A field-theoretical approach to the extended Hubbard model

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Abstract

We transform the quartic Hubbard terms in the extended Hubbard model to a quadratic form by making the Hubbard-Stratonovich transformation for the electron operators. This transformation allows us to derive exact results for mass operator and charge-charge and spin-spin correlation functions for s-wave superconductivity. We discuss the application of the method to the d-wave superconductivity.

Key words: extended Hubbard model; Dyson equation; Bethe-Salpeter equation; mass operator; correlation functions.

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1 Introduction

The Hubbard model predicts phase instabilities which give rise to a divergence of the charge and spin correlation functions, and therefore, it has been the focus of particular interest as a model for high-temperature superconductivity. The Hamiltonian of the standard Hubbard model contains only two terms representing the hopping of electrons between sites of the lattice and their on-site interaction. If the interaction between electrons on different sites of the lattice is included, the model is referred as the extended Hubbard model. In what follows we study the following Hamiltonian:

\[ H = - \sum_{i,j,\sigma} t_{ij} \psi_{i,\sigma}^\dagger \psi_{j,\sigma} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - V \sum_{<i,j>,\sigma\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}, \]  

(1)
where $\mu$ is the chemical potential. The Fermi operator $\psi_{i,\sigma}^\dagger$ ($\psi_{i,\sigma}$) creates (destroys) a fermion on the lattice site $i$ with spin projection $\sigma = \uparrow, \downarrow$ along a specified direction, and $\hat{n}_{i,\sigma} = \psi_{i,\sigma}^\dagger \psi_{i,\sigma}$ is the density operator on site $i$. The symbol $\Sigma_{<ij>}$ means sum over nearest-neighbor sites. The first term in (1) is the usual kinetic energy term in a tight-binding approximation, where $t_{ij}$ is the single electron hopping integral. Depending on the sign of $U$, the third term describes the on-site repulsive or attractive interaction between electrons with opposite spins. We assume that $V > 0$, so the last term is expected to stabilize the pairing by bringing in a nearest-neighbor attractive interaction. The lattice spacing is assumed to be $a = 1$ and the total number of sites is $N$.

The simplest method to study the possibility for the extended Hubbard model to show a superconducting instability is to apply mean-field analysis of pairing followed by general random phase approximation (GRPA) [12]. Going beyond the GRPA requires reliable approximation schemes to handle self-consistent relations between single- and two-particle quantities: the mass operator $\Sigma$ depends on the two-particle Green function $K$, and the kernel of the Bethe-Salpeter (BS) equation $\delta \Sigma / \delta G$ for the spectrum of the collective excitations itself does depend on the mass operator. A possible approximation to this problem is the so-called two-particle self-consistent (TPSC) approach [3]-[15]. The TPSC approach is a method for closing the set of equations for single-particle mass operator and the two-body density matrix operator. The later can be factorized by introducing the so-called equal-time pair-correlation function $g_{\sigma\sigma'}(i,j)$ [12,13] which itself depends on the density-density correlation function. In other words, the TPSC approach goes beyond the GRPA for single-particle mass operator by establishing a self-consistency relation between single-particle and two-particle quantities. By setting $g_{\sigma\sigma'}(i,j) = 1$ one should recover the GRPA results for the mass operator and charge and spin correlation functions.

In what follows, we first obtain exact formulas for the electron self-energy (electron mass operator), the charge and spin correlation functions. We also briefly discuss how our approach could be generalized in order to include d-wave instabilities of the types examined in Refs. [16]-[20].

### 2 Field-theoretical approach to extended Hubbard model

The interaction part of the Hamiltonian (1) is quartic in the Grassmann fermion fields so the functional integrals cannot be evaluated exactly. However, it is convenient to transform the quartic Hubbard terms in (1) to a quadratic form by making the Hubbard-Stratonovich transformation for the electron operators:
\[ \int \mu[A] \exp \left[ \tilde{\psi}(y) \hat{\Gamma}_\alpha^{(0)}(y; x) \psi(x) A_\alpha(z) \right] = \exp \left\{ -\frac{1}{2} \tilde{\psi}(y) \hat{\Gamma}_\alpha^{(0)}(y; x) \psi(x) \right\}. \]

The symbol ‘hat’ over any quantity \( O \) means that this quantity is a matrix. The functional measure \( D\mu[A] \) is chosen to be:

\[ \mu[A] = DA e^{\frac{1}{2} A_\alpha(z) D_{\alpha,\beta}(z, z') A_\beta(z')} \int \mu[A] = 1. \]

