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Hoang Anh Tuan
Nguyen Toan Thang
and
Nguyen Ngoc Thuan

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**SUPERCONDUCTING IN THE NEAR HALF-FILLING
HUBBARD MODEL**

Hoang Anh Tuan ¹
International Centre for Theoretical Physics, Trieste, Italy,

Nguyen Toan Thang and Nguyen Ngoc Thuan
Institute of Theoretical Physics, P.O.Box 429 Bo Ho, Hanoi 10000, Vietnam.

ABSTRACT

The near half-filling Hubbard model of strongly correlated electron systems is considered within the framework of the new functional integral method without slave boson. A dynamical system of equations determining the superconducting phase of the Hubbard model is derived. Both singlet and triplet Cooper pairings are studied.

MIRAMARE-TRIESTE

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¹Permanent address: Institute of Theoretical Physics, P.O.Box 429 Bo Ho, Hanoi 10000, Vietnam.

I. INTRODUCTION

Recently a good deal of effort has been undertaken in the study of possible superconducting states in the Hubbard model in connection with the discovery of high- T_c superconductivity [1-3]. However, the problem is still far from being resolved. The reason lies in the extreme complexity of the Hubbard model in the strong correlation limit. Some diagram techniques for Hubbard operators are supposed [4-7], but they are too complicated and therefore not very constructive. Also the slave boson method has been employed extensively in the Hubbard model [8-10]. However, there is a number of difficulties in this approach due to the local constrain [11]. Some time ago we applied the new functional method suggested by Sarker [12] to study the half-filling Hubbard model. We reobtained the well-known results of the Mott metal-insulator [13] and derived the system of equations for superconducting order parameters [14] for both singlet and triplet Cooper pairing. In the case of singlet pairing it gives back the result of Bogoliubov group [15].

In this paper by means of the Sarker's approach we consider the superconducting in the near half-filling Hubbard model.

II. SYSTEM OF EQUATIONS FOR THE GREEN FUNCTIONS

We start with the single Hubbard model defined by the following Hamiltonian in the Wannier representation:

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

Here, $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) annihilates (creates) an electron with spin σ in lattice site i , the chemical potential μ controls the total number of electrons, t_{ij} is the hopping integral between sites i and j , U is the one-site Coulomb repulsion between electrons of different spins which is assumed to be large in comparison with t_{ij} . In the new functional integral method [12] the initial system given by Hamiltonian (1) is mapped to another Fermi system, expressed in terms of the additional Grassmann variables $a(\tau)$ and $a^*(\tau)$ corresponding to the auxiliary fermions. Following [12], the partition function of the system is written as follows:

$$Z = Z_o^N \int Da^* Da \exp(S), \quad (2)$$

where N is the number of sites, Z_o is the single-site partition function that is given by

$$Z_o = 1 + 2 \exp(\beta\mu) + \exp[\beta(2\mu - U)].$$

Up to second order of the parameter t the action S has the form [12]:

$$\begin{aligned} S = & \sum_{k\sigma} \int_0^\beta \int_0^\beta d\tau d\tau' a_\sigma^*(k, \tau) g_\sigma(k, \tau, \tau') a_\sigma(k, \tau') \\ & + \frac{t^2}{4N} \sum_{\{k\sigma\}} \int_0^\beta \prod_i d\tau_i \left(\sqrt{\epsilon(k_i)} \right) \delta_{k_1+k_2, k_3+k_4} \Gamma_{\sigma\sigma'}(\tau_1, \tau_2, \tau_3, \tau_4) \cdot \\ & \cdot a_\sigma^*(k_1, \tau_1) a_{\sigma'}^*(k_2, \tau_2) a_{\sigma'}(k_3, \tau_3) a_\sigma(k_4, \tau_4), \end{aligned} \quad (3)$$

