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# ON THE ROLE OF KINEMATIC AND EXCHANGE INTERACTIONS IN SUPERCONDUCTING PAIRING OF ELECTRONS IN THE 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-Hubard system near the insulator-metal transition. He proposed the theory of superconductivity on the basis of the effective exchange Hamiltonian of the form[3]:

$$\mathcal{H} = t \sum_{\langle ij\rangle,\sigma} (1 - n_{i-\sigma}) c^{+}_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}) + J \sum_{\langle ij\rangle} (S_i S_j - \frac{1}{4} n_i n_j) \qquad (1)$$

with $\langle ij\rangle$ nearest neighbouring sites on a square lattice; $J = 4t^2/U$ is the antiferromagnetic coupling. The Hamiltonian (1) results form 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 factors $(1 - n_{i-\sigma})$ which restrict 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]

$$X_i^{\sigma 0} = c_{i\sigma}^{+}(1-n_{i-\sigma}),\quad X_i^{0\sigma} = \overset{+}{X}{}_i^{\sigma 0},\quad X_i^{\sigma\sigma} = n_{i\sigma}(1-n_{i-\sigma}),$$

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

Then we have

$$\mathcal{H} = t\sum_{\langle ij\rangle,\sigma} X_i^{\sigma0}X_j^{0\sigma} + \frac{1}{2} J\sum_{\langle ij\rangle,\sigma}\left(X_i^{\sigma\bar\sigma}X_j^{\bar\sigma\sigma} - X_i^{\sigma\sigma}X_j^{\bar\sigma\bar\sigma}\right) - \mu\sum_{i\sigma} X_i^{\bar\sigma\bar\sigma}, \quad (2)$$

where $\mu$ is the chemical potential and $\bar\sigma \equiv -\sigma$. The operators $X_i^{\sigma0}$ ($X_i^{0\sigma}$) correspond to creation (annihilation) of electrons in the lower Hubbard subband. Concerning the nature of commutation relations it should be noted that $X_i^{\sigma0}$, $X_i^{0\sigma}$ bahave like fermion operators; while $X_i^{\sigma\sigma'}$ like boson ones.

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

$$X_i^\sigma = \begin{pmatrix} X_i^{0\sigma} \\ \overset{+}{X}{}_i^{0\bar\sigma}\end{pmatrix},\qquad \overset{+}{X}{}_i^\sigma = \left(\overset{+}{X}{}_i^{0\sigma},\, X_i^{0\bar\sigma}\right) \quad (3)$$

and define two-time (anticommutator) matrix Green function

$$G_{ij}^\sigma(t-t') = \langle\langle X_i^\sigma(t)\,|\,\overset{+}{X}{}_j^\sigma(t')\rangle\rangle = \begin{pmatrix} \langle\langle X_i^{0\sigma}(t)\,|\,\overset{+}{X}{}_j^{0\sigma}(t')\rangle\rangle & \langle\langle X_i^{0\sigma}(t)\,|\,X_j^{0\bar\sigma}(t')\rangle\rangle \\ \langle\langle \overset{+}{X}{}_i^{0\bar\sigma}(t)\,|\,\overset{+}{X}{}_j^{0\sigma}(t')\rangle\rangle & \langle\langle \overset{+}{X}{}_i^{0\bar\sigma}(t)\,|\,X_j^{0\bar\sigma}(t')\rangle\rangle \end{pmatrix} \quad (4)$$

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 $X_\ell^\sigma(t)$ part due to time averaged forces and an irregular part $Z_i^\sigma(t)$ due to an inelastic quasiparticle scattering

$$i\frac{d}{dt}X_i^\sigma(t) = [X_i^\sigma(t), H] = \sum_\ell A_{i\ell}^\sigma X_\ell^\sigma(t) + Z_i^\sigma(t). \quad (6)$$

Here the irreducible part $Z_i^\sigma(t)$ of the operator $\dot X_i^\sigma(t)$ is defined as an orthogonal one to the linear term $\sum A_{i\ell}^\sigma X_\ell^\sigma(t)$ by the equation

$$\langle\{Z_i^\sigma, \overset{+}{X}{}_\ell^\sigma\}\rangle = 0. \quad (7)$$

Simultaneously this equation determines the coefficients $A_{i\ell}^\sigma$, as it will be shown below (see eq.(10)).

