Rigorous derivation of the mean-field Green functions of the two-band Hubbard model of superconductivity

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Abstract

The Green function (GF) equation of motion technique for solving the effective two-band Hubbard model of high-$T_c$ superconductivity in cuprates (Plakida et al 1995 Phys. Rev. B \textbf{51} 16599, Plakida et al 2003 JETP \textbf{97} 331) rests on the Hubbard operator (HO) algebra. We show that, if we take into account the invariance to translations and spin reversal, the HO algebra results in invariance properties of several specific correlation functions. The use of these properties allows rigorous derivation and simplification of the expressions of the frequency matrix (FM) and of the generalized mean-field approximation (GMFA) Green functions (GFs) of the model. For the normal singlet-hopping and anomalous exchange pairing correlation functions which enter the FM and GMFA-GFs, an approximation procedure based on the identification and elimination of exponentially small quantities is described. It secures the reduction of the correlation order to GMFA-GF expressions.

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1. Introduction

A consistent theoretical model of the high critical temperature superconductivity in cuprates is to be able to accommodate both the normal and superconducting states under incorporation of the essential features of these systems (see, e.g., [1] for a review): strong antiferromagnetic (AFM) superexchange interaction inside the CuO$_2$ planes, occurrence of two relatively isolated energy bands around the Fermi level, able to develop $d_{x^2−y^2}$ pairing: one stemming from single-particle copper $d_{x^2−y^2}$ states and the second one from singlet doubly occupied states generated [2] by crystal field interaction; hopping conduction for an extremely low density of the free charge carriers.
The p–d model [3], while incorporating all these features, is too cumbersome and the
cell-cluster perturbation theory [4, 5] providing a hierarchy of the various interaction terms
was used to derive simpler models from it. Extreme limit cases of this reduction procedure are
various effective one-band t–J models (see, e.g., [6, 7] and references therein) which, while
unveiling the role played by the AFM exchange interaction in the occurrence of the d-wave
pairing, address exclusively the superconducting state.

The reduction of the p–d model to an effective two-band Hubbard model considered
by Plakida et al [8], corroborated with the use of the equation of motion technique for
thermodynamic Green functions (GF) [9], provided the simplest approach to the description
of both the normal [8, 10] and the superconducting states [11–13] within a frame securing
rigorous fulfillment of the Pauli exclusion principle for fermionic states.

The Green function technique rests on the Hubbard operator algebra. Its rigorous
implementation onto a system characterized by specific symmetry properties (translation-
invariant two-dimensional spin lattice, spin-reversal invariance of the observables) results
either in characteristic invariance properties of several correlation functions, or in the
occurrence of some exactly vanishing correlation functions. The use of these results allows
rigorous derivation and simplification of the expressions of the frequency matrix and of the
generalized mean-field approximation (GMFA) Green functions of the model.

The obtained expressions contain higher order boson–boson correlation functions (CFs).
For the CFs involving singlets (normal singlet-hopping CFs and anomalous exchange pairing
CFs), an approximation procedure which avoids the usual decoupling schemes and, yet,
secures the correlation order reduction to GMFA-GF expressions, under the identification and
elimination of exponentially small quantities, is described.

The organization of the paper is as follows. Section 2 summarizes essentials of the
two-band Hubbard model and GMFA-GF equations. Section 3 describes the invariance
properties following from the translation invariance of the underlying spin lattice. Section 4
derives invariance properties and constraints following from the invariance of the macroscopic
properties of the system under spin reversal. On the basis of the results of sections 3 and 4,
rigorous derivation of the frequency matrix in the \((r, \omega)\)-representation is done in section 5.
The derivation of GMFA-GF expressions for the boson–boson correlation functions involving
singlets is discussed in section 6.

Collecting together the results of sections 5 and 6, expressions of the frequency matrix
and of the GMFA Green function matrix are derived in the \((q, \omega)\)-representation in sections 7
and 8, respectively. These results explicitly incorporate both hole-doping and electron-doping
features of the cuprate systems through the singlet-hopping and superconducting pairing terms.

The paper ends with conclusions in section 9.

2. Mean-field approximation

The Hamiltonian of the effective two-band singlet-hole Hubbard model [8] is written in the form
\[
H = E_1 \sum_{i,\sigma} X_1^{\sigma} + E_2 \sum_{i} X_2^{\sigma} + K_{11} \sum_{i,\sigma} \tau_{1,i}^{\sigma,0,\bar{\sigma}} + K_{22} \sum_{i,\sigma} \tau_{1,i}^{2\sigma,2\sigma} \\
+ K_{21} \sum_{i,\sigma} 2\sigma \left( \tau_{1,i}^{2\sigma,0,\bar{\sigma}} + \tau_{1,i}^{0,\sigma,2\sigma} \right). \tag{1}
\]

The summation label \(i\) runs over the sites of an infinite two-dimensional (2D) square array the
lattice constants of which, \(a_x = a_y\), are defined by the underlying single crystal structure.
The spin projection values in the sums over \(\sigma\) are \(\sigma = \pm 1/2\), \(\bar{\sigma} = -\sigma\).
The Hubbard operators (HOs) $X_i^{αβ} = |iα⟩⟨β|$ are defined for the four states of the model at each lattice site $i$: $|0⟩$ (vacuum), $|σ⟩ = |↑⟩$ and $|σ⟩ = |↓⟩$ (single-particle spin states inside the hole subband) and $|2⟩ = |↑↓⟩$ (singlet state in the singlet subband).

The multiplication rule holds $X_i^{αβ} X_j^{γη} = δ_{βγ} X_j^{αη}$. The HOs may be fermionic (single-spin-state creation/annihilation in a subband) or bosonic (singlet creation/annihilation, spin or charge densities, particle numbers). For a pair of fermionic HOs, the anticommutator rule holds $\{X_i^{αβ}, X_j^{γη}\} = δ_{ij} (δ_{βγ} X_j^{αη} + δ_{ηα} X_i^{βγ})$ whereas, if one or both HOs are bosonic, the commutation rule holds $[X_i^{αβ}, X_j^{γη}] = δ_{ij} (δ_{βγ} X_j^{αη} - δ_{ηα} X_i^{βγ})$. At each lattice site $i$, the constraint of no double occupancy of any quantum state $|iα⟩$ is rigorously fulfilled due to the completeness relation $X_i^{αα} + X_i^{σσ} + X_i^{ασ} + X_i^{σα} = 1$.

In (1), $E_i = \tilde{ε}_d - \mu$ denotes the hole subband energy for the renormalized energy $\tilde{ε}_d$ of a $d$-hole and the chemical potential $\mu$. The energy parameter of the singlet subband is $E_2 = 2E_1 + Δ$, where $Δ ≈ Δ_{pd} = ε_p - ε_d$ is an effective Coulomb energy $U_{\text{eff}}$ corresponding to the difference between the two energy levels of the model.

In the description of the hopping processes, label 1 points to the hole subband and 2 to the singlet subband. The hopping energy parameter $K_{ab} = 2t_{pd} K_{pd}$ depends on $t_{pd}$, the hopping p–d integral, and on energy band dependent form factors, $K_{ab}$, inband ($K_{11} = K_{12}$) and interband ($K_{21} = K_{22}$) processes are present. The Hubbard 1-forms

$$τ_{i,j}^{αβ,γη} = \sum_{m, \phi} v_{j\phi} X_{i}^{αβ} X_{m}^{γη}$$

(2)

incorporate the overall effects of specific hopping processes (through the labels $(αβ, γη)$ of the pair of Hubbard operators) involving the lattice site $i$ and its neighbouring sites.