where $t\epsilon(k)$ is the Fourier transform of the hopping integral t_{ij} ,

$$\begin{aligned}\Gamma_{\sigma\sigma'} = & (2 - \delta_{\sigma\sigma'}) \left[\langle c_\sigma(\tau_1) c_{\sigma'}(\tau_2) c_{\sigma'}^*(\tau_3) c_\sigma^*(\tau_4) \rangle_o - \langle c_\sigma(\tau_1) c_\sigma^*(\tau_4) \rangle_o \langle c_{\sigma'}(\tau_2) c_{\sigma'}^*(\tau_3) \rangle_o \right. \\ & \left. + \langle c_\sigma(\tau_1) c_{\sigma'}^*(\tau_3) \rangle_o \langle c_{\sigma'}(\tau_2) c_\sigma^*(\tau_4) \rangle_o \right],\end{aligned}\quad (4)$$

and $g_o(k, \tau, \tau')$ is given by its Fourier transform $g_o(k, \omega) = -1 + t\epsilon(k)G_o(\omega)$ with $G_o(\omega) = \frac{q}{i\omega + \mu} + \frac{1-q}{i\omega + \mu - U}$; $q = Z_o^{-1}(1 + e^{\beta\mu})$; $\langle \dots \rangle_o$ refers to single site averages for $t = 0$.

Using Gorkov formalism [16] for treating the superconducting problems, we define the normal Green function

$$g_{\alpha\beta}(k, \tau - \tau') = -\langle a_\alpha(k, \tau) a_\beta^*(k, \tau') \rangle \quad (5)$$

and the anomalous Green functions

$$\begin{aligned}f_{\alpha\beta}(k, \tau - \tau') &= -\langle a_\alpha(k, \tau) a_\beta(-k, \tau') \rangle, \\ \bar{f}_{\alpha\beta}(k, \tau - \tau') &= -\langle a_\alpha^*(k, \tau) a_\beta^*(-k, \tau') \rangle.\end{aligned}\quad (6)$$

Making the Gorkov factorization on the second order term of the action (3), it is straightforward to obtain the following equations for the Fourier transforms of the Green functions [14]

$$g_{\alpha\gamma}(k, \omega) Q_{\gamma\beta}^1(k, \omega) + f_{\alpha\gamma}(k, \omega) K_{\gamma\beta}^2(k, \omega) = \delta_{\alpha\beta} \quad (7)$$

$$g_{\alpha\gamma}(k, \omega) K_{\gamma\beta}^1(k, \omega) + f_{\alpha\gamma}(k, \omega) Q_{\gamma\beta}^2(k, \omega) = 0, \quad (8)$$

where the following notations are used:

$$\begin{aligned}Q_{\alpha\beta}^1(k, \omega) &= -\delta_{\alpha\beta} g_o(k, \omega) + \delta_{\alpha\beta} \frac{t^2 \epsilon(k)}{2N} \sum_{\gamma\omega k'} \epsilon(k') g_{\gamma\gamma}(k', \omega_1) \Gamma_{\alpha\gamma}(\omega, \omega_1, \omega_1, \omega) \\ &\quad - \frac{t^2 \epsilon(k)}{2N} \sum_{\omega_1 k'} \epsilon(k') g_{\alpha\beta}(k', \omega_1) \Gamma_{\alpha\beta}(\omega, \omega_1, \omega, \omega_1)\end{aligned}\quad (9)$$

$$Q_{\alpha\beta}^2(k, \omega) = -Q_{\beta\alpha}^1(-k, -\omega) \quad (10)$$

$$K_{\alpha\beta}^1(k, \omega) = -\frac{t^2 \sqrt{\epsilon(k)\epsilon(-k)}}{2N} \sum_{\omega_1 k'} \sqrt{\epsilon(k')\epsilon(-k')} f_{\beta\alpha}(k', \omega_1) \Gamma_{\alpha\beta}(\omega, -\omega, \omega_1, -\omega_1) \quad (11)$$

$$K_{\alpha\beta}^2(k, \omega) = -\frac{t^2 \sqrt{\epsilon(k)\epsilon(-k)}}{2N} \sum_{\omega_1 k'} \sqrt{\epsilon(k')\epsilon(-k')} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 \bar{f}_{\beta\alpha}(k', \omega_1) \Gamma_{\beta\alpha}(-\omega_1, \omega_1, -\omega, \omega). \quad (12)$$

The summation convention on repeated spin indices is used in the above equations (9)-(12).

