$\rho\ 7\ \prime$

N.M.Plakida, I.V.Stasyuk*

ON THE THEORY
OF SUPERCONDUCTIVITY
IN THE HUBBARD MODEL

* Lvov Division of the Institute for Theoretical
Physics, Lvov 290005, USSR

1. INTRODUCTION

Recently a large number of theoretical models has been proposed to explain the pairing mechanism in the new oxide high-T_c superconductors (see, e.g. [1]). An important role of strong single-site Coulomb correlation was pointed out in several models based on the Hubbard model. A theory of superconductivity was proposed in [2] where the pairing of holes (or particles) in the nearly half-filled band case was caused by the kinematical interaction in the Hubbard model.

But equations for gap functions, obtained in [2] by a sophisticated diagram technique, has no simple physical meaning, and the appearance of two gaps in the simple Hubbard model seems unreasonable.

In the present paper, we consider the theory of superconductivity in the Hubbard model by employing a much simpler and physically more clear equation of motion method for the two-time Green functions [3]. This method has been proved to be successful in obtaining interpolation solutions in the Hubbard model (see, e.g. [4]). By generalizing the well-known "Hubbard-I" approximation [5] to incorporate the superconducting pairing correlations we get a simple system of equations for the gap and T_c. In comparison with the results of [2], we get only one gap function with the wave-vector dependence of the extended s-type [6] and some corrected expression for T_c. These differences, as it seems to us, are due to a more consistent consideration of kinematic-type scattering processes in the equation of motion method than in the diagram technique [2].

2. EQUATIONS FOR THE GREEN FUNCTIONS

To describe a system of electrons with a strong Coulomb correlation, we consider the Hubbard Hamiltonian

$$H = E \sum_{i\sigma} n_{i\sigma} + \sum_{ij\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} , \qquad (1)$$

where $a^+_{i\sigma}$, $a_{i\sigma}$ are the creation and annihilation operators for electrons with spin σ on the lattice site i; t_{ij} is the transfer integral, $U > 0$ is the intra-atomic Coulomb repulsion and the atomic energy level E is measured from the chemical potential μ; $E = E_o - \mu$.

A complete set of orbitally nondegenerate localized electronic states $|n_{i\uparrow}, n_{i\downarrow}>$ at the lattice site i consists of 4 functions:

1
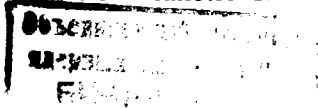
$$|1> = |0,0>, \quad |2> = |1,1>, \quad |3> = |0,1>, \quad |4> = |1,0>. \tag{2}$$

To distinguish whether an electron with inverse direction of the spin is present or not at a lattice site i, when operators $a_{i\sigma}^+$, $a_{i\sigma}$ act on the states (2), one should introduce the projection operators $\{n_{i-\sigma}, (1 - n_{i-\sigma})\}^{1/5}$. As a result, one obtains the Hubbard operators $X_i^{pq} = |ip> <iq|$ acting on the states (2). They can be written in terms of the Fermi operators as:

$$X_i^{14} = a_{i\uparrow}(1 - n_{i\downarrow}), \qquad X_i^{32} = a_{i\uparrow} n_{i\downarrow},$$
$$X_i^{13} = a_{i\downarrow}(1 - n_{i\uparrow}), \qquad X_i^{42} = -a_{i\downarrow} n_{i\uparrow}. \tag{3}$$

The Fermi operators $a_{i\sigma}$, $a_{i\sigma}^+$ are given by the equations:

$$a_{i\uparrow} = X_i^{14} + X_i^{32}, \qquad a_{i\uparrow}^\top = X_i^{41} + X_i^{23},$$
$$a_{i\downarrow} = X_i^{13} - X_i^{42}, \qquad a_{i\downarrow}^+ = X_i^{31} - X_i^{24}. \tag{4}$$