Up to three coordination spheres around the reference site $i$ do contribute [4, 5] to the sum (2), each being characterized by a small specific value of the overlap coefficients $v_{ij}$ ($v_1$ for the nearest neighbour (nn), $v_2$ for the next nearest neighbour (nnn), $v_3$ for the third coordination sphere).

The quasi-particle spectrum and superconducting pairing for the Hamiltonian (1) are obtained [11, 12] from the two-time $4 \times 4$ GF matrix (in Zubarev notation [9])

$$\tilde{G}_{iσ}(t - t') = \langle \hat{X}_{iσ}(t) | \hat{X}^\dagger_{iσ}(t') \rangle = -iθ(t - t') \{ \langle \hat{X}_{iσ}(t) | \hat{X}^\dagger_{jσ}(t') \rangle \} \,$$

(3)

where $⟨⟨ \cdots ⟩⟩$ denotes the statistical average over the Gibbs grand canonical ensemble.

The GF (3) is defined for the four-component Nambu column operator

$$\hat{X}_{iσ} = (X_{iσ}^{2σ} X_{iσ}^{1σ} X_{iσ}^{1σ} X_{iσ}^{2σ})^T$$

(4)

where the superscript $T$ denotes the transposition. In (3), $\hat{X}^\dagger_{iσ} = (X_{iσ}^{2σ} X_{jσ}^{1σ} X_{iσ}^{1σ} X_{jσ}^{2σ})$ is the adjoint operator of $\hat{X}_{iσ}$.

The GF matrix in the $(r, ω)$-representation is related to the expression (3) of the GF matrix in the $(r, t)$-representation by the non-unitary Fourier transform,

$$\tilde{G}_{ijσ}(t - t') = \frac{1}{2π} \int_{-∞}^{t∞} \tilde{G}_{iσ}(ω) e^{-iω(t-t')} \, dω.$$

(5)

The energy spectrum of the translation-invariant spin lattice of (1) is solved in the reciprocal space. The GF matrix in this $(q, ω)$-representation is related to the GF matrix in the $(r, ω)$-representation by the non-unitary discrete Fourier transform

$$\tilde{G}_{iσ}(ω) = \frac{1}{N} \sum_{q} e^{-iq(r-r')} \tilde{G}_{iσ}(q, ω).$$

(6)

For an elemental GF of labels $(αβ, γη)$, we use the notation $\langle \{X^{αβ}_i(t) | X^{γη}_j(t')\} \rangle$ in the $(r, t)$-representation and, similarly, $\langle \{X^{αβ}_i(t) | X^{γη}_j(t')\} \rangle_ω$ (assuming Hubbard operators at $t = 0$), in
the \((\mathbf{r}, \omega)\)-representation. In the \((\mathbf{q}, \omega)\)-representation, it is convenient to use the notation \(G^{a\beta, \gamma\eta}(\mathbf{q}, \omega)\).

We shall consider henceforth the GMFA-GF, \(\tilde{G}^{0}_{\sigma}(\mathbf{q}, \omega)\). Its derivation involves:

(i) Differentiation of the GF (3) with respect to \(t\) and use of the equations of motion for the Heisenberg operators \(X_{i}^{a\beta}(t)\).

(ii) Derivation of an algebraic equation for \(\tilde{G}_{ij\sigma}(\omega)\), equation (5).

(iii) Elimination of the contribution of the inelastic processes to the commutator \(\hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H]\) entering the equation of motion of \(\tilde{G}_{ij\sigma}(\omega)\).

(iv) Transformation to the \((\mathbf{q}, \omega)\)-representation of the obtained equation of \(\tilde{G}^{0}_{\sigma}(\mathbf{q}, \omega)\) by means of the Fourier transform (6).

This finally yields

\[
\tilde{G}^{0}_{\sigma}(\mathbf{q}, \omega) = \tilde{\chi}[\tilde{\chi} \omega - \tilde{\Delta}_{\sigma}(\mathbf{q})]^{-1} \tilde{\chi},
\]

\[
\tilde{\chi} = \{[\hat{X}_{i\sigma}, \hat{X}^{\dagger}_{i\sigma}]\},
\]

\[
\tilde{\Delta}_{\sigma}(\mathbf{q}) = \sum_{r_{ij}} e^{i\mathbf{q} \cdot (r_{j} - r_{i})} \tilde{\Delta}_{ij\sigma}, \quad r_{ij} = r_{j} - r_{i},
\]

\[
\tilde{\Delta}_{ij\sigma} = \{[\hat{X}_{i\sigma}, H], \hat{X}^{\dagger}_{j\sigma}\}.
\]

The matrix \(\tilde{\Delta}_{ij\sigma}\) is Hermitian.

3. Translation invariance of the spin lattice

Four consequences follow from the translation invariance of the spin lattice.

- The definition of the Hubbard 1-form (2) over a translation-invariant spin lattice results in the identity (which secures the Hermiticity of the Hamiltonian \(H\)):

\[
\tau_{a\beta, \gamma\eta}^{i,j} = -\tau_{\gamma\eta, a\beta}^{i,j}.
\]

- The Green function (3) of the model Hamiltonian (1) depends only on the distance \(r_{ij} = |\mathbf{r}_{j} - \mathbf{r}_{i}|\) between the position vectors at the lattice sites \(i\) and \(j\) [9].

- The one-site statistical averages are independent of the site label \(i\), \(\langle X_{i}^{a\beta}\rangle = \langle X_{j}^{a\beta}\rangle\) (\(\forall i, j\)).

For this reason, the site label in the one-site averages will be omitted.

- The two-site statistical averages \(\langle X_{i}^{a\beta} X_{j}^{\gamma\eta}\rangle\) remain invariant under the interchange of the site labels \(i\) and \(j\),

\[
\langle X_{i}^{a\beta} X_{j}^{\gamma\eta}\rangle = \langle X_{j}^{a\beta} X_{i}^{\gamma\eta}\rangle, \quad i \neq j
\]

4. Spin reversal invariance

The energy spectrum of the system described by the Hamiltonian (1) does not depend on the specific values \(\sigma = \pm 1/2\) of the spin projection. As a consequence, the definition of the GF (3) either in terms of the \(\sigma\)-Nambu operator (4) or the \(\tilde{\sigma}\)-Nambu operator

\[
\hat{\tilde{X}}_{i\sigma} = (X_{i}^{a\beta} X_{i}^{0\sigma} X_{i}^{\sigma a} X_{i}^{0\beta})^{T}
\]

has to result in mathematically equivalent descriptions of the observables. This means, however, that the mathematical structures of the frequency matrices \(\tilde{\Delta}_{ij\sigma}\), equation (10) and
\[ \mathcal{A}_{ij \sigma} = \{ [\hat{X}_{i \sigma}, H], \hat{X}_{j \sigma}^\dagger \} \] emerging from the \( \sigma \)-Nambu operator (13) have to be related to each other.

