function $\langle \{ \chi_i^\sigma(t), \tilde{X}_j^\sigma(t') \} \rangle$ are conserved^{13,14/}.

Now to calculate the Green function in this lowest order approximation, we should determine the coefficients \tilde{A}_{ie}^σ by means of (7). Since according to (6) $\tilde{X}_i^\sigma = [\chi_i^\sigma, \mathcal{H}] - \sum_e \tilde{A}_{ie}^\sigma \chi_e^\sigma$ one gets from (7) the following equations

$$\sum_e \tilde{A}_{ie}^\sigma \langle \{ \chi_e^\sigma, \tilde{X}_j^\sigma \} \rangle = \langle \{ [\chi_i^\sigma, \mathcal{H}], \tilde{X}_j^\sigma \} \rangle. \quad (10)$$

Remembering that the coefficients \tilde{A}_{ie}^σ are (2×2) matrices with components $(\tilde{A}_{ie}^\sigma)_{\alpha\beta}$ and using the commutation relations for the Hubbard operators one may express from (10) the components $(\tilde{A}_{ie}^\sigma)_{\alpha\beta}$ through correlation functions as

$$(A_{ii}^{\sigma})_{11} = \frac{1}{\langle Q_i^{\sigma} \rangle} \left\{ -t \sum_{\ell(i)} \langle X_i^{\bar{\sigma}0} X_{\ell}^{0\bar{\sigma}} \rangle + \mu \langle Q_i^{\sigma} \rangle + \mathcal{J} \sum_{\ell(i)} (\langle X_{\ell}^{\bar{\sigma}\bar{\sigma}} X_i^{\sigma\bar{\sigma}} \rangle - \langle X_{\ell}^{\bar{\sigma}\bar{\sigma}} Q_i^{\sigma} \rangle) \right\}, \quad (11)$$

$$(A_{ij}^{\sigma})_{11} = \frac{1}{\langle Q_i^{\sigma} \rangle} \left\{ t (\langle X_i^{\bar{\sigma}\bar{\sigma}} X_j^{\sigma\bar{\sigma}} \rangle + \langle Q_i^{\sigma} Q_j^{\sigma} \rangle) - \mathcal{J} \langle X_j^{\bar{\sigma}0} X_i^{0\bar{\sigma}} \rangle \right\}, \quad (i \neq j) \quad (12)$$

$$(A_{ii}^{\sigma})_{12} = \frac{1}{\langle Q_i^{\sigma} \rangle} t \sum_{\ell(i)} \langle X_i^{0\bar{\sigma}} X_{\ell}^{0\bar{\sigma}} - X_i^{0\bar{\sigma}} X_{\ell}^{0\sigma} \rangle, \quad (13)$$

$$(A_{ij}^{\sigma})_{12} = \frac{1}{\langle Q_i^{\sigma} \rangle} \mathcal{J} \langle X_i^{0\bar{\sigma}} X_j^{0\bar{\sigma}} - X_i^{0\bar{\sigma}} X_j^{0\sigma} \rangle, \quad (i \neq j) \quad (14)$$

$$(A_{ii}^{\sigma})_{21} = (A_{ii}^{\sigma})_{12}^*, \quad (A_{ij}^{\sigma})_{22} = -(A_{ij}^{\sigma})_{11}^*. \quad (15)$$

Here $Q_i^{\sigma} \equiv X_i^{00} + X_i^{\sigma\bar{\sigma}}$; the summation $\sum_{\ell(i)}$ runs over $\vec{\ell}$ sites nearest to the \vec{i} site; each pair $(i \neq j)$ denotes nearest neighbours too. Note that diagonal components $(A_{ii}^{\sigma})_{11}$ $(A_{ii}^{\sigma})_{22}$ are correlation functions of the normal type while nondiagonal ones are of the anomalous type corresponding to a singlet pairing.