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

$$\omega G_{ij}^\sigma(\omega) = \langle\{X_i^\sigma, \overset{+}{X}{}_j^\sigma\}\rangle + \sum_\ell A_{i\ell}^\sigma G_{\ell j}^\sigma(\omega) + \langle\langle Z_i^\sigma\,|\,\overset{+}{X}{}_j^\sigma\rangle\rangle_\omega. \quad (8)$$

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

$$-i\frac{d}{dt'}\langle\langle Z_i^\sigma(t)\,|\,\overset{+}{X}{}_j^\sigma(t')\rangle\rangle = \sum_\ell \overset{*}{A}{}_{j\ell}^\sigma \langle\langle Z_i^\sigma(t)\,|\,\overset{+}{X}{}_\ell^\sigma(t')\rangle\rangle + \langle\langle Z_i^\sigma(t)\,|\,\overset{+}{Z}{}_j^\sigma(t')\rangle\rangle, \quad (9)$$

where we have used eqs.(6) and (7). As it is easy to check that the irreducible Green function $\langle\langle Z_i^\sigma\,|\,\overset{+}{X}{}_j^\sigma\rangle\rangle_\omega$ is proportional to the scattering matrix $\langle\langle Z_i^\sigma\,|\,\overset{+}{Z}{}_j^\sigma\rangle\rangle$. This matrix defines all the inelastic scattering processes of quasiparticles and is proportional to the second and higher order in $t$ and $J$ interaction terms.

In the present paper we derive a renormalized quasiparticle spectrum only to the lowest order in interactions, keeping in (6) an (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 $\langle\{X_i^\sigma(t)\,,\,\overset{+}{X}{}_j^\sigma(t')\}\rangle$ are conserved [13,14].

Now to calculate the Green function in this lowest order approximation, we should determine the coefficients $A_{i\ell}^\sigma$ by means of (7). Since according to (6) $Z_i^\sigma=[X_i^\sigma,H] - \sum A_{i\ell}^\sigma X_\ell^\sigma$, one gets from (7) the following equations

$$\sum_\ell A_{i\ell}^\sigma \langle\{X_\ell^\sigma,\overset{+}{X}{}_j^\sigma\}\rangle = \langle\{[X_i^\sigma,H],\overset{+}{X}{}_j^\sigma\}\rangle . \qquad (10)$$

Remembering that the coefficients $A_{i\ell}^\sigma$ are (2x2) matrices with components $(A_{i\ell}^\sigma)_{\alpha\beta}$ and using the commutation relations for the Hubbard operators one may express from (10) the components $(A_{i\ell}^\sigma)_{\alpha\beta}$ through correlation functions as

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

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

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

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

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

Here, $Q_i^\sigma \equiv X_i^{00} + X_i^{\sigma\sigma}$; 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 $(A_{i\ell}^\sigma)_{11}$, $(A_{i\ell}^\sigma)_{22}$ 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

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

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

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

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

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

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

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

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

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

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

$$\Delta_{\vec q}^\sigma = \frac{2}{N}\sum_{\vec k}\frac{\Delta_{\vec k}^\sigma}{E_{\vec k}^\sigma}[t\gamma_{\vec k} + J\gamma_{\vec k+\vec q}]\,\mathrm{th}\left(\frac{E_{\vec k}^\sigma}{2T}\right) . \qquad (22)$$

where $\gamma_{\vec k} = \frac{1}{2}\sum_{\vec a(=n.n.)}\exp(i\vec k\vec a)$. The equation (22) includes both contributions $\sim t$ due to the kinematic interaction and $\sim J$ to the exchange one.