The identification of the existing relationships is constructive: we calculate and compare the corresponding matrix elements of \( \mathcal{A}_{ij \sigma} \) and \( \mathcal{A}_{ij \sigma} \). The multiplication rules and the commutation/anticommutation relations satisfied by the Hubbard operators result in the following general expression of the elemental anticommutators entering their definitions:

\[
\{ [X_{i \sigma}, H], X_{j \sigma}^\dagger \} = \delta_{ij} c_{i \sigma}^{\mu \nu, \psi} + (1 - \delta_{ij}) v_{ij} t_{ij}^{\mu \nu, \psi},
\]

with one-site contributions given by

\[
C_{i \sigma}^{\mu \nu, \psi} = \delta_{\mu \nu} \left[ \left( \sum_{\sigma} \delta_{\mu \sigma} \right) E_1 + \delta_{\mu 2} E_2 \right] X_{i \sigma}^{\psi}
+ \sum_{\sigma} \delta_{\sigma \sigma} \left[ - E_1 X_{i \sigma}^{\psi} + \mathcal{K}_{21} t_{i \sigma, 0}^{\psi, \sigma, 0} - \mathcal{K}_{22} t_{i \sigma, 2}^{\psi, \sigma, 2} + \mathcal{K}_{21} \cdot 2 \sigma \left( t_{i \sigma, 0}^{\psi, 2 \sigma} + t_{i \sigma, 2}^{\psi, 0 \sigma} \right) \right]
+ \delta_{\sigma 2} \left( - E_2 X_{i \sigma}^{\psi} + \mathcal{K}_{22} \sum_{\sigma} t_{i \sigma, 2}^{\psi, \sigma, 2} + \mathcal{K}_{21} \sum_{\sigma} 2 \sigma \left( t_{i \sigma, 0}^{\psi, 2 \sigma} + t_{i \sigma, 2}^{\psi, 0 \sigma} \right) \right)
- \delta_{\sigma 0} \left( \mathcal{K}_{21} \sum_{\sigma} t_{i \sigma, 0}^{\psi, 0, \sigma} + \mathcal{K}_{21} \sum_{\sigma} 2 \sigma t_{i \sigma, 2}^{\psi, 0, 2 \sigma} \right)
+ \delta_{\sigma 2} \left( E_2 X_{i \sigma}^{\psi} + \mathcal{K}_{22} \sum_{\sigma} t_{i \sigma, \sigma}^{\psi, 2 \sigma} + \mathcal{K}_{21} \sum_{\sigma} 2 \sigma t_{i \sigma, 2}^{\psi, 2 \sigma} \right)
- \delta_{\sigma 0} \left( \mathcal{K}_{21} \sum_{\sigma} t_{i \sigma, \sigma}^{\psi, \sigma, 2} + \mathcal{K}_{21} \sum_{\sigma} 2 \sigma t_{i \sigma, \sigma}^{\psi, \sigma, 2} \right)
\]

and two-site contributions given by

\[
T_{ij}^{\mu \nu, \psi} = \delta_{\mu \nu} \left[ \left( \sum_{\sigma} \delta_{\mu \sigma} \right) (\mathcal{K}_{11} X_{i \sigma}^{\psi} X_{j \sigma}^{0 \psi} - \mathcal{K}_{22} X_{i \sigma}^{2 \psi} X_{j \sigma}^{0 \psi}) + (-\delta_{\mu 0} \mathcal{K}_{11} + \delta_{\mu 2} \mathcal{K}_{22}) \sum_{\sigma} X_{i \sigma}^{\psi} X_{j \sigma}^{\sigma \psi} \right]
+ \delta_{\phi \sigma} \left[ \left( \sum_{\sigma} \delta_{\phi \sigma} \right) \left( -\mathcal{K}_{11} X_{i \sigma}^{0 \psi} X_{j \sigma}^{\psi} + \mathcal{K}_{22} X_{i \sigma}^{2 \psi} X_{j \sigma}^{\psi} \right) + (\delta_{\phi 0} \mathcal{K}_{11} - \delta_{\phi 2} \mathcal{K}_{22}) \sum_{\sigma} X_{i \sigma}^{\mu \sigma} X_{j \sigma}^{\nu \psi} \right]
- \sum_{\sigma} \delta_{\sigma \sigma} \left[ \delta_{\sigma 0} \mathcal{K}_{11} X_{i \sigma}^{0 \psi} X_{j \sigma}^{\sigma \psi} - \delta_{\sigma 2} \mathcal{K}_{22} X_{i \sigma}^{2 \psi} X_{j \sigma}^{\sigma \psi} \right]
\]
four distinct kinds of relationships:

The comparison of the results obtained from (14) for the corresponding matrix elements of $\hat{A}_{ij\sigma}$ and $\hat{A}_{ij\bar{\sigma}}$ and the use of the translation invariance properties (11) and (12) result in four distinct kinds of relationships:

- Under the spin reversal $\sigma \to \bar{\sigma}$, the following **invariance properties** hold for the normal one-site statistical averages:

  \[ \langle X_{i\sigma} \rangle = \langle X_{i\bar{\sigma}} \rangle \]  \hspace{1cm} (15)

  \[ \langle t_{i,\sigma}^{0,0} \rangle = \langle t_{i,\bar{\sigma}}^{0,0} \rangle, \quad \langle t_{i,\sigma}^{0,\bar{\sigma}} \rangle = \langle t_{i,\bar{\sigma}}^{0,\bar{\sigma}} \rangle \]  \hspace{1cm} (16)

  \[ 2\sigma \langle t_{i,\sigma}^{0,\bar{\sigma}} \rangle = 2\bar{\sigma} \langle t_{i,\bar{\sigma}}^{0,\bar{\sigma}} \rangle. \]  \hspace{1cm} (17)

- The identity $\langle C_{i}^{2,0\sigma} + C_{i}^{0,0,\sigma} \rangle = 0$ holds, from where we get for the one-site anomalous averages:

  \[ \langle X_{i}^{02} \rangle = 0 \]  \hspace{1cm} (18)

  \[ \langle t_{i,\sigma}^{0,\bar{\sigma}} \rangle = -\langle t_{i,\bar{\sigma}}^{0,\bar{\sigma}} \rangle \]  \hspace{1cm} (19)

  \[ \langle t_{i,\sigma}^{0,\sigma} \rangle = \langle t_{i,\bar{\sigma}}^{0,\bar{\sigma}} \rangle \]  \hspace{1cm} (20)

The first two equations imply that the contributions of the one-site terms $\langle X_{i}^{02} \rangle$ and $\sum_{\sigma} \langle t_{i,\sigma}^{0,\sigma} \rangle$ to the superconducting pairing **vanish identically irrespective of the model details** (like, e.g., the relationship between the lattice constants $a_x$ and $a_y$).

For a rectangular spin lattice ($a_x \neq a_y$), equation (20) points to the occurrence of a small non-vanishing one-site contribution to the superconducting pairing **equally** in both energy subbands. However, over the square spin lattice (1) ($a_x = a_y$), each term of (20) vanishes for d-wave pairing due to the symmetry in the reciprocal space [12].