Further introducing quantities $\Omega_{\vec{q}}^{\sigma}$ and $\Delta_{\vec{q}}^{\sigma}$ in the \vec{q} -representation as

$$\Omega_{\vec{q}}^{\sigma} = (A_{ii}^{\sigma})_{11} + \sum_{j(i)} (A_{ij}^{\sigma})_{11} e^{-i\vec{q} \cdot (\vec{i}-\vec{j})} \quad (16)$$

$$\Delta_{\vec{q}}^{\sigma} = (A_{ii}^{\sigma})_{12} + \sum_{j(i)} (A_{ij}^{\sigma})_{12} e^{-i\vec{q} \cdot (\vec{i}-\vec{j})} \quad (17)$$

one obtains from (8) under the assumptions made above the matrix equation for $G^{\sigma}(\vec{q}, \omega)$

$$\begin{pmatrix} \omega - \Omega_{\vec{q}}^{\sigma} + \mu & \Delta_{\vec{q}}^{\sigma} \\ (\Delta_{\vec{q}}^{\sigma})^* & \omega + \Omega_{\vec{q}}^{\sigma} - \mu \end{pmatrix} G^{\sigma}(\vec{q}, \omega) = \begin{pmatrix} \langle Q_i^{\sigma} \rangle & 0 \\ 0 & \langle Q_i^{\bar{\sigma}} \rangle \end{pmatrix}, \quad (18)$$

Finding solutions of (18), we obtain both normal and anomalous Green functions, respectively

$$\langle\langle X^{0\sigma} | \dot{X}^{0\sigma} \rangle\rangle_{\vec{q}, \omega} = \langle Q_i^\sigma \rangle \frac{\omega + \Omega_{\vec{q}}^\sigma - \mu}{\omega^2 - (E_{\vec{q}}^\sigma)^2} \quad (19)$$

$$\langle\langle \dot{X}^{0\bar{\sigma}} | \dot{X}^{0\bar{\sigma}} \rangle\rangle_{\vec{q}, \omega} = - \langle Q_i^\sigma \rangle \frac{(\Delta_{\vec{q}}^\sigma)^*}{\omega^2 - (E_{\vec{q}}^\sigma)^2}, \quad (20)$$

where the quasiparticle spectrum $E_{\vec{q}}^\sigma$ is given by

$$(E_{\vec{q}}^\sigma)^2 = (\Omega_{\vec{q}}^\sigma - \mu)^2 + |\Delta_{\vec{q}}^\sigma|^2. \quad (21)$$

By means of (13)-(15) and (17) we obtain in the usual way the following self-consistent equation for the gap $\Delta_{\vec{q}}^\sigma$ in the spectrum

$$\Delta_{\vec{q}}^\sigma = \frac{1}{N} \sum_{\vec{k}} \frac{\Delta_{\vec{k}}^\sigma}{E_{\vec{k}}^\sigma} [t \gamma_{\vec{k}} + \mathcal{J} \gamma_{\vec{k}+\vec{q}}] t h \left(\frac{E_{\vec{k}}^\sigma}{2T} \right), \quad (22)$$

where $\gamma_{\vec{k}} = \sum_{\vec{a}(\sigma n, n)} \exp(i\vec{k}\vec{a})$. Equation (22) includes both contributions $\sim t$ due to the kinematic interaction and $\sim \mathcal{J}$ due to the exchange one.

To solve equation (22), one should take into account the symmetry of superconducting states in the anomalous correlation functions (13), (14) and (17). For the singlet pairing both the *S*-wave $\Delta_{1,2S}(\vec{q}) = \Delta_{1S}, \Delta_{2S} \gamma_{\vec{q}}$ and *d*-wave, $\Delta_{1,2d}(\vec{q}) = \Delta_{1d}(\cos q_x a - \cos q_y a), \Delta_{2d} \sin q_x a \sin q_y a$, states are possible^{1/6}. To obtain some restriction on the symmetry of the gap function (17) in eq.(22), we consider an exact condition for the Hubbard operators $\langle X_i^{\sigma 0} X_i^{\bar{\sigma} 0} \rangle = 0$, that eliminate two-particle states at one site. By using eq.(20) this condition can be written in the form

$$\langle X_i^{\sigma 0} X_i^{\bar{\sigma} 0} \rangle = \frac{\langle Q_i^\sigma \rangle}{N} \sum_{\vec{k}} \frac{\Delta_{\vec{k}}^\sigma}{2E_{\vec{k}}^\sigma} t h \left(\frac{E_{\vec{k}}^\sigma}{2T} \right) = 0, \quad (23)$$