Let us for a moment neglect the linear in t contribution and assume in particular that $\Delta_{\vec q}^\sigma = 4\Delta\gamma_{\vec q}$. Then taking into account the equality following from a symmetry of the Brillouin zone

$$\sum_{\vec{k}} \frac{\gamma_{\vec{k}}}{E^{\sigma}_{\vec{k}}} \cos \vec{k}\vec{a}\, \mathrm{th}\left(\frac{E^{\sigma}_{\vec{k}}}{2T}\right) = \frac{1}{2} \sum_{\vec{k}} \frac{\gamma^2_{\vec{k}}}{E^{\sigma}_{\vec{k}}} \mathrm{th}\frac{E^{\sigma}_{\vec{k}}}{2T} \tag{23}$$

we find from (22) the gap equation

$$1 = \frac{I}{N} \sum_{\vec{k}} \frac{\gamma^2_{\vec{k}}}{E^{\sigma}_{\vec{k}}} \mathrm{th}\left(\frac{E^{\sigma}_{\vec{k}}}{2T}\right), \tag{24}$$

which coincides with that of paper[3].

## 3. APPROXIMATE CALCULATION OF THE SPECTRUM OF A NORMAL STATE

To calculate self-consistently the spectrum (21), one needs to estimate, besides the gap $\Delta^{\sigma}_{\vec{q}}$, the normal state spectrum $\Omega^{\sigma}_{\vec{q}}$ in (21). According to (11), (12), and (16) the value of $\Omega^{\sigma}_{\vec{q}}$ is determined by normal correlation functions of two types: first, the function $\langle X^{\sigma 0}_{i} X^{0\sigma}_{\ell} \rangle$ containing fermion-like operators and, second, the set of $\langle X^{\bar{\sigma}\sigma}_{i} X^{\sigma\bar{\sigma}}_{\ell} \rangle$, $\langle Q^{\sigma}_{i} Q^{\sigma}_{\ell} \rangle$, etc., with boson-like ones. The former may be calculated by means of Green function given by (19) while to estimate the boson-like correlation functions we use a decoupling procedure of the "Hubbard-I" type[10]:

$$\begin{aligned} &\langle X^{\bar{\sigma}\bar{\sigma}}_{i} (X^{00}_{\ell} + X^{\sigma\sigma}_{\ell}) \rangle \approx \langle X^{\bar{\sigma}\bar{\sigma}}_{i} \rangle \langle X^{00}_{\ell} + X^{\sigma\sigma}_{\ell} \rangle = \frac{n}{2}\left(1 - \frac{n}{2}\right), \\ &\langle (X^{00}_{i} + X^{\sigma\sigma}_{i})(X^{00}_{\ell} + X^{\sigma\sigma}_{\ell}) \rangle \approx \langle X^{00}_{i} + X^{\sigma\sigma}_{i} \rangle \langle X^{00}_{\ell} + X^{\sigma\sigma}_{\ell} \rangle = \left(1 - \frac{n}{2}\right)^2 . \end{aligned} \tag{25}$$

Moreover, because a possible ferro- or antiferromagnetic ordering in the system is not considered in this paper we assume

$$\langle X^{\bar{\sigma}\sigma}_{i} X^{\sigma\bar{\sigma}}_{\ell} \rangle \sim \langle S^{\pm}_{i} S^{\mp}_{\ell} \rangle \to 0 . \tag{26}$$

Finally we come to the following equation for $\Omega^{\sigma}_{q}$ and the chemical potential $\mu$

$$\Omega^{\sigma}_{\vec{q}} = 2\left(1 - \frac{n}{2}\right) t \gamma_{\vec{q}} - 2t \frac{1}{N} \sum \gamma_{\vec{k}} \left[1 - \frac{\Omega^{\sigma}_{\vec{k}} - \mu}{E^{\sigma}_{\vec{k}}} \mathrm{th}\left(\frac{E^{\sigma}_{\vec{k}}}{2T}\right)\right] - nJ\gamma_0 . \tag{27}$$



$$\frac{n}{1 - n/2} = \frac{1}{N} \sum_{\vec{k}} \left[1 - \frac{\Omega^{\sigma}_{\vec{k}} - \mu}{E^{\sigma}_{\vec{k}}} \mathrm{th}\left(\frac{E^{\sigma}_{\vec{k}}}{2T}\right)\right], \tag{28}$$

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 (22), (27), and (28). It should be noted that the "Hubbard-I" type approximation was adopted in deducing equations for the normal state spectrum $\Omega^{\sigma}_{\vec{q}}$ and the chemical potential $\mu$ while the form of eq.(22) for the superconducting gap $\Delta^{\sigma}_{\vec{q}}$ was found without this decoupling procedure. We emphasize also that handling with Hubbard operators up to now we have trated the problem in terms of "real" electron excitations.