- Under the spin reversal $\sigma \to \bar{\sigma}$, the following **invariance properties** hold for the two-site statistical averages:

  \[ \langle X_{i\sigma} X_{j\bar{\sigma}} \rangle = \langle X_{i\bar{\sigma}} X_{j\sigma} \rangle, \quad \langle X_{i\sigma} X_{j\bar{\sigma}} \rangle = \langle X_{i\bar{\sigma}} X_{j\sigma} \rangle \]  \hspace{1cm} (21)

  \[ \langle X_{i}^{02 \sigma} X_{j}^{\bar{\sigma}} \rangle = \langle X_{i}^{02 \bar{\sigma}} X_{j}^{\sigma} \rangle, \quad \langle X_{i}^{02 \sigma} X_{j}^{\bar{\sigma}} \rangle = \langle X_{i}^{02 \bar{\sigma}} X_{j}^{\sigma} \rangle \]  \hspace{1cm} (22)

  \[ \langle X_{i}^{02 \sigma} X_{j}^{\bar{\sigma}} \rangle = \langle X_{i}^{02 \bar{\sigma}} X_{j}^{\sigma} \rangle. \]  \hspace{1cm} (23)
• The operator of the number of particles at site \(i\) within the singlet subband, \(N_i\), is the sum of spin \(\sigma\) and \(\bar{\sigma}\) components,
\[
N_i = n_{i\sigma} + n_{i\bar{\sigma}}, \quad n_{i\sigma} = X_{i\sigma}^{\sigma\sigma} + X_{i\sigma}^{22}, \quad n_{i\bar{\sigma}} = X_{i\bar{\sigma}}^{\bar{\sigma}\sigma} + X_{i\bar{\sigma}}^{22}.
\]
(24)

Similar relationships hold for the number of particles at site \(i\) within the hole subband, \(N_i^h\),
\[
N_i^h = n_{i\sigma}^h + n_{i\bar{\sigma}}^h, \quad n_{i\sigma}^h = X_{i\sigma}^{\sigma\sigma} + X_{i\sigma}^{00}, \quad n_{i\bar{\sigma}}^h = X_{i\bar{\sigma}}^{\bar{\sigma}\sigma} + X_{i\bar{\sigma}}^{00}.
\]
(25)

Due to the completeness relation,
\[
N_i + N_i^h = 2, \quad n_{i\sigma} + n_{i\bar{\sigma}}^h = n_{i\sigma} + n_{i\bar{\sigma}}^h = 1.
\]
(26)

These equalities simply reflect the fact that, at a given lattice site \(i\), there is a single spin state of predefined spin projection, whereas the total number of spin states equals 2.

Therefore, the operator \(N_i\), equation (24), provides unique characterization of the occupied states within the model [8, 10, 12].

5. Frequency matrix in the \((r, \omega)\)-representation

A straightforward consequence of the results established in section 4 is the simplest general expression of the frequency matrix \(\mathcal{A}_{ij\sigma}\), equation (10):
\[
\mathcal{A}_{ij\sigma} = \delta_{ij} \begin{pmatrix} \hat{c}_\sigma & 0 \\ 0 & -\hat{c}_\sigma \end{pmatrix} + (1 - \delta_{ij}) \begin{pmatrix} \hat{D}_{ij\sigma} & \hat{A}_{ij\sigma} \\ (\hat{A}_{ij\sigma})^\dagger & -(\hat{D}_{ij\sigma})^\dagger \end{pmatrix}.
\]
(27)

The one-site \(2 \times 2\) matrix \(\mathcal{A}_{ij\sigma}\) is Hermitian, its elements do not depend on the particular lattice site \(i\),
\[
\hat{c}_\sigma = \begin{pmatrix} (E_i + \Delta) \chi_2 + a_{22} \\ 2\sigma a_{21} \\ 2\sigma a_{21} \end{pmatrix},
\]
(28)

and are expressed in terms of the spin-reversal invariant quantities
\[
\chi_2 = \langle n_{i\sigma} \rangle = \langle n_{i\bar{\sigma}} \rangle
\]
(29)
\[
\chi_1 = \langle n_{i\sigma}^h \rangle = \langle n_{i\bar{\sigma}}^h \rangle = 1 - \chi_2
\]
(30)
\[
a_{22} = \mathcal{K}_{11} \chi_1^{(\bar{\sigma},\sigma)} - \mathcal{K}_{22} \chi_1^{2(\sigma)}
\]
(31)
\[
a_{21} = (\mathcal{K}_{11} - \mathcal{K}_{22}) \cdot 2\sigma \chi_1^{(\bar{\sigma},\sigma)} + \mathcal{K}_{21}(\chi_1^{0(\bar{\sigma},\sigma)} - \chi_1^{2(\sigma)})
\]
(32)

The normal hopping \(2 \times 2\) matrix \(\hat{D}_{ij\sigma}\) is symmetric,
\[
\hat{D}_{ij\sigma} = \begin{pmatrix} d_{ij}^{22} & 2\sigma d_{ij}^{11} \\ 2\sigma d_{ij}^{11} & d_{ij}^{11} \end{pmatrix}.
\]
(33)

Due to constraints (21) and (22), the charge-spin correlations entering the matrix elements of (33) get exactly decoupled from each other, such that
\[
d_{ij}^{22} = \mathcal{K}_{22}(\chi_{ij}^{\bar{\sigma}} + \chi_{ij}^{\sigma}) - \mathcal{K}_{11}\chi_{ij}^{\bar{\sigma} - \bar{\sigma}}
\]
\[
d_{ij}^{11} = \mathcal{K}_{11}[\chi_{ij}^{\bar{\sigma}} + (\chi_1 - \chi_2)\nu_{ij} + \chi_{ij}^{\sigma}] - \mathcal{K}_{22}\chi_{ij}^{\bar{\sigma} - \bar{\sigma}}
\]
\[
d_{ij}^{21} = \mathcal{K}_{21}[\chi_{ij}^{\bar{\sigma}} - \chi_2 \nu_{ij}] + \chi_{ij}^{\sigma} - \mathcal{K}_{21}\chi_{ij}^{\bar{\sigma} - \bar{\sigma}}
\]

with the three spin-reversal invariant weighted boson–boson correlation functions representing respectively charge–charge (c), spin–spin (S) and singlet-hopping (s-h) correlations:
\[
\chi_{ij}^e = v_{ij}(N_iN_j)/4, \tag{34}
\]
\[
\chi_{ij}^S = v_{ij}(S_iS_j) \tag{35}
\]
\[
\chi_{ij}^{\text{spin}} = v_{ij}[X_{ij}^{02}X_{ij}^{20}]. \tag{36}
\]

In (35), \(S_i = (S_i^x, S_i^y)\), with \(S_i^x = (X_i^{\sigma\sigma} - X_i^{\bar{\sigma}\bar{\sigma}})/2\) and \(S_i^y = X_i^{\sigma\bar{\sigma}}\).