where $\langle Q_i^\sigma \rangle = 1 - n/2 \neq 0$ for $n < 1$. As follows from this equation, a nonzero solution for the gap is possible only for the d -wave state, $\Delta_{\vec{k}} = \Delta_{1d}(\vec{k})$. But for the d -wave pairing the kinematic interaction $\sim t$ does not contribute to eq.(22) and the latter comes to

$$\Delta_{1d}(\vec{q}) = \frac{J}{N} \sum_{\vec{k}} \frac{\Delta_{1d}(\vec{k})}{E_{\vec{k}}^\sigma} \gamma_{\vec{k}+\vec{q}} t h \left(\frac{E_{\vec{k}}^\sigma}{2T} \right). \quad (24)$$

3. Approximate calculation of the spectrum of a normal state.

To calculate spectrum (21), self-consistently, one needs to estimate, besides the gap $\Delta(\vec{q})$, the normal state spectrum $\Omega_{\vec{q}}^\sigma$. According to (11), (12) and (16) the value of $\Omega_{\vec{q}}^\sigma$ is determined by normal correlation functions of two types: first, the function $\langle X_i^{\sigma\sigma} X_l^{\sigma\sigma} \rangle$ containing fermion-like operators and, second, the set of $\langle X_i^{\sigma\sigma} X_l^{\sigma'\sigma'} \rangle$, $\langle Q_i^\sigma Q_l^\sigma \rangle$ etc., with boson-like ones. The former may be calculated by means of Green function (19), while to estimate the boson-like correlation functions, we use a decoupling procedure of the "Hubbard-I" type ^{110/} ($i \neq l$):

$$\langle X_i^{\sigma\sigma} X_l^{\sigma'\sigma'} \rangle \approx \langle X_i^{\sigma\sigma} \rangle \langle X_l^{\sigma'\sigma'} \rangle = \left(\frac{n}{2} \right)^2$$

$$\langle (X_i^{00} + X_i^{\sigma\sigma})(X_l^{00} + X_l^{\sigma'\sigma'}) \rangle \approx \langle X_i^{00} + X_i^{\sigma\sigma} \rangle \langle X_l^{00} + X_l^{\sigma'\sigma'} \rangle = \left(1 - \frac{n}{2} \right)^2 \quad (25)$$

$$\langle X_i^{\sigma\bar{\sigma}} X_l^{\bar{\sigma}\sigma} \rangle \approx \langle X_i^{\sigma\bar{\sigma}} \rangle \langle X_l^{\bar{\sigma}\sigma} \rangle = 0. \quad (26)$$

The validity of these approximations (25), (26) is discussed in Appendix A.

Finally, we come to the following equation for $\Omega_{\vec{q}}^\sigma$ and the chemical potential μ

$$\Omega_{\vec{q}}^\sigma = \left(1 - \frac{n}{2} \right) t \gamma_{\vec{q}} - \frac{t}{2N} \sum_{\vec{k}} \gamma_{\vec{k}} \left[1 - \frac{\Omega_{\vec{k}}^\sigma - \mu}{E_{\vec{k}}^\sigma} t h \left(\frac{E_{\vec{k}}^\sigma}{2T} \right) \right] - \frac{n}{2} J \gamma_0 \quad (27)$$

$$\frac{n}{1 - n/2} = \frac{1}{N} \sum_{\vec{k}} \left[1 - \frac{\Omega_{\vec{k}}^\sigma - \mu}{E_{\vec{k}}^\sigma} t h \left(\frac{E_{\vec{k}}^\sigma}{2T} \right) \right], \quad (28)$$

where $n = \sum_{\sigma} \langle n_{i\sigma} \rangle$ is the average occupation number.

Thus the quasiparticle spectrum (21) for the superconducting state is determined self-consistently by the set of equations (24), (27) and (28). It should be noted that the "Hubbard-I" type approximation was adopted in deducing the equation for the normal state spectrum Σ_{σ}^{ω} and chemical potential μ , while the form of eqs. (22), (24) for the superconducting gap $\Delta(\bar{q})$ was found without this decoupling procedure. We emphasize also that handling with Hubbard operators up to now we have treated the problem in terms of "real" electron excitations.