The Hubbard-Stratonovich transformation converts the quartic problem of interacting electrons to the more tractable quadratic problem of noninteracting Nambu fermion fields

\[ \tilde{\psi}(y) = \left( \psi^\dagger(y) \psi_\uparrow(y) \right), \quad \hat{\psi}(x) = \begin{pmatrix} \psi^\dagger(x) \\ \psi_\uparrow(x) \end{pmatrix} \]

coupled to a Bose field \( A_\alpha(z) \) where \( \alpha = \uparrow, \downarrow \) is the spin degree of freedom which reflects the spin-dependent nature of the Hubbard interaction. The bare boson propagator in (2) provides an instantaneous spin-dependent interaction, and in accordance with the Hamiltonian (1), it should have the following form:

\[ D^{(0)}_{\alpha,\beta}(z, z') = D^{(0)}_{\alpha,\beta}(j, j'; v - v') = \delta(v - v') \left[ U \delta_{jj'} \delta_{\alpha,\beta} - 2V_{<jj'>} (\delta_{\bar{\alpha},\beta} + \delta_{\alpha,\beta}) \right] \]

\[ = \frac{1}{N} \sum_k \sum_{\omega_p} e^{i \left[ k \cdot (r_j - r_{j'}) - \omega_p (v - v') \right]} \left\{ 1 \right\} D^{(0)}_{\alpha,\beta}(k; \omega_p), \]

\[ D^{(0)}_{\alpha,\beta}(k; \omega_p) = U \delta_{\bar{\alpha},\beta} - V(k) \left( \delta_{\bar{\alpha},\beta} + \delta_{\alpha,\beta} \right). \]

Here \( \bar{\alpha} \) is complimentary of \( \alpha \), and \( V(k) = 4V (\cos k_x + \cos k_y) \) is the nearest-neighbor interaction in momentum space. The symbol \( V_{<jj'>} \) is equal to \( V \) if \( j \) and \( j' \) sites are nearest neighbors, and zero otherwise. We have used composite variables \( y = \{ r_i, u \} = \{ i, u \}, x = \{ r_\uparrow, u \} = \{ i', u' \}, z = \{ r_j, v \} = \{ j, v \} \) and \( z' = \{ r_{j'}, v' \} = \{ j', v' \} \), where \( r_i, r_\uparrow, r_j \) and \( r_{j'} \) are the lattice site vectors. The symbol \( \sum_{\omega_p} \) is used to denote \( \beta^{-1} \sum_p \). For boson fields we have \( \omega_p = (2\pi/\beta)p; p = 0, \pm 1, \pm 2, \ldots \).

After performing the Hubbard-Stratonovich transformation, the action of the system becomes

\[ S = S^{(e)}_0 + S^{(A)}_0 + S^{(e-A)}, \]

where:

\[ S^{(e)}_0 = \tilde{\psi}(y) \hat{G}^{(0)-1}(y; x) \psi(x), \]

\[ (5) \]
\[ S_0^{(A)} = \frac{1}{2} A_\alpha(z) D^{(0)-1}_{\alpha\beta}(z, z') A_\beta(z'), \quad (6) \]

\[ S^{(e-A)} = \overline{\psi(y)} \hat{G}^{(0)}(y, x \mid z) \hat{\psi}(x) A_\alpha(z). \quad (7) \]

The inverse Green function of free electrons \( \hat{G}^{(0)-1}(y; x) \) is diagonal with respect to the spin indices and has its usual form:

\[
\hat{G}^{(0)-1}(y; x) = \begin{pmatrix}
G^{(0)-1}(\uparrow, \uparrow; x) & 0 \\
0 & -G^{(0)-1}(\downarrow, \downarrow; x)
\end{pmatrix} \\
= \frac{1}{N} \sum_k \sum_{\omega_m} \exp\{i \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_\nu) - \omega_m (u - u')\} \times
\begin{pmatrix}
G^{(0)-1}(\mathbf{k}, \omega_m) & 0 \\
0 & -G^{(0)-1}(\mathbf{k}, \omega_m)
\end{pmatrix},
\quad (8)
\]

where \( G^{(0)-1}(\mathbf{k}, \omega_m) = [\omega_m - (\epsilon(\mathbf{k}) - \mu)]^{-1} \), and \( G^{(0)-1}(\mathbf{k}, \omega_m) = [\omega_m + (\epsilon(\mathbf{k}) - \mu)]^{-1} \).

Here \( \epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \) is the non-interacting dispersion on a square lattice, \( \mu \) is the electron chemical potential, and the symbol \( \sum_{\omega_m} \) is used to denote \( \beta^{-1} \sum_m \). For fermion fields we have \( \omega_m = (2\pi/\beta)(m + 1/2); m = 0, 1, 2, \ldots \).