The anomalous hopping 2 \times 2 matrix \(\hat{\Delta}_{ij}^{\sigma\bar{\sigma}}\) has a very special form, namely
\[
\hat{\Delta}_{ij}^{\sigma\bar{\sigma}} = \left( \begin{array}{cc} -K_{21} \cdot 2\sigma & -\frac{1}{2}(K_{11} + K_{22})/K_{21} \cdot 2\sigma \\ \frac{1}{2}(K_{11} + K_{22})/K_{21} \cdot 2\sigma & -K_{21} \cdot 2\sigma \end{array} \right) \chi_{ij}^{\text{pair}}, \tag{37}
\]
where the spin-reversal-invariant weighted boson–boson pairing (pair) correlation function is given by
\[
\chi_{ij}^{\text{pair}} = v_{ij}[X_{ij}^{02}X_{ij}^{20}] = 2v_{ij}[X_{ij}^{20} X_{ij}^{\sigma\sigma} + X_{ij}^{10} X_{ij}^{\bar{\sigma}\bar{\sigma}}] \tag{38}
\]
\[
= -v_{ij}[N_i^0 X_j^{02}] = -2v_{ij}[\langle X_i^{\sigma\sigma} + X_i^{\bar{\sigma}\bar{\sigma}} \rangle X_j^{02}]. \tag{39}
\]

In equations (38) and (39), the derivation of the second expression from the first one makes use of the spin-reversal invariance property (23).

To get a workable expression of the frequency matrix, approximations have to be derived for the boson–boson statistical averages entering the two-site hopping matrix elements. In the following section we show that the method of reference [12], yielding the pairing correlation for the boson–boson statistical averages entering the two-site hopping matrix elements. In the exponentially small terms, can be extended to the singlet-hopping correlations \(X_i^{02}X_j^{20}\) as well.

6. Hopping processes involving singlets

The right approach to the reduction of the order of correlation of the boson–boson statistical averages \(\langle X_i^{02}X_j^{\mu\nu} \rangle = \langle X_i^{\mu\nu}X_j^{02} \rangle\) goes differently for the hole-doped and electron-doped cuprates.

6.1. Reduction of the correlation order for the hole-doped cuprates

In these systems, the Fermi level (the zero-point energy) stays in the singlet subband. We get the estimates \(E_2 \simeq -\Delta\), \(E_2 - \Delta \simeq -2\Delta\), \(E_2 + \Delta \simeq 0\). With \(\Delta \sim 3\) eV, \(\beta\Delta \sim 3.5 \times 10^4\) T\(^{-1}\). Therefore, at \(T \lesssim 300\) K, the quantities containing the factor \(e^{\beta E_2} \simeq e^{-\beta\Delta} \lesssim e^{-100} < 10^{-44}\) are negligible.

We start with the following form of the spectral theorem [9]
\[
\langle X_i^{02}X_j^{\mu\nu} \rangle = \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{1 + e^{\beta \omega}} \text{Tr} \left[ \langle X_i^{02} | X_j^{\mu\nu} \rangle \right]_{\omega+\epsilon} - \text{Tr} \left[ \langle X_i^{02} | X_j^{\mu\nu} \rangle \right]_{\omega-\epsilon}, \tag{40}
\]
written for anticommutator retarded \((\omega + i\epsilon)\), respectively advanced \((\omega - i\epsilon)\) Green functions. Their equation of motion in the \((\tau, \omega)\)-representation is
\[
(\omega - E_2) \langle X_i^{02} | X_j^{i\sigma\bar{\sigma}} \rangle_{\omega} \simeq 2\langle X_i^{02} | X_j^{\mu\nu} \rangle_{\omega} + K_{21} \sum_\sigma \text{Tr} \left[ \langle X_i^{02} | X_j^{\mu\nu} \rangle \right]_{\omega} - \text{Tr} \left[ \langle X_i^{02} | X_j^{\mu\nu} \rangle \right]_{\omega}, \tag{41}
\]
where, for the sake of simplicity, the labels \(+i\epsilon, \epsilon = 0^+\), describing respectively the retarded and the advanced Green functions have been omitted. In (41), the higher order rhs
contributions coming from the inband hopping terms have been dropped off. Replacing (41) in (40), we get
\[ \langle X_{i}^{02} X_{j}^{μν} \rangle \simeq K_{21} \sum_{σ} 2σ \int_{-∞}^{+∞} \frac{dω}{1 + e^{−βω} \rho_σ} \times \left( \frac{1}{π} \right) \text{Im} \left[ \frac{1}{ω - E_{2} + iε} \left( \langle X_{i}^{σ0,0σ} X_{j}^{μν} \rangle \rangle_{\text{artic}} - \langle X_{i}^{σ2,σ2} X_{j}^{μν} \rangle \rangle_{\text{artic}} \right) \right]. \]

To evaluate the imaginary part, we use the identity [9]
\[ \frac{1}{ω - E_2 + iε} = P \frac{1}{ω - E_2} - iπ δ(ω - E_2). \]

The integrals over the δ-function yield (finite) GF real parts at ω = E_2, multiplied by a thermodynamic factor \( ∼ e^{-βΔ} \ll 1 \). The imaginary part of the hole subband GF \( \langle X_{i}^{σ0,0σ} X_{j}^{μν} \rangle \rangle_{\text{artic}} \) shows a δ-like maximum at \( ω = E_2 - Δ \), where \( (ω - E_2)^{-1} \simeq Δ^{-1} \) and the thermodynamic factor reaches a value \( ∼ e^{-2Δ} \). The only non-negligible contribution to the principal part integral comes from the singlet subband GF \( \langle X_{i}^{σ2,σ2} X_{j}^{μν} \rangle \rangle_{\text{artic}} \) the imaginary part of which shows a δ-like maximum at \( ω = E_2 + Δ \). This allows us to approximate \( (ω - E_2)^{-1} \simeq Δ^{-1} \) within the integral over the singlet subband GF to get
\[ \langle X_{i}^{02} X_{j}^{μν} \rangle \simeq (1 - δ_{ij}) \frac{K_{21}}{Δ} \sum_{σ} 2σ \langle X_{i}^{σ2,σ2} X_{j}^{μν} \rangle. \]

Replacing this result in equation (38) and using (2) we get
\[ \chi^{\text{pair}}_{ij} \simeq (1 - δ_{ij}) \frac{K_{21} v_{ij}}{Δ} \left[ 4 v_{ij} \cdot 2σ \langle X_{i}^{σ2} X_{j}^{σ2} \rangle - 2 \sum_{m \neq (i,j)} v_{im} \sum_{σ} 2σ \langle X_{i}^{σ2} X_{j}^{σ2} N_{j}^{σ} \rangle \right]. \]

Omitting the three-site terms, we get the two-site approximation of the superconducting pairing originating in the singlet subband.
\[ \chi^{\text{pair}}_{ij} \simeq (1 - δ_{ij}) \frac{4K_{21} v_{ij}}{Δ} \cdot 2σ \langle X_{i}^{σ2} X_{j}^{σ2} \rangle, \]
which reproduces the well-known two-site exchange term of the t-J model.

For the singlet-hopping correlation function, (42) yields the two-site approximation
\[ \chi^{s-h}_{ij} \simeq (1 - δ_{ij}) \frac{2K_{21} v_{ij}^{2}}{Δ} \cdot 2σ \langle X_{i}^{σ2} X_{j}^{σ0} \rangle. \]

6.2. Reduction of the correlation order for electron-doped cuprates

The Fermi level (the zero-point energy) stays now in the hole subband. We have the estimates \( E_2 \simeq Δ, E_2 + Δ \simeq 2Δ, E_2 - Δ \simeq 0. \)

It is convenient now to start with the alternative form of the spectral theorem [9]
\[ \langle X_{i}^{μν} X_{i}^{02} \rangle = \frac{i}{2π} \int_{-∞}^{+∞} \frac{dω}{e^{βω} + 1} \left[ \langle X_{i}^{02} X_{j}^{μν} \rangle \rangle_{\text{artic}} - \langle X_{i}^{02} X_{j}^{μν} \rangle \rangle_{\text{artic}} \right]. \]

with the retarded and advanced GFs following from the same equation (41).