4. Comparison with mean-field theories^{/3,6,7/}

Let us now compare our results (22), (24), (27) and (28) derived here for the "real" electron spectrum with analogous expressions obtained in^{/3,6,7/}. To do this, we employ the slave boson representation^{/8,9/} which allows the mapping from Hubbard operators to new fermion $f_{i\sigma}^+$, $f_{i\sigma}$ and boson b_i^+ , b_i operators as

$$X_i^{\sigma\sigma} \rightarrow b_i^+ f_{i\sigma}, \quad X_i^{\sigma\sigma'} \rightarrow f_{i\sigma}^+ f_{i\sigma'}, \quad X_i^{\sigma\sigma} \rightarrow b_i^+ b_i, \quad \text{etc.} \quad (29)$$

with the completeness relation

$$b_i^+ b_i + \sum_{\sigma} f_{i\sigma}^+ f_{i\sigma} = 1 \quad (30)$$

for each site i . Then the Hamiltonian (2) may be rewritten in the form

$$\mathcal{H} = t \sum_{\langle ij \rangle \sigma} b_i b_j^+ f_{i\sigma}^+ f_{j\sigma} + \frac{1}{2} g \sum_{\langle ij \rangle \sigma} (f_{i\sigma}^+ f_{i-\sigma} f_{j-\sigma}^+ f_{j\sigma} - f_{i\sigma}^+ f_{i\sigma} f_{j-\sigma}^+ f_{j-\sigma}) - \mu \sum_{i,\sigma} f_{i\sigma}^+ f_{i\sigma} + \sum_i \lambda_i (b_i^+ b_i + \sum_{\sigma} f_{i\sigma}^+ f_{i\sigma} - 1), \quad (31)$$

where the constraints (30) are taken into account by means of Lagrange multipliers λ_i .

Considering a purely fermion ("spinon") part of an excitation

spectrum for the Hamiltonian (31) one should first define by analogy with (3) two-component fermion operators ψ_i^σ :

$$X_i^\sigma = \begin{pmatrix} b_i^+ f_{i\sigma} \\ b_i f_{i-\sigma}^+ \end{pmatrix} \rightarrow \psi_i^\sigma \equiv \begin{pmatrix} f_{i\sigma} \\ f_{i-\sigma}^+ \end{pmatrix} \quad (32)$$

and introduce a new Green function $F_{ij}^\sigma(t-t')$ as

$$\begin{aligned} F_{ij}^\sigma(t-t') &= \langle\langle \psi_i^\sigma(t) | \psi_j^{\sigma\dagger}(t') \rangle\rangle = \\ &= \begin{pmatrix} \langle\langle f_{i\sigma}(t) | f_{j\sigma}^+(t') \rangle\rangle & \langle\langle f_{i\sigma}(t) | f_{j-\sigma}(t') \rangle\rangle \\ \langle\langle f_{i-\sigma}^+(t) | f_{j\sigma}^+(t') \rangle\rangle & \langle\langle f_{i-\sigma}^+(t) | f_{j-\sigma}(t') \rangle\rangle \end{pmatrix}. \end{aligned} \quad (33)$$

As before we find a spectrum to the first order in interaction by projecting the equation of motion for $F_{ij}^\sigma(t-t')$ onto the original set of operators ψ_i^σ and neglecting the irreducible Green functions which describe higher order scattering processes for new effective fermions. Then, after the Fourier transform we get the equation analogous to (18):

$$\begin{pmatrix} \omega - \varepsilon_{\vec{q}}^\sigma + \tilde{\mu} & \tilde{\Delta}_{\vec{q}} \\ \tilde{\Delta}_{\vec{q}}^* & \omega + \varepsilon_{\vec{q}}^\sigma - \mu \end{pmatrix} \mathcal{F}^\sigma(\vec{q}, \omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (34)$$

where

$$\varepsilon_{\vec{q}}^\sigma = t \gamma_{\vec{q}} \langle b_i b_j^+ \rangle - \mathcal{J} \gamma_{\vec{q}} \langle f_{i\sigma}^+ f_{j\sigma} \rangle - \frac{\eta}{2} \mathcal{J} \gamma_0 \quad (35)$$

$$\tilde{\Delta}_{\vec{q}} = \mathcal{J} \sum_{\ell(m)} (\langle f_{\ell\sigma} f_{m\sigma} \rangle - \langle f_{\ell\sigma} f_{m-\sigma} \rangle) e^{-i\vec{q}(\vec{\ell} - \vec{m})} \quad (36)$$

$$\tilde{\mu} = \mu - \lambda \quad (37)$$

and we assumed also that the restriction (30) is satisfied only in the average, therefore λ_i is not depend on the site \vec{i} .