The bare vertex \( \hat{\Gamma}^{(0)}_\alpha(y; x \mid z) \) is a \( 2 \times 2 \) matrix defined as follows:

\[
\hat{\Gamma}^{(0)}_\alpha(y; x \mid z) = \begin{pmatrix}
\Gamma^{(0)}_\alpha(\uparrow, \uparrow; x \mid z) & 0 \\
0 & -\Gamma^{(0)}_\alpha(\downarrow, \downarrow; x \mid z)
\end{pmatrix},
\quad \Gamma^{(0)}_\alpha(\sigma, y; \sigma, x \mid z) = \Gamma^{(0)}_\alpha(\sigma, i, u; \sigma, i', u' \mid i'', v)
\]

\[
= \delta(u - v)\delta(u - u')\delta_{\sigma,\sigma'}\delta_{i,i'}\delta_{i,i''}.
\quad (9)
\]

Since the electrons polarize the boson field, and the boson field acts onto the electrons, our approach describes the correlated motion of the electrons and the surrounding polarization field.

In field theory the expectation value of a general operator \( \hat{O}(u) \) is expressed as a functional integral over the boson field \( A \) and the Grassmann fermion fields \( \hat{\psi} \) and \( \hat{\psi} \)

\[
< \hat{T}_u(\hat{O}(u)) >= \frac{1}{Z[J, M]} \int D\mu(\hat{\psi}, \hat{\psi}, A) \hat{O}(u) \times
\exp \left[ J_\alpha(z) A_\alpha(z) - \hat{\psi}(y) \hat{M}(y; x) \hat{\psi}(x) \right] |_{J = M = 0},
\quad (10)
\]
where the symbol $< ... >$ means that the thermodynamic average is made, and $\hat{T}_u$ is an $u$—ordering operator. $J, M$ are the sources of the boson and fermion fields, respectively. The functional $Z[J, M]$ is defined by

$$Z[J, M] = \int D\mu[\hat{\psi}, \hat{\psi}, A] e^{[J_\alpha(z)A_\alpha(z)-\hat{\psi}(y)\hat{\psi}(y)]},$$

(11)

where the functional measure $D\mu[\hat{\psi}, \hat{\psi}, A] = DAD\hat{\psi}D\hat{\psi}\exp (S)$ satisfies the condition $\int D\mu[\hat{\psi}, \hat{\psi}, A] = 1$.

It is convenient to introduce complex indices $1 = \{\sigma_1, x_1\}$, $2 = \{\sigma_2, y_2\}$, ...,

where, $\sigma_1, \sigma_2 = \{\uparrow, \downarrow\}$ and $x_1 = \{r_i, u_1\}$, and $y_2 = \{r_i, u_2\}$. We define a functional derivative $\delta / \delta M(1; 2)$, and depending on the spin degrees of freedom $\sigma_1$ and $\sigma_2$, there are four possible derivatives:

$$\frac{\delta}{\delta M(\uparrow, y_2; \uparrow, x_1)}; \frac{\delta}{\delta M(\uparrow, y_2; \downarrow, x_1)}; \frac{\delta}{\delta M(\downarrow, y_2; \uparrow, x_1)}; \frac{\delta}{\delta M(\downarrow, y_2; \downarrow, x_1)}.$$

The reason to write the expectation value (10) as a functional integral is that all Green functions related to system under consideration can be expressed in terms of the functional derivatives of the generating functional of the connected Green functions $W[J, M] = \ln Z[J, M]$. By means of the functional $W[J, M]$, we define the following Green and vertex functions of the extended Hubbard model:

Boson Green function:

$$D_{\alpha\beta}(z, z') = -\frac{\delta^2 W}{\delta J_\alpha(z)\delta J_\beta(z')};$$

(12)

The single-electron Green function $G(1; 2) = -\delta W/\delta M(2; 1)$ in the Hubbard model assumes the form:

$$\hat{G}(1; 2) = -\begin{pmatrix}
< \hat{T}_u \left( \psi_\uparrow(x_1)\psi_\uparrow^\dagger(y_2) \right) > & < \hat{T}_u \left( \psi_\uparrow(x_1)\psi_\downarrow(y_2) \right) > \\
< \hat{T}_u \left( \psi_\downarrow(x_1)\psi_\uparrow^\dagger(y_2) \right) > & < \hat{T}_u \left( \psi_\downarrow(x_1)\psi_\downarrow(y_2) \right) > 
\end{pmatrix}. $$

(13)