Now we consider the two-time thermodynamic Green function

$$G_{ij\sigma}|t - t'| = \ll a_{i\sigma}(t) ; a_{j\sigma}^+(t') \gg,$$

where the usual notation is used. In the atomic limit $t_{ij} = 0$ its Fourier-transform is given by

$$G_{ij\sigma}(\omega) = \delta_{ij} g(\omega); \quad g(\omega) = (1 - \tfrac{n}{2}) g_1(\omega) + \tfrac{n}{2} g_2(\omega), \tag{5}$$

$$g_1(\omega) = (\omega - E)^{-1}, \qquad g_2(\omega) = (\omega - E - U)^{-1}, \tag{6}$$

where $n = \sum_\sigma <n_{i\sigma}>$ is the average occupation number: $0 \le n \le 2$ (we consider the non-magnetic system, $<n_{i\sigma}> = <n_{i-\sigma}> = n/2$. Two terms in (5) correspond to electron excitations at a lattice site being empty or occupied by another electron with inverse spin projection, respectively.

For $t_{ij} \neq 0$ we derive an equation for $G_{ij\sigma}(\omega)$ by using equations of motion for the Hubbard operators (3), e.g.:

$$[X_i^{14}, H] = [a_{i\uparrow}(1 - n_{i\downarrow}), H] = E a_{i\uparrow}(1 - n_{i\downarrow}) +$$
$$+ \sum_j t_{ij} \{a_{i\downarrow} a_{i\downarrow}^+ a_{j\uparrow} - a_{i\downarrow}^+ a_{i\uparrow} a_{j\downarrow} + a_{i\downarrow} a_{i\uparrow} a_{j\downarrow}^+\}. \tag{7}$$

The last three terms in eq. (7) are due to the commutations of the operators $a_{i\uparrow}$, $a_{i\downarrow}$, $a_{i\downarrow}^+$ in X_i^{14} with the Hamiltonian. Effective four-particle interactions can be introduced to describe each of the three contributions in (7). They have the following form

$$V_1 \sim t_{ij} a_{i\uparrow}^+(1 - n_{i\downarrow}) a_{j\uparrow}; \qquad V_2 \sim t_{ij} a_{i\downarrow}^+|1 - n_{i\uparrow}) a_{j\downarrow};$$
$$V_3 \sim t_{ij} a_{j\downarrow}^+ a_{i\downarrow} n_{i\uparrow}, \tag{8}$$

and can be illustrated by the diagrams
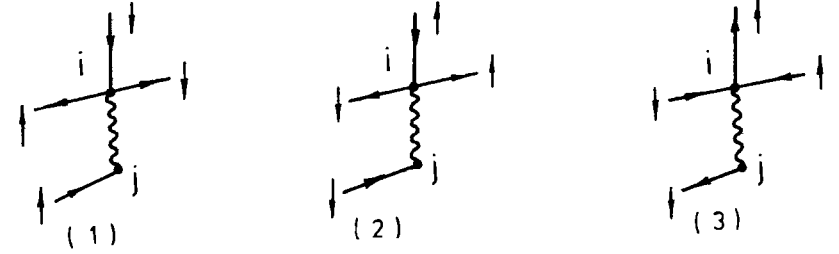
These are the kinematic-type interactions caused by some limitations due to the projection operators $n_{i-\sigma}$, $(1 - n_{i-\sigma})$.

The same type of interactions (9) appears in the diagram technique for the Hubbard operators (see, e.g. [7,8]) as zero-order vertices Γ_0.

As is well known, to obtain equations for the Green functions in the theory of superconductivity, one should introduce an anomalous pairing of the Fermi-operators with the same direction of lines in diagrams for the dressed vertex Γ. For this aim we should perform the following decoupling in the equation of motion (7):

$$a_{i\downarrow} a_{i\downarrow}^+ a_{j\uparrow} \to <a_{i\downarrow} a_{i\downarrow}^+> a_{j\uparrow} - <a_{i\downarrow} a_{j\uparrow}> a_{i\downarrow}^+,$$
$$a_{i\downarrow}^+ a_{i\uparrow} a_{j\downarrow} \to <a_{i\uparrow} a_{j\downarrow}> a_{i\downarrow}^+ - <a_{i\downarrow}^+ a_{j\downarrow}> a_{i\uparrow}, \tag{10}$$
$$a_{i\downarrow} a_{i\uparrow} a_{j\downarrow}^+ \to <a_{i\downarrow} a_{i\uparrow}> a_{j\downarrow}^+ - a_{i\uparrow} <a_{i\downarrow} a_{j\downarrow}^+>,$$

where both the normal and anomalous pairing are taken into account.