The solutions of (34) are

$$\langle\langle f_{\sigma} | f_{\sigma}^{\dagger} \rangle\rangle_{\vec{q}, \omega} = \frac{\omega + \varepsilon_{\vec{q}}^{\sigma} - \tilde{\mu}}{\omega^2 - (\tilde{E}_{\vec{q}}^{\sigma})^2}, \quad (38)$$

$$\langle\langle f_{-\sigma}^{\dagger} | f_{\sigma}^{\dagger} \rangle\rangle_{\vec{q}, \omega} = - \frac{\tilde{\Delta}_{\vec{q}}^{\sigma*}}{\omega^2 - (\tilde{E}_{\vec{q}}^{\sigma})^2}, \quad (39)$$

with the quasiparticle spectrum

$$(\tilde{E}_{\vec{q}}^{\sigma})^2 = (\varepsilon_{\vec{q}}^{\sigma} - \tilde{\mu})^2 + |\tilde{\Delta}_{\vec{q}}^{\sigma}|^2. \quad (40)$$

Finally, by means of (35)-(39) we obtain the following set of self-consistent equations for $\varepsilon_{\vec{q}}^{\sigma}$, $\tilde{\Delta}_{\vec{q}}^{\sigma}$ and $\tilde{\mu}$:

$$\varepsilon_{\vec{q}}^{\sigma} = t \gamma_{\vec{q}} \langle b_i | b_j^{\dagger} \rangle - \gamma_{\vec{q}} \frac{1}{8N} \sum_{\vec{k}} \gamma_{\vec{k}} \left[1 - \frac{\varepsilon_{\vec{k}}^{\sigma} - \tilde{\mu}}{\tilde{E}_{\vec{k}}^{\sigma}} \tanh \left(\frac{\tilde{E}_{\vec{k}}^{\sigma}}{2T} \right) \right] - \frac{n}{2} \gamma_{\vec{q}} \quad (41)$$

$$\tilde{\Delta}_{\vec{q}}^{\sigma} = \frac{\gamma}{N} \sum_{\vec{k}} \gamma_{\vec{q}+\vec{k}} \frac{\tilde{\Delta}_{\vec{k}}^{\sigma}}{\tilde{E}_{\vec{k}}^{\sigma}} \tanh \left(\frac{\tilde{E}_{\vec{k}}^{\sigma}}{2T} \right) \quad (42)$$

$$n = \frac{1}{N} \sum_{\vec{k}} \left[1 - \frac{\varepsilon_{\vec{k}}^{\sigma} - \tilde{\mu}}{\tilde{E}_{\vec{k}}^{\sigma}} \tanh \left(\frac{\tilde{E}_{\vec{k}}^{\sigma}}{2T} \right) \right]. \quad (43)$$

Assuming in (42) the S-wave pairing $\tilde{\Delta}_{\vec{k}}^{\sigma} = \Delta_{2S} \delta_{\vec{k}}$, one comes to the same set of equations as deduced in [3,6,7]. It is clear that eq.(42) permits the d-wave pairing as well. However, the mean-field approach based on the slave-boson approximation replaces the local constraint (30) by a global one, $\gamma_i \rightarrow \lambda$, and therefore misses the kinematic condition similar to (23) that restricts the type of a pairing state.

5. Discussion

In the present paper, the superconducting pairing in a system of electrons with strong correlations is considered by employing the projections techniques for the Green functions. To describe electrons in the lower Hubbard subband, the Hubbard operators were introduced to avoid any decoupling of fermion and boson degrees of