Depending on the two spin degrees of freedom $\sigma_1$ and $\sigma_2$, there exist two ”normal” Green functions

$$G(\uparrow, x_1; \uparrow, y_2) = G_{\uparrow,\uparrow}(x_1, y_2) = -< \hat{T}_u \left( \psi_\uparrow(x_1)\psi_\uparrow^\dagger(y_2) \right) > = -\frac{\delta W}{\delta M(\uparrow, y_2; \uparrow, x_1)},$$

$$G(\downarrow, x_1; \downarrow, y_2) = G_{\downarrow,\downarrow}(x_1, y_2) = -< \hat{T}_u \left( \psi_\downarrow(x_1)\psi_\downarrow^\dagger(y_2) \right) > = -\frac{\delta W}{\delta M(\downarrow, y_2; \downarrow, x_1)},$$

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and two "anomalous" Green functions

\[ G(\downarrow, x_1; \uparrow, y_2) = G_{\downarrow, \uparrow}(x_1, y_2) = \left< \hat{T}_u \left( \hat{\psi}_{\uparrow}^\dagger(x_1) \hat{\psi}_{\uparrow}(y_2) \right) \right> \equiv \frac{\delta W}{\delta M(\uparrow, y_2; \downarrow, x_1)}, \]

\[ G(\uparrow, x_1; \downarrow, y_2) = G_{\uparrow, \downarrow}(x_1, y_2) = \left< \hat{T}_u \left( \hat{\psi}_{\uparrow}(x_1) \hat{\psi}_{\downarrow}(y_2) \right) \right> \equiv \frac{\delta W}{\delta M(\downarrow, y_2; \uparrow, x_1)}. \]

We introduce Fourier transforms of the "normal" \( G_{\uparrow, \uparrow}(k, u - u') = \left< \hat{T}_u \left( \hat{\psi}_{\uparrow,k}^\dagger(u') \hat{\psi}_{\uparrow,k}(u) \right) \right> \) and "anomalous" \( G_{\downarrow, \uparrow}(k, u - u') = \left< \hat{T}_u \left( \hat{\psi}_{\downarrow,k}^\dagger(u') \hat{\psi}_{\uparrow,k}(u) \right) \right> \) one-particle Green functions. Here \( \hat{\psi}_{\uparrow,k}^\dagger(u), \hat{\psi}_{\uparrow,k}(u) \) and \( \hat{\psi}_{\downarrow,k}^\dagger(u), \hat{\psi}_{\downarrow,k}(u) \) are the creation-annihilation Heisenberg operators. The final form of single-particle Green function is given by

\[
\hat{G}(1; 2) = \frac{1}{N} \sum_k \sum_{\omega_m} \exp\{i \mathbf{k} \cdot (\mathbf{r}_{x_1} - \mathbf{r}_{x_2}) - \omega_m (u_1 - u_2)\} \left( \begin{array}{ccc} G_{\uparrow, \uparrow}(k, \omega_m) & G_{\uparrow, \downarrow}(k, \omega_m) \\ G_{\downarrow, \uparrow}(k, \omega_m) & G_{\downarrow, \downarrow}(k, \omega_m) \end{array} \right). \tag{14}
\]

The two-particle Green function is defined by:

\[
K \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = \frac{\delta^2 W}{\delta M(2; 1) \delta M(3; 4)} = -\frac{\delta G(1; 2)}{\delta M(3; 4)}. \tag{15}
\]

Depending on the four spin degrees of freedom \( \sigma_1, \sigma_2, \sigma_3 \) and \( \sigma_4 \), there are sixteen different components of the two-particle Green function.

The vertex function \( \Gamma_{\sigma\alpha}(2; 1 \mid z) \) is given by:

\[
\Gamma_{\sigma\alpha}(2; 1 \mid z) = -\frac{\delta G^{-1}(2; 1)}{\delta J_{\beta}(z')} D_{\beta\alpha}^{-1}(z', z) = G^{-1}(2; 3) \frac{\delta^2 G(3; 4)}{\delta J_{\beta}(z')} G^{-1}(4; 1) D_{\beta\alpha}^{-1}(z', z). \tag{16}
\]

If the spin variable \( \alpha \) is fixed, then depending on the spin degrees of freedom \( \sigma_1 \) and \( \sigma_2 \), there are four different vertex functions.