By performing the same procedure in all other equations for the Hubbard operators in (4) we obtain a closed system of equations for the Green functions. For the Fourier components of the Green functions in the q-space one gets the following equations:

$$\ll a_\uparrow |a_\uparrow^+ \gg_{\vec{q}\omega} = g(\omega) + g(\omega) t(\vec{q}) \ll a_\uparrow |a_\uparrow^+ \gg_{\vec{q}\omega} +$$
$$+ \gamma(\omega)[\Delta + F t(\vec{q})] \ll a_\downarrow^+ |a_\uparrow^+ \gg_{\vec{q}\omega}, \tag{11}$$

$$\langle\langle a_\downarrow^+ | a_\uparrow^+ \rangle\rangle_{\vec{q}\omega} = -\gamma(-\omega) F^* + g(-\omega) t(\vec{q}) \langle\langle a_\downarrow^+ | a_\uparrow^+ \rangle\rangle_{\vec{q}\omega} -$$
$$-\gamma(-\omega)[\Delta^* + F^* t(\vec{q})] \langle\langle a_\uparrow | a_\uparrow^+ \rangle\rangle_{\vec{q}\omega},$$

where

$$\gamma(\omega) = g_1(\omega) - g_2(\omega) \tag{12}$$

$$\Delta = 2 \sum_j t_{ij} \langle a_{i\uparrow} a_{j\downarrow} \rangle; \quad F = \langle a_{i\downarrow} a_{i\uparrow} \rangle. \tag{13}$$

The parameters Δ and F depend on the anomalous averages for electron pairs at different and the same lattice sites, respectively. By employing the identity $\langle [a_{i\downarrow} a_{i\uparrow}, H] \rangle = 0$ one can find the equation

$$(2E + U) F = \Delta. \tag{14}$$

that couples them.

Equations (11) are Gorkov's system of equations for the normal and anomalous Green functions. An analogous system of equations can be written for the matrix Green function $\langle\langle X^{pq}, X^{rs} \rangle\rangle_{\vec{q}\omega}$. It is convenient to write it in the form:

$$\hat{G} = \hat{g}\hat{N} + \hat{g}\hat{a}\hat{G} + \hat{g}\hat{N}\hat{t}\hat{G}, \tag{15}$$

where for the spin $\sigma = \uparrow$ the matrix $\hat{G}$ is constructed for $(p, q) = (14, 32, 31, 24)$ and for the spin $\sigma = \downarrow$ is constructed for $(p, q) = (13, 42, 41, 23)$. For $\sigma = \uparrow$ the matrices in (15) are given by:

$$\hat{g} = \begin{pmatrix} g_1(\omega) & 0 & 0 & 0 \\ 0 & g_2(\omega) & 0 & 0 \\ 0 & 0 & -g_1(-\omega) & 0 \\ 0 & 0 & 0 & -g_2(-\omega) \end{pmatrix}; \quad \hat{t} = \begin{pmatrix} t & t & 0 & 0 \\ t & t & 0 & 0 \\ 0 & 0 & -t & t \\ 0 & 0 & t & -t \end{pmatrix}.$$

$$\hat{N} = \begin{pmatrix} 1-n/2 & 0 & 0 & F \\ 0 & n/2 & F & 0 \\ 0 & F^* & 1-n/2 & 0 \\ F^* & 0 & 0 & n/2 \end{pmatrix}; \quad \hat{a} = \begin{pmatrix} 0 & 0 & \Delta & -\Delta \\ 0 & 0 & -\Delta & \Delta \\ \Delta^* & \Delta^* & 0 & 0 \\ \Delta^* & \Delta^* & 0 & 0 \end{pmatrix}. \tag{16}$$

Eq. (15) can also be written as

$$\hat{N}\hat{G}^{-1} = \hat{\Sigma}^{-1} - \hat{N}\hat{t}. \tag{17}$$

where $\hat{\Sigma}^{-1} = \hat{g}^{-1} - \hat{a}$. The matrix $\hat{\Sigma}$ is an irreducible part of the Green function.