freedom usually used in the slave-boson representation. As a result, we obtain the quasiparticle spectrum of electrons (21), (22), (27) and (28) to be different from that one for fermions (spinons), (40)-(42), deduced in the slave-boson representation. The most important difference is the appearance, in the gap equation (22), of a kinematic-type interaction ^{/15/} which comes from the kinetic energy term. Being proportional to t it would give the main contribution since in the limit of strong correlations $\mathcal{J} \sim t^2/u \ll t$. But only the d -wave pairing is allowed in this limit due to the exact condition (23) that forbids two-particle states on one site. Since in the case of d -wave pairing the kinematic interaction does not contribute to the gap equation, only the superexchange one $\sim \mathcal{J}$ survives giving Eq.(24), as in the superexchange theory of superconductivity proposed by Cyrot ^{/17/}. Therefore a kinematic type attraction for the superconducting pairing in the strong correlation limit, $u \rightarrow \infty$, proposed in ^{/4/} and considered lately in our paper ^{/5/} (see also ^{/18/}) does not work due to the d -wave symmetry of the gap in this case.

In the recent paper by Kotliar et al. ^{/19/}, the infinite Hubbard model with an N -fold-degenerate band has been treated approximately and a possibility of the superconducting pairing has been pointed out. By taking into account fluctuation corrections to the mean-field results in the slave-boson picture (see sect. 4) a weak attraction $\sim t$ for the d -wave (p-wave) states was obtained for a low concentration of holes (electrons). In the present paper, we consider only a linearized equation of motion for the Green function in (8) and ignore all inelastic scattering processes that are responsible for fluctuations. To take them into account, one should consider the renormalization of the quasiparticle spectrum originating from the scattering matrix $\langle\langle \mathcal{X}_i^{\sigma} / \mathcal{X}_j^{\sigma} \rangle\rangle$ in eq.(9) which can lead to an additional contribution to the pairing attraction of the order t in the $u \rightarrow \infty$ limit.

One should note also that an important contribution to the renormalization of spectrum (16) in the normal phase may come from the short-range correlations neglected in the Hubbard-I type approximation (25) and (26) (see Appendix A, (A.4), (A.5)). Some of these renormalizations as well as an effect of an antiferromagnetic ordering in the system will be considered elsewhere.

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Appendix A

Following the method applied in /20/ we demonstrate here in a short manner how the boson-like pair correlation functions $\langle X_i^{\sigma\sigma} X_e^{\sigma'\sigma'} \rangle$, $\langle X_i^{\sigma\bar{\sigma}} X_e^{\bar{\sigma}\sigma} \rangle$, $\langle X_i^{00} X_e^{\sigma\sigma} \rangle$ can be calculated by the same projection procedure as defined by (6). Let us introduce the set of operators $P_{\vec{q}}^{(i)}(\vec{R})$ defined as

$$\begin{aligned} P_{\vec{q}}^{(1)}(\vec{R}) &= \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\vec{J}} X_{j+\vec{h}}^{\sigma\sigma} X_j^{\sigma\sigma}, \\ P_{\vec{q}}^{(2)}(\vec{R}) &= \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\vec{J}} X_{j+\vec{h}}^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma}, \\ P_{\vec{q}}^{(3)}(\vec{R}) &= \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\vec{J}} X_{j+\vec{h}}^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma}. \end{aligned} \quad (\text{A.1})$$

Then the correlation functions under consideration can be now expressed as

$$\begin{aligned} \langle X_{j+\vec{h}}^{\sigma\sigma} X_j^{\sigma\sigma} \rangle &= \frac{1}{N} \sum_{\vec{q}} \langle P_{\vec{q}}^{(1)}(\vec{R}) X_{\vec{q}}^{0\sigma} \rangle \\ \langle X_{j+\vec{h}}^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \rangle &= \frac{1}{N} \sum_{\vec{q}} \langle P_{\vec{q}}^{(2)}(\vec{h}) X_{\vec{q}}^{0\bar{\sigma}} \rangle \\ \langle X_{j+\vec{h}}^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \rangle &= \frac{1}{N} \sum_{\vec{q}} \langle P_{\vec{q}}^{(3)}(\vec{h}) X_{\vec{q}}^{0\bar{\sigma}} \rangle \end{aligned} \quad (\text{A.2})$$

and, besides $\langle X_i^{00} X_j^{\sigma\sigma} \rangle = \langle X_j^{\sigma\sigma} \rangle - \sum_{\vec{\sigma}} \langle X_i^{\sigma\bar{\sigma}'} X_j^{\bar{\sigma}\sigma} \rangle$.