The action \( H \) as well as all of the above definitions allow us to map the extended Hubbard model onto the polariton model that describes the light propagation in semiconductors \[21\]. This mapping allows us to apply directly to the Hubbard model all exact equations and relationships derived for the case of light propagation in crystals. For example, we can write the mass
operator $\Sigma(1; 2) = \Sigma_H(1; 2) + \Sigma_F(1; 2)$ as a sum of Hartree and Fock parts [21]. The Hartree contribution to the mass operator is diagonal with respect to the spin indices:

$$\Sigma_H(1; 2) = \Sigma_H(\sigma_1, i_1, u_1; \sigma_2, i_2, u_2) = \Gamma^{(0)}_\alpha(1; 2 | z)G(4; 3)\Gamma^{(0)}_\beta(3; 4 | z')D^{(0)}_{\alpha\beta}(z, z') = \delta(1 - 2) \times$$

$$\{-UG_{\sigma_1, \sigma_1}(i_1, u_1; i_1, u_1) - 2V\sum_a[G_{\sigma_1, \sigma_1}(i_1, u_1; i_1 + a, u_1) - G_{\sigma_1, \sigma_1}(i_1, u_1; i_1 + a, u_1)]\}, \quad (17)$$

where the summation on $a$ runs over the nearest-neighbor sites of site $i_1$.

The Fock part depends on the boson Green function $D$, or equivalently, depends on the two-particle Green function $K$:

$$\Sigma_F(1; 2) = \Sigma_F(\sigma_1, i_1, u_1; \sigma_2, i_2, u_2) = -\Gamma^{(0)}_\alpha(1; 3 | z)G(3; 4)\Gamma^{(0)}_\beta(4; 2 | z')D^{(0)}_{\alpha\beta}(z, z'),$$

$$= -\Gamma^{(0)}_\alpha(1; 6 | z)D^{(0)}_{\alpha\beta}(z, z')\Gamma^{(0)}_\beta(4; 5 | z')K \begin{pmatrix} 5 & 3 \\ 4 & 6 \end{pmatrix} G^{-1}(3; 2)$$

$$= \{UK \begin{pmatrix} \sigma_1, i_1, u_1 & \sigma_3, i_3, u_3 \\ \sigma_1, i_1, u_1 & \sigma_1, i_1, u_1 \end{pmatrix} + 2V\sum_a[K \begin{pmatrix} \sigma_1, i_1 + a, u_1 & \sigma_3, i_3, u_3 \\ \sigma_1, i_1 + a, u_1 & \sigma_1, i_1, u_1 \end{pmatrix}$$

$$-K \begin{pmatrix} \sigma_1, i_1 + a, u_1 & \sigma_1, i_1 + a, u_1 \end{pmatrix} \}]G^{-1}(3; 2) \begin{pmatrix} 5 & 3 \\ 4 & 6 \end{pmatrix} G^{-1}(3; 2),$$

$$\{ -UG_{\sigma_1, \sigma_1}(i_1, u_1; i_1, u_1) - 2V\sum_a[G_{\sigma_1, \sigma_1}(i_1, u_1; i_1 + a, u_1) - G_{\sigma_1, \sigma_1}(i_1, u_1; i_1 + a, u_1)]\}, \quad (18)$$

The $V$-terms in (18) differ from the corresponding result in [12,13].

3 Spectrum of the collective modes

Spectrum of the two-particle excitations (or collective modes) $\omega(Q)$ can be obtained by locating the positions of the common poles of the Fourier transform of the two-particle fermion Green function (15) and the Fourier transform of the boson Green function (12). In other words, collective modes are defined by the solutions of the BS equation for the function $K$ or the Dyson equation for the boson function $D$.

The BS equation is $K^{-1} \Psi = [K^{(0)-1} - I] \Psi = 0$, where $I$ is the kernel, and

$$K^{(0)-1} \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} = G^{-1}(1; 3)G^{-1}(4; 2)$$
is the two-particle free propagator constructed from a pair of fully dressed single-particle Green functions. The kernel $I = \frac{\delta \Sigma_F}{\delta G} + \frac{\delta \Sigma_F}{\delta G^*}$ depends on the functional derivative of the Fock contribution to the mass operator. Since the Fock term itself depends on the two-particle Green function $K$ (see Eq. [18]), we have to solve self-consistently a set of two equations, namely the BS equation and the Dyson equation $G^{-1} = G^{(0)^{-1}} - \Sigma$ for the single-particle Green function.