To proceed further one needs the explicit expression of the effective interaction vertex $\Gamma_{\sigma\sigma'}$ defined by (4). A lengthy but straightforward calculation yields for $\Gamma_{\alpha\beta}(\omega_1, \omega_2, \omega_3, \omega_4)$

$$\Gamma_{\alpha\beta}(\omega_1, \omega_2, \omega_3, \omega_4) = \delta_{\alpha\beta} \Gamma_o(\omega_1, \omega_2, \omega_3, \omega_4) + (\sigma_1)_{\alpha\beta} \Gamma_1(\omega_1, \omega_2, \omega_3, \omega_4), \quad (13)$$

where

$$\Gamma_o(\omega_1, \omega_2, \omega_3, \omega_4) = (\delta_{\omega_1, \omega_4} \delta_{\omega_2, \omega_3} - \delta_{\omega_1, \omega_3} \delta_{\omega_2, \omega_4}) q(1-q) \frac{U^2}{\lambda_1 \bar{\lambda}_1 \lambda_2 \bar{\lambda}_2}, \quad (14)$$

$$\begin{aligned} \Gamma_1(\omega_1, \omega_2, \omega_3, \omega_4) = & -\frac{2U^2(e^{2\beta\mu} - e^{(2\mu-U)\beta})\delta_{\omega_1, \omega_4}\delta_{\omega_2, \omega_3}}{Z_o^2 \lambda_1 \bar{\lambda}_1 \lambda_2 \bar{\lambda}_2} - \frac{2U^2 e^{\beta\mu} \delta_{\omega_1, \omega_3} \delta_{\omega_2, \omega_4}}{Z_o \lambda_1 \bar{\lambda}_1 \lambda_2 \bar{\lambda}_2} \\ & + \frac{2qU(\lambda_1 + \lambda_2)\delta_{\omega_1+\omega_2, \omega_3+\omega_4}}{\beta(\bar{\lambda}_2 - \lambda_1)\lambda_1 \lambda_2 \lambda_3 \lambda_4} - \frac{2(1-q)U(\bar{\lambda}_1 + \bar{\lambda}_2)\delta_{\omega_1+\omega_2, \omega_3+\omega_4}}{\beta(\bar{\lambda}_2 - \lambda_1)\bar{\lambda}_1 \bar{\lambda}_2 \bar{\lambda}_3 \bar{\lambda}_4}, \end{aligned} \quad (15)$$

with $\lambda_i = i\omega_i + \mu$, $\bar{\lambda}_i = -i\omega_i + \alpha$, $\alpha = U - \mu$, $i = \bar{1}, \bar{4}$.

Hereafter $\sigma_i (i = 1, 2, 3)$ denotes a Pauli matrix. In the paramagnetic state the normal Green function is diagonal in spin indices:

$$g_{\alpha\beta}(k, \omega) = g(k, \omega) \delta_{\alpha\beta} \quad (16)$$

while the anomalous Green functions have the following general form:

$$f_{\alpha\beta}(k, \omega) = f_s(k, \omega) \epsilon_{\alpha\beta} + (\sigma_2 \vec{\sigma})_{\alpha\beta} \vec{f}_t(k, \omega), \quad (17)$$

where $\epsilon_{\alpha\beta}$ is the second rank antisymmetric spinor, the scalar $f_s(k, \omega)$ is even and the vector $\vec{f}_t(k, \omega)$ is odd function of k and ω :

$$\begin{aligned} f_s(k, \omega) &= f_s(-k, -\omega) \\ \vec{f}_t(k, \omega) &= -\vec{f}_t(-k, -\omega) \end{aligned} \quad (18)$$