Exponentially small quantities result from the δ-term of \( (ω - E_2 + iε)^{-1} \) and from the singlet subband GF \( \langle X_{i}^{σ0,0σ} X_{j}^{μν} \rangle \rangle_{\text{artic}} \). The hole subband GF \( \langle X_{i}^{σ2,σ2} X_{j}^{μν} \rangle \rangle_{\text{artic}} \), yields the non-negligible contribution
\[ \langle X_{i}^{μν} X_{i}^{02} \rangle \simeq (1 - δ_{ij}) \frac{K_{21}}{Δ} \sum_{σ} 2σ \langle X_{j}^{μν} X_{i}^{σ0,σ0} \rangle. \]
Replacing in (39) and omitting the three-site terms, we get the two-site approximation of the superconducting pairing originating in the hole subband,
\[
\chi_{ij}^{\text{pair}} \simeq (1 - \delta_{ij}) \frac{4K_{21}v_i^2}{\Delta} \cdot 2\sigma \langle X_i^{0\sigma} X_j^{0\sigma} \rangle.
\] (48)

Finally, the two-site approximation of the singlet-hopping correlation function is
\[
\langle X_i^{0\sigma} X_j^{2\sigma} \rangle \simeq (1 - \delta_{ij}) \frac{2K_{21}v_i^2}{\Delta} \cdot 2\bar{\sigma} \langle X_i^{0\sigma} X_j^{2\sigma} \rangle.
\] (49)

In conclusion, the GMFA superconducting pairing is a second-order effect. The lowest order contribution to it originates in interband hopping correlating annihilation (or creation) of pairs of spins at neighbouring lattice sites \(i\) and \(j\) within that energy subband which crosses the Fermi level.

Similarly, the singlet hopping is a second-order effect as well. It mainly proceeds by interband single particle jumps from the upper energy subband to the lower energy subband.

7. Frequency matrix in the \((\mathbf{q}, \omega)\)-representation

The calculation of the matrix elements of \(\tilde{A}_\sigma(\mathbf{q})\) from equation (9) asks for three essentially different kinds of Fourier transforms, namely

- The averages of the Hubbard 1-forms entering equations (31) and (32) result in sums of products of \(q\)-space averages and geometrical form factors:
\[
\langle X_\lambda^\mu X_\nu^\psi \rangle_q = \frac{1}{N} \sum_{\mathbf{q}} \langle X_\lambda^\mu X_\nu^\psi \rangle_q \gamma_\alpha(q)
\] (50)

for label sets \([\lambda, \mu, \nu, \psi] \in \{(0\bar{\sigma}, \bar{\sigma} 0); (\sigma 2, 2\sigma); (\bar{\sigma} 2, \bar{\sigma} 0);\}\).

The quantity \(\langle X_\lambda^\mu X_\nu^\psi \rangle_q\) denotes the average of the \(q\)-space image of the product of Hubbard operators of labels \(\lambda, \mu\) and \(\nu, \psi\) respectively,
\[
\langle X_\lambda^\mu X_\nu^\psi \rangle_q = \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{1 + e^{\beta\omega}} [G_\lambda^\mu, \nu^\psi(\mathbf{q}, \omega + i\epsilon) - G_\lambda^\mu, \nu^\psi(\mathbf{q}, \omega - i\epsilon)]
\] (51)

Finally, in equation (50), \(\gamma_\alpha(q)\) denote the nn \((\alpha = 1)\), nnn \((\alpha = 2)\) and third neighbour \((\alpha = 3)\) geometrical form factors, \(\gamma_1(q) = 2[\cos(q_1a_1) + \cos(q_2a_2)]\), \(\gamma_2(q) = 4 \cos(q_1a_1) \cos(q_2a_2)\) and \(\gamma_3(q) = 2[\cos(2q_1a_1) + \cos(2q_2a_2)]\).

- For the two-site weighted singlet hopping (36) and the superconducting pairing (38), the Fourier transforms result in convolutions of specific averages and geometrical form factors. The results are as follows:
  - Singlet hopping
\[
\chi^{s-h}(\mathbf{q}) = \sum_{\alpha=1}^{3} v_\alpha^2 \cdot \frac{1}{N} \sum_{\mathbf{k}} \Xi_k \gamma_\alpha(q - k)
\] (52)

where \(\Xi_k = 2\sigma \langle X_{\sigma\sigma} X_{\delta\delta} \rangle_k\), while \(\Xi_k = 2\sigma \langle X_{0\sigma} X_{2\sigma} \rangle_k\) for hole-doped and electron-doped cuprates respectively, with averages defined in (51).
  - Superconducting pairing
\[
\chi^{\text{pair}}(\mathbf{q}) = \sum_{\alpha=1}^{3} v_\alpha^2 \cdot \frac{1}{N} \sum_{\mathbf{k}} \Pi_k \gamma_\alpha(q - k)
\] (53)
where $\Pi_k = 2\delta (X^{s\bar{s}} X^{s\bar{s}})_k$, while $\Pi_k = 2\sigma (X^{s\bar{s}} X^{s\bar{s}})_k$ for hole-doped and electron-doped cuprates respectively, with averages defined in (51).

- The charge–charge and spin–spin correlation functions (34) and (35) are treated approximately following [8, 10]:
  - The order of the charge–charge correlation function $\langle N_i N_j \rangle$ is lowered using a Hubbard type I approximation decoupling procedure $\langle N_i N_j \rangle \simeq \langle N_i \rangle \langle N_j \rangle = 2\chi_2$.
  - The spin–spin correlation function $\langle S_i S_j \rangle$ is kept undecoupled, but treated phenomenologically. Equation (2) implies the occurrence of up to three non-vanishing spin–spin correlation functions: $nn$, $\chi_S^\delta = \langle S_i S_{\pm 2\alpha, \pm \alpha} \rangle$, $nnn$, $\chi_S^2 = \langle S_i S_{\pm 2\alpha, \pm \alpha} \rangle$. These are site-independent quantities.