Similar obstruction arises if we start from the Dyson equation for boson Green function:

$$D^{-1}_{\alpha\beta}(z, z') = D^{(0)^{-1}}_{\alpha\beta}(z, z') - \Pi_{\alpha\beta}(z, z'),$$

(19)

where $\Pi_{\alpha\beta}(z, z')$ is the proper self-energy of the boson field. The obstruction now is that the proper self-energy depends on the vertex function $\Gamma$, or on the two-particle Green function $\tilde{K}$:

$$\Pi_{\alpha\beta}(z, z') = \Gamma^{(0)}_{\alpha}(1; 2 | z) \tilde{K} \left( \begin{array}{c} 2 \\ 3 \\ 1 \\ 4 \end{array} \right)^{(0)} \Gamma^{(0)}_{\beta}(3; 4 | z').$$

(20)

The Green function $\tilde{K}$, which we shall call the Green function of electronic excitations, satisfies the following BS equation:

$$\tilde{K}^{-1} \left( \begin{array}{c} 1 \\ 3 \\ 2 \\ 4 \end{array} \right) = K^{(0)^{-1}} \left( \begin{array}{c} 1 \\ 3 \\ 2 \\ 4 \end{array} \right) - \frac{\delta \Sigma_F(1; 2)}{\delta G(3; 4)}.$$  

(21)

Let us introduce the so-called general response function $\Pi_{\alpha\beta}$:

$$\Pi_{\alpha\beta}(z; z') = \Gamma^{(0)}_{\alpha}(1; 2 | z) \tilde{K} \left( \begin{array}{c} 2 \\ 3 \\ 1 \\ 4 \end{array} \right)^{(0)} \Gamma^{(0)}_{\beta}(3; 4 | z').$$

(22)

By means of (22), we can rewrite the BS and Dyson equations as follows: $K = K^{(0)} + K^{(0)} \Gamma^{(0)}_{\alpha} \Pi_{\alpha\beta} \Gamma^{(0)}_{\beta} K^{(0)}$, $D = D^{(0)} + D^{(0)} \Pi D^{(0)}$. The Fourier transforms of the general response function $\Pi_{\alpha\beta}(Q; \omega)$ and the proper self-energy $\tilde{\Pi}_{\alpha\beta}(Q; \omega)$ are connected by the following equation:

$$\Pi_{\alpha\beta}(Q; \omega) = \tilde{\Pi}_{\alpha\beta}(Q; \omega) + \tilde{\Pi}_{\alpha\gamma}(Q; \omega) (-U + V(Q)) \Pi_{\gamma\beta}(Q; \omega)$$

$$+ \Pi_{\alpha\gamma}(Q; \omega) V(Q) \tilde{\Pi}_{\gamma\beta}(Q; \omega),$$

(23)
According to Eq. (20), the proper self-energy $\Pi$, the Green function $\tilde{K}$ and the vertex function $\Gamma$ must have common poles. Let $E_l(Q)$ and $Q$ denote the energy and momentum of these common poles. Close to $E_l(Q)$ one can write:

$$
\tilde{K} = \begin{pmatrix} 1 & 3 \\
2 & 4 \end{pmatrix} = \begin{pmatrix} \sigma_1, i_1, u_1 & \sigma_3, i_3, u_3 \\
\sigma_2, i_2, u_2 & \sigma_4, i_4, u_4 \end{pmatrix}
$$

$$
\approx \sum_{\omega_p} e^{-\omega_p (u_1-u_3)} \Phi^{l \sigma_1, \sigma_2}_{\alpha} (r_{i_2}, r_{i_1}; u_2 - u_1) \Phi^{l \sigma_3, \sigma_4}_{\alpha} (r_{i_4}, r_{i_3}; u_4 - u_3),
$$

where $\Phi^{l \sigma_1, \sigma_2}_{\alpha} (r_{i_2}, r_{i_1}; u_2 - u_1)$ are the BS amplitudes:

$$
\phi^{l \sigma_1, \sigma_2}_{\alpha} (r_{i_2} - r_{i_1}; u_1 - u_2) = \frac{1}{N} \sum_k \exp \{ i k \cdot (r_{i_1} - r_{i_2}) \} \phi^{l \sigma_1, \sigma_2}_{\alpha} (k, Q),
$$

Due to the form of the bare vertex $\tilde{\Gamma}^{(0)}$, we have to take into account only the equal "time" $u_1 = u_2$ amplitudes:

$$
\phi^{l \sigma_1, \sigma_2}_{\alpha} (r_{i_2} - r_{i_1}; u_1 - u_2) = \frac{1}{N} \sum_k \exp \{ i k \cdot (r_{i_1} - r_{i_2}) \} \phi^{l \sigma_1, \sigma_2}_{\alpha} (k, Q),
$$

where $\phi^{l \alpha \beta}_{\uparrow \uparrow} (k, Q), \phi^{l \alpha \beta}_{\uparrow \downarrow} (k, Q), \phi^{l \alpha \beta}_{\downarrow \uparrow} (k, Q)$ and $\phi^{l \alpha \beta}_{\downarrow \downarrow} (k, Q)$ are the equal "time" two-particle wave functions in $k$-representation. By means of (24) and (20) we obtain:

$$
\Pi^{l \alpha \beta}_{\alpha \beta} (Q, \omega) = \sum_l \left[ \frac{\phi^{l \alpha, \alpha}_{\uparrow \downarrow} (0; 0) \phi^{l \alpha, \beta}_{\uparrow \downarrow} (0; 0)}{\omega - \omega_{lQ} + i0^+} - \frac{\phi^{l \alpha, \alpha}_{\uparrow \downarrow} (0; 0) \phi^{l \alpha, \beta}_{\uparrow \downarrow} (0; 0)}{\omega + \omega_{lQ} + i0^+} \right],
$$

where $\omega_{lQ} = E_l(Q) - \mu$. If the proper self-energy is known, the spectrum of the collective excitations $\omega(Q)$ could be obtained assuming the vanishing of the following 2 × 2 determinant:

$$
\text{det} \| \delta_{\alpha, \beta} - (-U + V(Q)) \Pi^{l \alpha \beta}_{\alpha \beta} (Q, \omega) + V(Q) \Pi^{l \alpha \beta}_{\alpha \beta} (Q, \omega) \| = 0.
$$

By solving Eq. (20) (with the help of $\Pi^{l \alpha \beta}_{\alpha \beta} = \Pi^{l \beta \alpha}_{\beta \alpha}$) we find two different types of collective modes. The first one is governed by $U$ interaction:

$$
0 = 1 - U \left[ \Pi^{l \uparrow \uparrow}_{\uparrow \uparrow} (Q, \omega) - \Pi^{l \uparrow \downarrow}_{\uparrow \downarrow} (Q, \omega) \right].
$$

Strictly speaking the $V$ interaction is included indirectly in Eq. (27) through BS amplitudes and poles of the function $\tilde{K}$. This collective mode manifests itself as a pole of the spin response function $\chi_{ss}(Q; \omega) = 2 [\Pi^{l \uparrow \uparrow}_{\uparrow \uparrow} (Q; \omega) - \Pi^{l \uparrow \downarrow}_{\uparrow \downarrow} (Q; \omega)]$, 

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and therefore, gives rise to the spin instabilities. The spin correlation function is defined by

$$\chi_{ss}(Q; \omega) = \frac{\bar{\chi}_{ss}(Q; \omega)}{1 - \bar{\chi}_{ss}(Q; \omega)U/2}, \quad (28)$$

where $\bar{\chi}_{ss}(Q; \omega) = 2 \left[ \bar{\Pi}^{++}(Q; \omega) - \bar{\Pi}^{++}(Q; \omega) \right]$. The second type of collective modes satisfies the following equation:

$$0 = 1 + [U - 2V(Q)] \left[ \bar{\Pi}^{++}(Q, \omega) + \bar{\Pi}^{++}(Q, \omega) \right]. \quad (29)$$

The second collective mode manifests itself as a pole of the charge response function $\chi_{cc}(Q; \omega) = 2 \left[ \Pi^{++}(Q; \omega) + \Pi^{++}(Q; \omega) \right]$ which is determined by the following equations:

$$\chi_{cc}(Q; \omega) = \frac{\bar{\chi}_{cc}(Q; \omega)}{1 + \bar{\chi}_{cc}(Q; \omega) \left[ U/2 - V(Q) \right]}, \quad (30)$$

where $\bar{\chi}_{cc}(Q; \omega) = 2 \left[ \bar{\Pi}^{++}(Q; \omega) + \bar{\Pi}^{++}(Q; \omega) \right]$.

Within the GRPA, one should replace $\bar{K}$ in (20) by $K^{(0)}$, thus obtaining the free response functions $\chi^{(0)}$ instead of the exact $\bar{\chi}$ expressions. In other words, the exact relations (28) and (30) in the GRPA are given by

$$\chi_{ss}(Q; \omega) = \frac{\chi_{ss}^{(0)}(Q; \omega)}{1 - \chi_{ss}^{(0)}(Q; \omega)U/2}, \quad (31)$$

$$\chi_{cc}(Q; \omega) = \frac{\chi_{cc}^{(0)}(Q; \omega)}{1 + \chi_{cc}^{(0)}(Q; \omega) \left[ U/2 - V(Q) \right]}.$$  