## 4. COMPARISON WITH MEAN-FIELD THEORIES[3,6,7]

Let us now compare our results (22), (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

$$X^{0\sigma}_{i} \to b^{+}_{i} f_{i\sigma}, \quad X^{\sigma\sigma'}_{i} \to f^{+}_{i\sigma} f_{i\sigma'}, \quad X^{00}_{i} \to b^{+}_{i} b_{i}, \text{ etc.}, \tag{29}$$

with the completeness relation

$$b^{+}_{i} b_{i} + \sum_{\sigma} f^{+}_{i\sigma} f_{i\sigma} = 1 \tag{30}$$

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

$$\begin{aligned} \mathcal{H} = t \sum_{\langle ij\rangle,\sigma} b_i b^{+}_{j} f^{+}_{i\sigma} f_{j\sigma} + \frac{1}{2} J \sum_{\langle ij\rangle,\sigma} (f^{+}_{i\sigma} f_{i-\sigma} f^{+}_{j-\sigma} f_{j\sigma} - f^{+}_{i\sigma} f_{i\sigma} f^{+}_{j-\sigma} f_{j-\sigma}) - \\ - \mu \sum_{i,\sigma} f^{+}_{i\sigma} f_{i\sigma} + \sum_{i} \lambda_i \left(b^{+}_{i} b_i + \sum_{\sigma} f^{+}_{i\sigma} f_{i\sigma} - 1\right), \end{aligned} \tag{31}$$

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

Considering a purely fermion ("spinon") part of an excitation spectrum for the Hamiltonian (31) one should first dezone

$$\sum_{\vec k} \frac{\gamma_{\vec k}}{E^\sigma_{\vec k}} \cos \vec k \vec a \, \mathrm{th}\left(\frac{E^\sigma_{\vec k}}{2T}\right) = \frac{1}{2} \sum_{\vec k} \frac{\gamma^2_{\vec k}}{E^\sigma_{\vec k}} \mathrm{th}\frac{E^\sigma_{\vec k}}{2T} \qquad (23)$$

we find from (22) the gap equation

$$1 = \frac{I}{N} \sum_{\vec k} \frac{\gamma^2_{\vec k}}{E^\sigma_{\vec k}} \mathrm{th}\left(\frac{E^\sigma_{\vec k}}{2T}\right), \qquad (24)$$

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$$\langle X_i^{\bar\sigma\bar\sigma}(X_\ell^{00} + X_\ell^{\sigma\sigma})\rangle \approx \langle X_i^{\bar\sigma\bar\sigma}\rangle \langle X_\ell^{00} + X_\ell^{\sigma\sigma}\rangle = \frac{n}{2}\left(1-\frac{n}{2}\right),$$

$$\langle (X_i^{00} + X_i^{\sigma\sigma})(X_\ell^{00} + X_\ell^{\sigma\sigma})\rangle \approx \langle X_i^{00} + X_i^{\sigma\sigma}\rangle \langle X_\ell^{00} + X_\ell^{\sigma\sigma}\rangle = \left(1-\frac{n}{2}\right)^2. \qquad (25)$$

Moreover, because a possible ferro- or antiferromagnetic ordering in the system is not considered in this paper we assume

$$\langle X_i^{\bar\sigma\sigma} X_\ell^{\sigma\bar\sigma}\rangle \sim \langle S_i^\pm S_\ell^\mp\rangle \to 0. \qquad (26)$$

Finally we come to the following equation for $\Omega^\sigma_q$ and the chemical potential $\mu$

$$\Omega^\sigma_{\vec q} = 2\left(1-\frac{n}{2}\right) t \gamma_{\vec q} - 2t \frac{1}{N} \sum \gamma_{\vec k}\left[1 - \frac{\Omega^\sigma_{\vec k} - \mu}{E^\sigma_{\vec k}} \mathrm{th}\left(\frac{E^\sigma_{\vec k}}{2T}\right)\right] - nJ\gamma_0, \qquad (27)$$



$$\frac{n}{1-n/2} = \frac{1}{N} \sum_{\vec k}\left[1 - \frac{\Omega^\sigma_{\vec k} - \mu}{E^\sigma_{\vec k}} \mathrm{th}\left(\frac{E^\sigma_{\vec k}}{2T}\right)\right], \qquad (28)$$