It should be pointed out that the decoupling (10) is a natural generalization of the Hubbard-I approximation [5] to the case of anomalous averages. For $\Delta = F = 0$ one gets from (11) a standard equation for the Green function $\langle\langle a_\sigma | a_\sigma^+ \rangle\rangle_{\vec{q}\omega}$ in this approximation.

3. SPECTRUM OF EXCITATIONS AND GAP EQUATION

By solving eq. (17) one can obtain the electronic spectrum of excitations. It is defined by the equation $\text{Det}|\hat{N}^{-1}\hat{\Sigma}^{-1} - \hat{t}| = 0$ and is given by

$$\lambda_{1,2}^2(\vec{q}) = \frac{1}{2}[\epsilon_1^2(\vec{q}) + \epsilon_2^2(\vec{q})] \pm$$
$$\pm [(\frac{\epsilon_1^2(\vec{q}) - \epsilon_2^2(\vec{q})}{2})^2 - U^2|\Delta + Ft(\vec{q})|^2]^{1/2}, \tag{18}$$

where $\epsilon_{1,2}(\vec{q})$ are the Hubbard subband energies:

$$\epsilon_{1,2}(\vec{q}) = E + \frac{1}{2}[U + t(\vec{q})] \pm [\frac{1}{4}(U - t(\vec{q}))^2 - (1 - \frac{n}{2}) U t(\vec{q})]^{1/2}. \tag{19}$$

They correspond to the Hubbard-I approximation. For $t \ll U$ they can be written as

$$\epsilon_1(\vec{q}) = E + U + \frac{n}{2} t(\vec{q}); \quad \epsilon_2(\vec{q}) = E + (1 - \frac{n}{2}) t(\vec{q}). \tag{20}$$

and respectively

$$\lambda_{1,2}^2(\vec{q}) = \epsilon_{1,2}^2(\vec{q}) \mp \frac{U^2}{\epsilon_1^2 - \epsilon_2^2}|\Delta + Ft(\vec{q})|^2. \tag{21}$$

Let us consider two cases $0 < n < 1$ and $1 < n < 2$. In the first case the Fermi energy level is in the lower subband, where $\epsilon_2 = 0$ at the Fermi level μ. In that case $\epsilon_1^2 - \epsilon_2^2 \simeq U^2$ and one gets

$$\lambda_{1,2}^2(\vec{q}) = \epsilon_{1,2}^2(\vec{q}) \mp |\Delta(\vec{q})|^2 \tag{22}$$

There is a gap in the energy spectrum in the lower subband:

$$\Delta(\vec{q}) = \Delta + Ft(\vec{q})\{1 - \frac{1}{U}[\epsilon_2(q) - (1 - n) t(\vec{q})]\} \tag{23}$$

In the second case $1 < n < 2$, an analogous situation takes place for the upper subband. Now, since $\epsilon_1^2 - \epsilon_2^2 \simeq -U^2$, one gets

$$\lambda_{1,2}^2 = \epsilon_{1,2}^2 \pm |\tilde{\Delta}(\vec{q})|^2 \tag{24}$$

and the gap appears in the $\lambda_1(\vec{q})$ spectrum.

It is important that the gap (23) depends on the wave vector $\vec{q}$. This dependence is caused by the scattering processes of the third type in (9) that after the decoupling in (9) brings about the single-site correlation function F (13). The $\vec{q}$-dependence of the gap (23) is the same as that of the band energy $t(\vec{q})$. This type of pairing is called an extended s-type [8]. In the limit $U \to \infty$ when all two-electron states are eliminated, $F \to 0$ and the gap does not depend on $\vec{q}$: $\Delta(\vec{q}) \to \Delta$. Since the anomalous single-site correlation function has not been taken into account in [2], there is another $\vec{q}$-dependence of the gap function. It should be also stressed that we have only one gap parameter Δ, and not two Δ_1, Δ_2, as in [2].