4 Discussion

We have established exact results for mass operator and spin and charge correlation functions in the case of s-wave superconductivity described by the extended Hubbard Hamiltonian. The Hamiltonian depends on an on-site repulsive interactions $U$, which drives antiferromagnetism, and a near-neighbor attractive interactions $V$, which drives d-wave superconductivity. Let us discuss consider the extended Hubbard model with a nearest-neighbor repulsion $V$. In this case the near-neighbor repulsive interaction $V$ drives instabilities related to the change in Fermi surface topology (Pomeranchuk instability) [18][19]. The Fermi surface is related to the diagonal elements of matrix (18).
In the RPA we replace \( K \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} \) by \( G(1;3)G(4;2) \), and therefore, the \( U \) term in [18] does not create any changes in the non-interacting Fermi surface \( \mu = \epsilon(k) \). In RPA only the near-neighbor repulsive interaction \( (V \rightarrow -V) \) changes the Fermi surface topology through the diagonal elements of the mass operator [18]:

\[
(\Sigma_F(k))_{\sigma\sigma} = -4V \sum_q \{ \cos(k_x - q_x) + \cos(k_y - q_y) \} n_\sigma(q),
\]

(33)

where \( n_\sigma(k) = \sum_{\omega_m} G_{\sigma\sigma}(k, \omega_m) \) is the occupation of the site \( k \) in momentum space. Note that the \( V \)-terms of \( \Sigma_F(1,2) \) in Refs. [12,13] are proportional to the delta function \( \delta(1 - 2) \), and therefore, \( \Sigma_F(k) \) does not depend on \( k \).

It is found [18] that the near-neighbor repulsive interaction \( V \) enhance small anisotropies producing deformations of the Fermi surface that break the point group symmetry of the square lattice at the Van Hove filling. Since the antiferromagnetic order is favored by \( U \) but suppressed by \( V \), one has to expect that the Pomeranchuk instability competes with magnetic instabilities and will be suppressed at some critical value \( V \).

The analog of the BCS reduced Hamiltonian for singlet density-wave order is the so-called f-Hamiltonian [17,19,20]:

\[
H = \sum_{k,\sigma}(\epsilon(k) - \mu)n_{k,\sigma} + \frac{1}{2V} \sum_{k,p,q} S(q)d_kd_p n_{k}(q)n_{p}(-q),
\]

(34)

where \( d_k = \cos(k_x) - \cos(k_y) \) and the operator \( n_{k}(q) \) is \( n_{k}(q) = \sum_{\sigma} \psi^\dagger_{\sigma}(k + \frac{1}{2}q)\psi_{\sigma}(k - \frac{1}{2}q) \). In momentum space the corresponding order parameter can be defined through the following operator (for more general definition of \( O(q) \), see Ref. [20])

\[
O(q) = \sum_k d_k \tilde{\psi}(k + \frac{1}{2}q)\tilde{\sigma}_z \tilde{\psi}(k - \frac{1}{2}q),
\]

(35)

where \( \tilde{\psi}(k) \) and \( \tilde{\psi}(k) \) are the Fourier transforms of the Nambu fermion fields, and \( \tilde{\sigma}_z \) is the Pauli matrix. The interaction term in the above Hamiltonian in coordinate space is \( \frac{1}{2} \sum_{i,j} S(r_i - r_j)O(r_i)O(r_j) \), where the Fourier transform of \( S(r_i) \) is \( S(k) \). Now, we introduce a boson field \( B(z) = B(r_j;v) \) with a free propagator \( S^{(0)}(z,z') = \delta(v - v')S^{(0)}(r_j - r_{j'}) \) and a bare vertex function \( \Gamma^{(0)}(y, x|z) = \Gamma^{(0)}(r_i, u; r_{j'}, u'|r_{j}, v) = \delta(u - u')\delta(u - v)\delta(r_i - r_{j'})\delta(r_i - r_{j}) \). Now, we can perform exactly the same steps as in the case of s-wave superconductivity. As a result, one can obtain the following equation for d-wave response.
function $\Pi(Q, \omega)$:

$$\Pi(Q, \omega) = \tilde{\Pi}(Q, \omega) + \tilde{\Pi}(Q, \omega)S^{(0)}(Q)\Pi(Q, \omega),$$

(36)

where the proper self-energy is defined as

$$\tilde{\Pi}(z, z') = \Gamma^{(0)}(1; 2|z)G(2; 3)G(3; 4)\Gamma(3; 4|z).$$

Solving (36) we obtain the GRPA result for the d-wave response function:

$$\chi(Q, \omega) = \frac{\chi^{(0)}(Q, \omega)}{1 - S^{(0)}(Q)\chi^{(0)}(Q, \omega)},$$

where $\chi^{(0)}$ is the d-wave proper self-energy in RPA (see eq. (7) in Ref. [19]).

In summary, we have used the Hubbard-Stratonovich transformation to convert the quartic Hubbard problem of interacting electrons into more tractable quadratic problem of noninteracting electrons coupled to a Bose field. This field-theoretical approach allows us to express all quantities of interest in terms of the corresponding Green functions and obtain exact relations between single- and two-particle quantities.

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