Employing the projection (6),(7) to the equation of motion for Green functions $\langle\langle X_{\vec{q}}^{\sigma\sigma}(t) | P_{\vec{q}}^{(i)}(\vec{R}; 0) \rangle\rangle$ and keeping in (6), as before, the part linear in $X_i^{\sigma\sigma}(t)$ one comes to the

matrix equation

$$\begin{pmatrix} \omega - \Omega_{\bar{q}}^{\sigma} + \mu & \Delta_{\bar{q}}^{\sigma} \\ (\Delta_{\bar{q}}^{\sigma})^* & \omega + \Omega_{\bar{q}}^{\bar{\sigma}} - \mu \end{pmatrix} \begin{pmatrix} \langle\langle X_{\bar{q}}^{\sigma\sigma} | \rho_{\bar{q}}^{(i)}(\bar{R}) \rangle\rangle_{\omega} \\ \langle\langle X_{\bar{q}}^{\bar{\sigma}\bar{\sigma}} | \rho_{\bar{q}}^{(i)}(\bar{R}) \rangle\rangle_{\omega} \end{pmatrix} = \begin{pmatrix} \langle\{X_{\bar{q}}^{\sigma\sigma}, \rho_{\bar{q}}^{(i)}(\bar{R})\}\rangle \\ \langle\{X_{\bar{q}}^{\bar{\sigma}\bar{\sigma}}, \rho_{\bar{q}}^{(i)}(\bar{R})\}\rangle \end{pmatrix}$$

In particular, choosing $\rho_{\bar{q}} = X_{-\bar{q}}^{\sigma\sigma}$, one arrives at (18). After calculating the anticommutators in the right-hand side of (A.3) and taking into account that $\langle X_i^{\sigma\sigma} \rangle = \langle X_i^{\bar{\sigma}\bar{\sigma}} \rangle = \frac{n}{2}$ we obtain the results ($\bar{R} \neq 0$):

$$\langle X_{j+h}^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \rangle = \left(\frac{n}{2}\right)^2 - \frac{1-n/2}{1-n} \left| \langle X_{j+h}^{\sigma\sigma} X_j^{\sigma\sigma} \rangle \right|^2 \quad (\text{A.4})$$

$$\langle X_{j+h}^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \rangle = \left(\frac{n}{2}\right)^2 + \frac{n/2}{1-n} \left| \langle X_{j+h}^{\sigma\sigma} X_j^{\sigma\sigma} \rangle \right|^2$$

$$\langle X_{j+h}^{\bar{\sigma}\bar{\sigma}} X_j^{\sigma\sigma} \rangle = \frac{-1}{1-n} \left[\left| \langle X_{j+h}^{\sigma\sigma} X_j^{\sigma\sigma} \rangle \right|^2 + \left| \langle X_{j+h}^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \rangle \right|^2 \right].$$

One may check that the approach developed here leads also to correct consequences for the case $\bar{h} = 0$, i.e. $\langle X_i^{\sigma\sigma} X_i^{\bar{\sigma}\bar{\sigma}} \rangle = \langle X_i^{\bar{\sigma}\bar{\sigma}} \rangle = n/2$, etc. Thus the boson-like correlation functions can be expressed by (A.4) through fermion-like ones given by eqs. (19), (20). The solution of this self-consistent system of equations will be presented elsewhere. Here we obtain, at least at $T=0$, an estimation for the dependence of correlation functions in the right-hand side of (A.4) on the electron concentration n by the Gutzwiller approximation developed recently by Zhang et al.^{/21/}. This gives for nearest sites:

$$\begin{aligned} \langle X_{j+h}^{\sigma\sigma} X_j^{\sigma\sigma} \rangle &\approx g_t \langle c_{j+h\sigma}^+ c_{j\sigma} \rangle_0, \\ \langle X_{j+h}^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \rangle &\approx g_t \langle c_{j+h\sigma}^+ c_{j\bar{\sigma}} \rangle_0, \end{aligned} \quad (\text{A.5})$$

where $g_t = 2(1-n)/[1+(1-n)]$ and $\langle A \rangle_0$ is the expectation value in the BCS state^{/21/}. One can see from (A.4) and (A.5) that the

"Hubbard-I" decoupling procedure adopted in this paper neglects the terms in the right-hand side of (A.4) proportional to $(1-n) \ll 1$.

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