Substituting formulas (16) and (17) into equations (7)-(8) we obtain:

$$g(k, \omega) = \frac{Q(-k, -\omega)}{D(k, \omega)} \quad (19)$$

$$f_s(k, \omega) = \frac{K_o(k, \omega)}{D(k, \omega)} \quad (20)$$

$$\vec{f}_t(k, \omega) = \frac{\vec{K}_1(k, \omega)}{D(k, \omega)} \quad (21)$$

where

$$\begin{aligned} Q(k, \omega) &= -g_o(k, \omega) + \frac{t^2 \epsilon(k)}{N} \sum_{k' \omega'} \epsilon(k') [\Gamma_o(\omega, \omega', \omega', \omega) \\ &+ \frac{1}{2} \Gamma_1(\omega, \omega', \omega', \omega)] g(k', \omega') \end{aligned} \quad (22)$$

$$D(k, \omega) = -Q(k, \omega) Q(-k, -\omega) - |K_o|^2 - |\vec{K}_1|^2 \quad (23)$$

$$K_o(k, \omega) = -\frac{t^2 \sqrt{\epsilon(k) \epsilon(-k)}}{2N} \sum_{k' \omega'} \sqrt{\epsilon(k') \epsilon(-k')} f_s(k', \omega') O_s(\omega, \omega') \quad (24)$$

$$\begin{aligned} K_{1i} &= -\frac{t^2 \sqrt{\epsilon(k) \epsilon(-k)}}{2N} \sum_{k' \omega'} \sqrt{\epsilon(k') \epsilon(-k')} f_{ti}(k', \omega') O_i(\omega, \omega') \\ &(i = 1, 2, 3) \end{aligned} \quad (25)$$

$$\begin{aligned} O_s(\omega, \omega') &= O_3(\omega, \omega') = \Gamma_1(\omega, -\omega, \omega', -\omega') \\ O_1(\omega, \omega') &= O_2(\omega, \omega') = \Gamma_o(\omega, -\omega, \omega', -\omega') \end{aligned} \quad (26)$$

The above equations (19)-(26) form the closed system of equations for the Green functions defined by (5) and (6).

III. DISCUSSIONS

It is convenient to introduce the following notations:

$$\Delta_s(\omega) = -\frac{K_o(k, \omega)}{t^2 \sqrt{\epsilon(k) \epsilon(-k)}} \quad (27)$$

$$\vec{\Delta}_t(\omega) = -\frac{\vec{K}_1(k, \omega)}{t^2 \sqrt{\epsilon(k) \epsilon(-k)}} \quad (28)$$

Then from the equations (20)-(26) it follows:

$$\Delta_s(\omega) = \frac{t^2}{2N} \sum_{\omega' k'} \frac{O_s(\omega, \omega') \Delta_s(\omega')}{D(k', \omega')} \epsilon(k') \epsilon(-k') \quad (29)$$

$$\Delta_{ti}(\omega) = \frac{t^2}{2N} \sum_{\omega' k'} \frac{O_{ti}(\omega, \omega') \Delta_{ti}(\omega')}{D(k', \omega')} \epsilon(k') \epsilon(-k') \quad (30)$$

where $D(k, \omega)$ may be rewritten as:

$$D(k, \omega) = -Q(k, \omega)Q(-k, -\omega) - t^2 \epsilon(k) \epsilon(-k) (|\Delta_s|^2 + |\Delta_t|^2). \quad (31)$$

To relate the chemical potential with doping δ we need the electron Green function:

$$\tilde{g}_{\alpha\beta}(k, \omega) = - \langle c_\alpha(k, \omega) c_\beta^*(k, \omega) \rangle \quad (32)$$

which is related to the corresponding Green function for the auxiliary a - particle by the relationship

$$t \epsilon(k) \tilde{g}_{\alpha\beta}(k, \omega) = -[\delta_{\alpha\beta} + g_{\alpha\beta}(k, \omega)] \quad (33)$$

In order to determine the transition temperature it is sufficient to write $\tilde{g}_{\alpha\beta}(k, \omega)$ for the normal phase

$$\tilde{g}(k, \omega) = \frac{\Lambda(k, \omega)}{1 - \epsilon(k) \Lambda(k, \omega)} \quad (34)$$

with

$$\Lambda(k, \omega) = G_o(\omega) - \frac{1}{N} \sum_{k' \omega'} \epsilon^2(k') [\Gamma_o(\omega', \omega, \omega, \omega') + \frac{1}{2} \Gamma_1(\omega', \omega, \omega, \omega')] \tilde{g}(k, \omega) \quad (35)$$