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 (22), (27), and (28). It should be noted that the "Hubbard-I" type approximation was adopted in deducing equations for the normal state spectrum $\Omega^\sigma_{\vec q}$ and the chemical potential $\mu$ while the form of eq.(22) for the superconducting gap $\Delta^\sigma_{\vec q}$ was found without this decoupling procedure. We emphasize also that handling with Hubbard operators up to now we have trated the problem in terms of "real" electron excitations.

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$$X_i^{0\sigma} \to b_i^+ f_{i\sigma}, \quad X_i^{\sigma\sigma'} \to f^+_{i\sigma} f_{i\sigma'}, \quad X_i^{00} \to b_i^+ b_i, \text{ etc.}, \qquad (29)$$

with the completeness relation

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

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

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

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

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 $\Psi_i^\sigma$:

$$X_i^\sigma = \begin{pmatrix} b_i^+ f_{i\sigma} \\ b_i f_{i-\sigma}^+ \end{pmatrix} \to \Psi_i^\sigma \equiv \begin{pmatrix} f_{i\sigma} \\ f_{i-\sigma}^+ \end{pmatrix} \qquad (32)$$

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

$$\mathcal{F}_{ij}^\sigma(t-t') = \langle\langle \Psi_i^\sigma(t) \mid \Psi_j^{+\sigma}(t') \rangle\rangle =$$

$$= \begin{pmatrix} \langle\langle f_{i\sigma}(t) \mid f_{j\sigma}^+(t') \rangle\rangle & \langle\langle f_{i\sigma}(t) \mid f_{j-\sigma}(t') \rangle\rangle \\ \langle\langle f_{i-\sigma}^+(t) \mid f_{j\sigma}^+(t') \rangle\rangle & \langle\langle f_{i-\sigma}^+(t) \mid f_{j-\sigma}(t') \rangle\rangle \end{pmatrix} . \qquad (33)$$

As before we find a spectrum to the first order in interaction by projecting the equation of motion for $\mathcal{F}_{ij}^\sigma(t-t')$ onto the original set of operators $\Psi_\ell^\sigma$ 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):

$$\begin{pmatrix} \omega - \epsilon_{\vec q}^\sigma + \tilde\mu & \tilde\Delta_{\vec q}^\sigma \\ (\tilde\Delta_{\vec q}^\sigma)^* & \omega + \epsilon_{\vec q}^\sigma - \tilde\mu \end{pmatrix} \mathcal{F}^\sigma(\vec q, \omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \qquad (34)$$

where

$$\epsilon_{\vec q}^\sigma = 2t\gamma_{\vec q} \langle b_i b_j^+ \rangle - 2J\gamma_{\vec q} \langle f_{i\sigma}^+ f_{j\sigma} \rangle - nJ\gamma_0 , \qquad (35)$$

$$\tilde\Delta_{\vec q}^\sigma = 4J\gamma_{\vec q} \langle f_{i\sigma} f_{j-\sigma} \rangle , \qquad (36)$$

$$\tilde\mu = \mu - \lambda \qquad (37)$$

and we assumed also that the restriction (30) is satisfied only in the average, therefore $\lambda_i$ is independent of the site i .

The solutions of (34) are

$$\langle\langle f_\sigma \mid f_\sigma^+ \rangle\rangle_{\vec q, \omega} = \frac{\omega + \epsilon_{\vec q}^\sigma - \tilde\mu}{\omega^2 - (\tilde E_{\vec q}^\sigma)^2} , \qquad (38)$$

$$\langle\langle f_{-\sigma}^+ \mid f_\sigma^+ \rangle\rangle_{\vec q, \omega} = - \frac{(\tilde\Delta_{\vec q}^\sigma)^*}{\omega^2 - (\tilde E_{\vec q}^\sigma)^2} \qquad (39)$$



with the quasiparticle spectrum

$$(\tilde E_{\vec q}^\sigma)^2 = (\epsilon_{\vec q}^\sigma - \tilde\mu)^2 + |\tilde\Delta_{\vec q}^\sigma|^2 . \qquad (40)$$