Using the above results, we get from (9) and (27) the mathematical structure of the frequency matrix $\tilde{A}_\sigma (q)$ as follows:

$$
\tilde{A}_\sigma (q) = \begin{pmatrix}
\tilde{E}_\sigma (q) & \Phi_\sigma (q) \\
(\Phi_\sigma (q))^\dagger & -(\tilde{E}_\sigma (q))^\top
\end{pmatrix}.
$$

The normal $2 \times 2$ contributions to $\tilde{A}_\sigma (q)$ show the characteristic $\sigma$-dependence,

$$
\tilde{E}_\sigma (q) = \begin{pmatrix}
c_{22} & 2\sigma c_{21} \\
2\sigma c_{21} & c_{11}
\end{pmatrix} ;
-(\tilde{E}_\sigma (q))^\top = \begin{pmatrix}
-c_{22} & 2\sigma c_{21} \\
2\sigma c_{21} & -c_{11}
\end{pmatrix},
$$

with the $\sigma$-independent terms $c_{ab}$ carrying normal one-site and two-site matrix elements,

$$
c_{22} \equiv c_{22}(q) = (E_1 + \Delta)\chi_2 + a_{22} + d_{22}(q)
$$

$$
c_{11} \equiv c_{11}(q) = E_1\chi_1 + a_{22} + d_{11}(q)
$$

$$
c_{21} \equiv c_{21}(q) = a_{21} + d_{21}(q)
$$

$$
d_{ab}(q) = K_{ab} \sum_{\alpha=1}^3 v_{ab} q_{\alpha} \left[ \chi_{\alpha}^\delta + (-1)^{a+b} \chi_{\alpha} \right] + \frac{1}{2} J_{ab} X^{a-b}(q).
$$

The one-site terms are defined by equations (31), (32) and (50). The exchange energy parameters are given by

$$
J_{ab} = 4K_{ab} K_{21}/\Delta, \quad \{ab\} \in \{22, 11, 21\},
$$

while the singlet-hopping contribution $X^{a-b}(q)$ is given by equation (52).

The anomalous $2 \times 2$ matrix contributions to $\tilde{A}_\sigma (q)$, obtained from (37), show the characteristic $\sigma$-dependence,

$$
\Phi_\sigma (q) = \begin{pmatrix}
-2\sigma \xi_1 b & \xi_2 b \\
-\xi_2 b & 2\sigma \xi_1 b
\end{pmatrix} ;
(\Phi_\sigma (q))^\dagger = \begin{pmatrix}
-2\sigma \xi_1 b^* & -\xi_2 b^* \\
\xi_2 b^* & 2\sigma \xi_1 b^*
\end{pmatrix},
$$

with $\xi_1 = J_{21}$, $\xi_2 = (J_{11} + J_{22})/2$, whereas $b \equiv b(q)$ is a shorthand notation for the pairing matrix element (53).

**Remark 1.** The spin-reversal $\sigma \to \sigma$ symmetry properties of the elemental Green functions entering the matrix GF (3) are identical to those established for the underlying frequency matrix $\tilde{A}_\sigma (q)$.
8. GMFA Green function

From equations (15) and (18) it follows that the matrix $\hat{\chi}$, equation (8), is diagonal and spin-reversal invariant, with two nonvanishing matrix elements,

$$\hat{\chi} = \begin{pmatrix} \hat{\chi}_2 & 0 \\ 0 & \hat{\chi}_1 \end{pmatrix}$$

where $\chi_2$ and $\chi_1$ are given by equations (29) and (30) respectively.

Replacing in (7) the expressions (58) of the matrix $\hat{\chi}$ and (54) of the frequency matrix $\hat{\Lambda}_0(q)$, we get a structure of the GMFA-GF matrix obeying the general symmetry properties established in [11],

$$\hat{\tilde{G}}^0_\sigma(q, \omega) = \begin{pmatrix} \hat{\tilde{G}}^0_\sigma(q, \omega) & \hat{\tilde{F}}^0_\sigma(q, \omega) \\ \hat{\tilde{F}}^0_\sigma(q, \omega)^\dagger & -\hat{\tilde{G}}^0_\sigma(q, -\omega) \end{pmatrix},$$

where the argument $\omega$ carries, in fact, the complex value $\omega + i\varepsilon$, $\varepsilon = 0^+$. (Hence the elemental GFs containing the argument $\omega$ point to retarded GFs, while those containing the argument $-\omega$ point to advanced GFs.)

The normal $2 \times 2$ matrix $\hat{\tilde{G}}^0_\sigma(q, \omega)$ shows the characteristic $\sigma$-dependence,

$$\hat{\tilde{G}}^0_\sigma(q, \omega) = \begin{pmatrix} g_{22}(q, \omega) & 2\sigma g_{21}(q, \omega) \\ 2\sigma g_{21}^*(q, \omega) & g_{11}(q, \omega) \end{pmatrix} \cdot \frac{1}{\mathcal{D}(q, \omega)},$$

with the $\sigma$-independent components $g_{ab}(q, \omega)$ found from

$$g_{ab}(q, \omega) = A_{ab}\omega^3 + B_{ab}\omega^2 + C_{ab}\omega + D_{ab}, \quad [ab] \in \{22, 11, 21\}.$$

Here the coefficients $A_{ab}$ are given respectively by

$$A_{22} = \chi_2, \quad A_{11} = \chi_1, \quad A_{21} = 0,$$

while $B_{ab}, C_{ab}, D_{ab}$ are $q$-dependent coefficients:

$$B_{22}(q) = c_{22}, \quad B_{11}(q) = c_{11}, \quad B_{21}(q) = c_{21}$$

$$C_{22}(q) = -\left[\chi_2(c_1^2 + \xi_1^2|b|^2) + \chi_1(c_2|b|^2 + \xi_2^2|b|^2)\right]/\chi_1^2$$

$$C_{11}(q) = -\left[\chi_1(c_2^2 + \xi_2^2|b|^2) + \chi_2(c_1|b|^2 + \xi_1^2|b|^2)\right]/\chi_2^2$$

$$C_{21}(q) = \left[c_2(c_1 \chi_1 + \chi_2 c_2) - \xi_1 \xi_2 |b|^2\right]/(\chi_1 \chi_2)$$

$$D_{22}(q) = -\left[c_{11}(c_{22} - |c_{21}|^2) + (c_{22}^2 \xi_1^2 + c_{11} \xi_1^2 + 2\Im(c_{21}) \xi_1 \xi_2)|b|^2\right]/\chi_1^2$$

$$D_{11}(q) = -\left[c_{22}(c_{22} - |c_{21}|^2) + (c_{22} \xi_2^2 + c_{22}^2 \xi_2^2 + 2\Im(c_{21}) \xi_1 \xi_2)|b|^2\right]/\chi_2^2$$

$$D_{21}(q) = \left[c_{22}(c_{22} - |c_{21}|^2) - [c_{22}^2 \xi_1^2 + c_{22} \xi_2^2 + (c_{22} + c_{11}) \xi_1 \xi_2]|b|^2\right]/(\chi_1 \chi_2)$$