Now we can from eq. (11) calculate the anomalous Green function and find out the corresponding correlation function. As a result, we obtain from eq. (13) the following equation for the gap parameter Δ:

$$\Delta = -\frac{1}{N} \sum_q \frac{t(\vec{q}) U \Delta}{2E + U} \{ \frac{\lambda_1^2(\vec{q}) - E^2 - (2E + U)U(1 - n/2)}{\lambda_1(\vec{q})[\lambda_2^2(\vec{q}) - \lambda_1^2(\vec{q})]} \text{th} \frac{\lambda_1(\vec{q})}{2T} +$$

$$+ \frac{\lambda_2^2(\vec{q}) - E^2 - (2E + U)U(1 - n/2)}{\lambda_2(\vec{q})[\lambda_1^2(\vec{q}) - \lambda_2^2(\vec{q})]} \text{th} \frac{\lambda_2(\vec{q})}{2T} \}. \tag{25}$$

Further we consider only the case $t \ll U$. For the occupation numbers $0 < n < 1$ the main contribution comes from the second term in (25). In the limiting case $U \to \infty$ the equation for the superconducting transition temperature T_c below which a nontrivial solution for Δ exists has the form

$$1 = \frac{1}{N} \sum_q \frac{t(\vec{q})(1 - n/2)}{\epsilon_2(\vec{q})} \text{th} \frac{\epsilon_2(\vec{q})}{2T_c}. \tag{26}$$

The summation over $\vec{q}$ will be replaced by the integration over $t(\vec{q})$ with a model density of states that is constant in the interval $[-w, w]$. By using the equation $n = (1/N) \sum_{q\sigma} < n_{q\sigma} >$ we eliminate the chemical potential μ in the Hubbard-I approximation for the average occupation number n. As a result, the electronic excitation spectrum reads

$$\epsilon_2(\vec{q}) = (1 - \frac{3}{2}n)w + (1 - \frac{n}{2})t(\vec{q}). \tag{27}$$

The equation for T_c (26) then takes the form

$$1 = \frac{1}{2} \int_{-1-a}^{1-a} dy (1 + \frac{a}{y}) \text{th} \frac{y}{2\theta_c}, \tag{28}$$

where the dimensionless temperature $\theta_c = T_c / w(1 - n/2)$ and the para-

meter $a = (3n - 2)/(2 - n)$ are introduced. In the logarithmic approximation we get for $1 - a \gg \theta_c$

$$\theta_c = \frac{2\gamma}{\pi} \sqrt{1 - a^2} \exp \{ - \frac{1 + a}{a} \}, \tag{29}$$

$(\ln \gamma = C, \gamma/\pi \approx 0.57)$, or

$$T_c = \frac{4\gamma}{\pi} w \sqrt{n(1 - n)/2} \exp \{ - \frac{2n}{3n - 2} \}. \tag{30}$$

The nontrivial solution for the gap exists in the range of concentration $3/2 < < n < 1$ (the critical value for the hole concentration $x_c = 1 - n = 1/3$).

The equation for the gap at zero temperature, $\Delta_0 = \Delta(T = 0)$, in the same approximation as eq. (26), has the form

$$1 = \frac{1}{N} \sum_q \frac{(1 - n/2) t(\vec{q})}{(\epsilon_2^2(q) + |\Delta_0|^2)^{1/2}}. \tag{31}$$

In the logarithmic approximation we get $2\Delta_0/T_c = 2\pi/\gamma \approx 3,5$, that is the BCS weak coupling value.

For the occupation numbers $1 < n < 2$, when the gap appears in the spectrum of the upper Hubbard subband, equations for T_c and Δ_0 have the forms

$$1 = -\frac{1}{N} \sum_q \frac{(n/2) t(\vec{q})}{\epsilon_1(\vec{q})} \text{th} \frac{\epsilon_1(\vec{q})}{2T_c}, \tag{32}$$

$$1 = -\frac{1}{N} \sum_q \frac{(n/2) t(\vec{q})}{(\epsilon_1^2(q) + |\Delta_0|^2)^{1/2}},$$

where $\epsilon_1(\vec{q}) = [2 - (3n/2)]w + (n/2)t(\vec{q})$. For the critical temperature T_c in this case we get for $(1 - n) \gg \theta_c$

$$T_c = \frac{4\gamma}{\pi} w \sqrt{\frac{(2 - n)(n - 1)}{2}} \exp \{ - \frac{2(2 - n)}{4 - 3n} \}. \tag{33}$$

The nonzero solution for the gap exists in the range $1 < n < 4/3$.