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

$$\epsilon_{\vec q}^\sigma = 2t_{\vec q} \langle b_i b_j^+ \rangle - J\gamma_{\vec q} \frac{1}{2N} \sum_{\vec k} \gamma_{\vec k} \left[1 - \frac{\epsilon_{\vec k}^\sigma - \tilde\mu}{\tilde E_{\vec k}^\sigma} \mathrm{th}\left(\frac{\tilde E_{\vec k}^\sigma}{2T}\right)\right] - nJ\gamma_0 , \qquad (41)$$

$$1 = J \frac{1}{N} \sum_{\vec k} \gamma_{\vec k}^2 \, \mathrm{th}\left(\frac{\tilde E_{\vec k}^\sigma}{2T}\right) , \qquad (42)$$

$$n = \frac{1}{N} \sum_{\vec k} \left[1 - \frac{\epsilon_{\vec k}^\sigma - \tilde\mu}{\tilde E_{\vec k}^\sigma} \mathrm{th}\left(\frac{\tilde E_{\vec k}^\sigma}{2T}\right)\right] . \qquad (43)$$

In principle, these are the same equations as deduced in [3,6,7] to describe the fermion (spinon) excitation spectrum for which according (42) the gap $\tilde\Delta_{\vec q}^\sigma$ is of purely exchange origin and does not include a kinematic contribution.

Thus we see that the method adopted here which is based on the projection technique for the Green function is equivalent to the mean-field approximation used in [3,6,7] . Therefore, it is clear that the distinction of the quasiparticle spectrum determined by (21), (22), (27), and (28) from that of papers [3,6,7] is not due to approximations used for Green functions but rather due to a different consideration of the interaction between boson ($b_i$, $b_i^+$) degrees of freedom and fermion ($f_{i\sigma}$, $f_{i\sigma}^+$) ones. The result (40)-(43) and analogous ones derived in [3,6,7] follow from a somewhat independent consideration of these two classes of excitations that causes the purely fermionic character of the Green function (33). While treating the problem in terms of Hubbard operators by means of the Green function (4) that describe the real electrons in the lower Hubbard subband we avoid any decoupling of fermion and boson degrees of freedom. As a result, a kinematic-type interaction well-known in the spin-wave theory (see e.g. Dyson [15]) manifests itself in the gap equation (22). Being proportional to t , it gives the main contribution in the case of strong repulsion $U \gg t$ . Therefore, one can in this case consider the limit $J \to 0$ in equations (22), (27), and (28) which bring about the result of [4,5] for the transition temperature and other physical quantities. A detailed analysis and numerical solutions of equations (22), (27), and (28) will be considered elsewhere.

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Плакида Н.М., Юшанхай В.Ю., Стасюк И.В. E17-88-749
О роли кинематического и обменного взаимодействий в сверхпроводящем спаривании электронов в модели Хаббарда

На основе эффективного обменного гамильтониана рассмотрена система электронов в нижней хаббардовской подзоне при сильном внутриатомном отталкивании $U \gg t$. С помощью функций Грина, определенных на операторах Хаббарда, методом проектирования получен спектр возбуждений с учетом сверхпроводящего спаривания. Показано, что наиболее важный вклад в уравнение для щели определяется кинематическим линейным по $t$ взаимодействием, а не обменным с $J \sim t^2/U$, как предложено Андерсоном и др.

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Plakida N.M., Yushankhai V.Yu., Stasyuk I.V. E17-88-749
On the Role of Kinematic and Exchange Interactions in Superconducting Pairing of Electrons in the Hubbard Model

A system of electrons with strong intraatomic repulsion $U \gg t$ in the lower Hubbard subband is considered on the basis of the effective exchange Hamiltonian. An excitation spectrum allowing for the superconducting pairing is obtained by employing the projection technique for the Green function in terms of Hubbard operators. It is shown that the most important contribution to the gap equation comes from the kinematic interaction being linear in $t$ and not from the exchange one with $J \sim t^2/U$ as considered by Anderson et al.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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