Then the equation for chemical potential reads:

$$\frac{1}{N} \sum_k \frac{1}{\beta} \sum_\omega \frac{\Lambda(k, \omega)}{1 - \epsilon(k) \Lambda(k, \omega)} = 1 - \delta \quad (36)$$

The equations (29), (30) and (36) form the closed system of equations for the superconducting order parameters $\Delta_s(\omega)$, $\Delta_t(\omega)$ and μ , taking into account both singlet and triplet pairing contributions.

In the case of the singlet pairing only, by setting $\tilde{\Delta}_t(\omega) = 0$, from equation (29) one obtains the equation determining the transition temperature of the singlet superconducting state:

$$\begin{aligned} \Delta_s(\omega) = & - \frac{U^2(e^{2\beta\mu} - e^{(2\mu-U)\beta} + Z_o e^{\beta\mu})\Delta_s(\omega)\Phi(\omega)}{Z_o^2(\omega^2 + \mu^2)(\omega^2 + \alpha^2)} + \frac{2U\mu q\psi_1}{(\alpha - \mu)(\omega^2 + \mu^2)} \\ & - \frac{2U(1-q)\psi_2}{(\alpha - \mu)(\mu^2 + \alpha^2)}, \end{aligned} \quad (37)$$

where

$$\Phi(\omega) = \frac{1}{N} \sum_k \frac{\epsilon(k)\epsilon(-k)}{Q(k, \omega)Q(-k, -\omega)} \quad (38)$$

$$\psi_1 = \frac{1}{\beta} \sum_{\omega} \frac{\Delta_s(\omega)\Phi(\omega)}{\omega^2 + \mu^2} \quad (39)$$

$$\psi_2 = \frac{1}{\beta} \sum_{\omega} \frac{\Delta_s(\omega)\Phi(\omega)}{\omega^2 + \alpha^2} \quad (40)$$

The obtained system of equations (36)-(40) is equivalent to the one derived by Bogoliubov and Moskalenko [17].

In the case of the triplet pairing, by setting $\Delta_s(\omega) = 0$, substituting the formulas (14), (15) and (26) into equation (30) and taking into account the oddness of the function $\Delta_{ti}(\omega)$ we have the following equation, determining the critical temperature:

$$q(1-q)U^2\phi(\omega) = (\omega^2 + \mu^2)(\omega^2 + \alpha^2). \quad (41)$$

If a nontrivial solution of $\Delta_s(\omega)(\Delta_{ti}(\omega))$ of the system of equations (36), (37) ((36), (41)) exists then the singlet (triplet) superconducting phase exists for the Hubbard model. The dependence of critical temperature T_c on the doping δ may be obtained by numerically investigating the above systems of equations. It would be done in our subsequent work.

We would like to note that in the static approximation ($\omega = 0$), keeping the leading terms from equations (36), (37) we obtain the well-known result of Baskaran - Zou - Anderson [18]. Indeed, for a square lattice with nearest neighbor coupling t we have:

$$\frac{1}{N} \sum_k \frac{t\hbar\beta E(k)/2}{E(k)} (\epsilon(k) - \mu) = \delta \quad (42)$$

$$\frac{1}{N} \sum_k \frac{t\hbar\beta E(k)/2}{E(k)} \gamma^2(k) = \frac{2}{J} \quad (43)$$

where $E(k) = \sqrt{\frac{(\epsilon(k) - \mu)^2 + \epsilon(k)^2 \mu^2 \Delta^2}{1 + \epsilon(k)^2 \Delta^2}}$; $\gamma(k) = 2(\cos k_x + \cos k_y)$; $J = \frac{4t^2}{U}$.

We conclude by noting that within the framework of the above functional method one may consider the extended two band Hubbard model, which is our future problem.

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