By comparing the results for $n < 1$ and $n > 1$ we find out the electron-hole symmetry: the formulae for $n < 1$ transform into the corresponding one for $n > 1$ under the substitution $n \to 2 - n$, $t(\vec{q}) \to - t(\vec{q})$ and $\epsilon_{1,2}(\vec{q}) \to - \epsilon_{2,1}(\vec{q})$.

The main results obtained here in the limit $U \to \infty$ are in accordance with the conclusions of the theory [2], though there are some deviations. For instance, the n-dependence in the exponent in formulae (30) for T_c does not coincide with that in [2] though the critical value for the hole-

concentration $x_c = 1/3$ is the same. Equations (32) and (33) for the upper subband obtained here in the explicit form permit us to check the electron-hole symmetry of the solutions.

4. DISCUSSION

We present a simple approximate scheme in the equation-of-motion method for the two-time Green function for the Hubbard model that generalizes the well-known first order approximation (the Hubbard-I approximation[5]) to the case of superconducting correlation.The proposed method permits one to obtain in an explicit form the gap equation (25) for a finite value of the single-site Coulomb repulsion U. Different scattering processes in (9) were analyzed, which show the role of the kinematical interaction in the pairing mechanisms for both of the Hubbard subbands and in the appearance of $\vec{q}$-dependence of the gap (23). In comparison with[2] we get only one gap function of the extended s-type. In the limit of strong Coulomb correlation, $U \to \infty$, equations for T_c (26) and the gap (31) give the results of the theory[2] but with a slightly different numerical coefficient. These deviations from the results of[2] are due to another coefficient in the matrix equation for the Green functions (15), (16). An explicit form of equations for T_c and the gap (26), (31), (32) both for the lower (0 < < n < 1) and upper (1 < n < 2) Hubbard subbands reveals the electron-hole symmetry of the problem.

The proposed method allows one to take into account the correlation of higher orders in (t/U) as well as to consider, in the framework of the Hubbard-III[5] approximation, the role of finite lifetime effects due to the nonelastic scattering of excitations. These problems would be considered in another paper. To apply the results of the present investigation to the new oxide superconductors of $La_{2-x} Sr_x Cu O_4$ and $Y Ba_2 Cu_3 O_7$ types, one should take into account a realistic crystal structure of the compounds and the existence of the long-range antiferromagnetic order in the nearly half-filled band for copper ions.

The authors are greatly indebted to Academician N.N.Bogolubov for helpful discussions.

REFERENCES

1. Fulde P. – Physica Scripta, 1987, (to be published).

2. Zaitsev R.O., Ivanov V.A. – Soviet Phys. Solid State, 1987, 10, p.2554, 3111.

3. Bogolubov N.N., Tyablikov S.V. – Soviet Phys. Doklady, 1959, 4, p.604.

4. Kuzemsky A.L. – Theor. and Math. Phys., 1978, 36, p.208.

5. Hubbard J. – Proc.Roy. Soc.A, 1963, 276, p.238; ibid 1964, 281, p.401.

6. Rice T.T. – Z.Phys., 1987, 68, p.9.

7. Slobodyan P.M., Stasyuk I.V. – Theor. and Math. Phys., 1974, 19, p.423.

8. Zaitsev R.O. – Soviet Phys. JETPh., 1976, 70, p.1100.

Плакида Н.М., Стасюк И.В.   E17-88-96
К теории сверхпроводимости в модели Хаббарда

Рассмотрен случай сильных внутриатомных корреляций в модели Хаббарда. На основе уравнений движения для двухвременных функций Грина с учетом аномальных спариваний получено уравнение для сверхпроводящей щели нелокального s -типа.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Plakida N.M., Stasyuk I.V.   E17-88-96
On the Theory of Superconductivity in the
Hubbard Model

A pairing mechanism caused by the kinematical interaction in the Hubbard model is considered. On the basis of equations of motion for two-time Green functions with anomalous pairings taken into account, equations are derived for the superconducting gap of an extended S-type and T_c .

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