The anomalous $2 \times 2$ matrix $\hat{\tilde{F}}^0_\sigma(q, \omega)$ shows the characteristic $\sigma$-dependence,

$$\hat{\tilde{F}}^0_\sigma(q, \omega) = \begin{pmatrix} 2\sigma f_{22}(q, \omega) & f_{21}(q, \omega) \\ -f_{21}(q, -\omega) & 2\sigma f_{11}(q, \omega) \end{pmatrix} \cdot \frac{1}{\mathcal{D}(q, \omega)},$$

with the elemental GFs $f_{ab}(q, \omega)$ given by

$$f_{aa}(q, \omega) = (P_{aa}\omega^2 + R_{aa})b, \quad [aa] \in \{22, 11\},$$

$$f_{21}(q, \omega) = (P_{21}\omega^2 + Q_{21}\omega + R_{21})b.$$
Here, $P_{22} = -\xi_1$, $P_{11} = \xi_1$ and $P_{21} = -\xi_2$ are $q$-independent, while

$$R_{22}(q) = \left[ (c_{21}^2 + c_{22}^2)\xi_1 + 2c_{11}c_{21}\xi_2 + \xi_1(\xi_1^2 - \xi_2^2) \right]/\chi^2_1$$

$$R_{11}(q) = -\left[ (c_{22}^2 + c_{21}^2)\xi_1 + 2c_{22}c_{21}^2\xi_2 + \xi_1(\xi_1^2 - \xi_2^2) \right]/\chi^2_2$$

$$R_{21}(q) = \left[ (c_{11}c_{21}^2 + c_{22}c_{21})\xi_1 + (c_{22}c_{21} + |c_{21}|^2)\xi_2 - \xi_2(\xi_1^2 - \xi_2^2) |b|^2 \right]/(\chi_1\chi_2)$$

$$Q_{21}(q) = \left[ (\chi_2c_{21} - c_{11}c_{21})\xi_1 + (\chi_2c_{21} - c_{11}c_{21})\xi_2 \right]/(\chi_1\chi_2).$$

The determinant $D(q, \omega)$ occurring in equations (60) and (61), which is proportional to the determinant of the matrix $\hat{J} - \hat{A}_\sigma(q)$ in (7), shows the following monic bi-quadratic dependence in $\omega$:

$$D(q, \omega) = (\omega^2 - u\omega + v)(\omega^2 + u\omega + v),$$

where $v = v(q)$ and $u = u(q)$ are found respectively from

$$v^2 = \left[ (c_{22}c_{11} - |c_{21}|^2 - (\xi_1^2 - \xi_2^2)|b|^2)^2 + \left[ (c_{22} + c_{11}) + 2\text{Re}(c_{21})^2 \xi_1^2 - 4(c_{22} + c_{11})\text{Re}(c_{21})\xi_2 - 4|c_{21}|^2(\xi_1^2 - \xi_2^2) \right]|b|^2 \right]/(\chi_1^2\chi_2^2)$$

$$u^2 - 2v = \frac{1}{\chi_1^2}(c_{22}^2 + \xi_1^2|b|^2) + \frac{1}{\chi_2^2}(c_{22}^2 + \xi_1^2|b|^2) + \frac{2}{\chi_1^2\chi_2^2}(|c_{21}|^2 + \xi_2^2|b|^2).$$

A necessary consistency condition to be satisfied by the parameters of the model at any vector $q$ inside the Brillouin zone is $v^2(q) \geq 0$.

**Remark 2.** The zeros of the determinant of the GMFA-GF,

$$D(q, \omega) = 0$$

provide the GMFA energy spectrum of the system.

At every wave vector $q$ inside the Brillouin zone, this yields for the superconducting state the energy eigenvalue set

$$\left[ \Omega_1(q), \Omega_2(q), -\Omega_2(q), -\Omega_1(q) \right], \quad \Omega_{1,2}(q) = (u/2) \pm \sqrt{(u/2)^2 - v}.$$

In the normal state ($b = 0$), equations (63) and (64) reduce respectively to

$$v_0 = (c_{22}/\chi_2)(c_{11}/\chi_1) - |c_{21}|^2/(\chi_1\chi_2)$$

$$u_0 = (c_{22}/\chi_2) + (c_{11}/\chi_1)$$

such that the energy spectrum is given by the roots of the second-order equation $\omega^2 - u_0\omega + v_0 = 0$ solved in [8].

Finally, if we assume a pure Hubbard model (i.e., energy band independent hopping parameters, $K_{11} = K_{22} = K_{21} \equiv t$, [10]), then a significant simplification of the equations derived in the last two sections is obtained. The normal 2 × 2 matrix $\tilde{E}_\sigma(q)$ becomes symmetric and so is the normal GMFA-GF $\tilde{G}_\sigma(q, \omega)$. Moreover, there is a single exchange energy parameter in (57), $\xi_1 \equiv \xi_2 \equiv J = 4t^2/\Delta$, which simplifies the anomalous 2 × 2 frequency matrix in $\tilde{\Phi}_\sigma(q) = (\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}) J b$, such that the quantities $u$ and $v$ in the expression (62) of the GF determinant reduce to

$$v^2 = \left[ (c_{22}c_{11} - c_{21}^2)^2 + (c_{22} + c_{11} + 2c_{21})^2 J^2 |b|^2 \right]/(\chi_1^2\chi_2^2)$$

$$u^2 - 2v = \left[ c_{22}^2 + c_{22}^2 + 2\chi_1\chi_2c_{21} + J^2 |b|^2 \right]/(\chi_1^2\chi_2^2).$$

A non-negative value $v \geq 0$ always follows from equation (67), however, the reality of the solutions (66) needs investigation of the domain of variation of the adjustable parameters of the model.
9. Conclusions

The two-band Hubbard model of the high-$T_c$ superconductivity in cuprates [8, 12] uses Hubbard operator algebra on a physical system characterized by specific invariance symmetries with respect to translations and spin reversal.

In the present paper, we have shown that the system symmetries result either in invariance properties or exact vanishing of several characteristic statistical averages. The vanishing of the one-site anomalous matrix elements is shown to be a property which is embedded in the Hubbard operator algebra. Another worth mentioning consequence following from the spin-reversal invariance properties of the two-site statistical averages is the exact decoupling from each other of the charge and spin correlations entering the matrix elements of the frequency matrix. The use of these results allowed rigorous derivation and simplification of the expression of the frequency matrix of the generalized mean-field approximation (GMFA) Green function (GF) matrix of the model.

For the higher order boson–boson averages $\langle X_0^{2i} X_0^{2j} \rangle$ and $\langle X_0^{2i} N_j \rangle$, which enter respectively the normal singlet-hopping and anomalous exchange pairing contributions to the frequency matrix, an approximation procedure resulting in GMFA-GF expressions was described. The procedure avoids the current decoupling schemes [14, 15]. Its principle, first formulated in [12], consists in the identification and elimination of exponentially small contributions to the spectral theorem representations of these statistical averages.

A point worth noting is that the proper identification of exponentially small quantities asks for the use of different starting expressions of the spectral theorem for the hole-doped and electron-doped cuprates.

The results of the reduction procedure may be summarized as follows:

- The singlet hopping is a second-order effect which may be described as interband $i \leftrightarrow j$ single particle jumps from the upper to the lower energy subband.
- The GMFA superconducting pairing is a second-order effect, the lowest order contribution to which originates in interband hopping correlating the annihilation (creation) of spin pairs at neighbouring lattice sites $i$ and $j$ within that energy subband which crosses the Fermi level.

The derivation of the most general and simplest possible expressions of the frequency matrix and of the GMFA-GF matrix in the $(q, \omega)$-representation enables reliable numerical investigation of the consequences coming from the adjustable parameters of the model (the degree of hole/electron doping, the energy gap $\Delta$, the hopping parameters).

Another open question of the GF approach to the solution of the present model is the use of the Hubbard operator algebra to get rigorous derivation and simplification of the Dyson equation of the complete Green function. As shown previously in [12], the self-energy corrections induce a spin fluctuation d-wave pairing originating in kinematic interaction in the second order.

These investigations are underway and results will be reported in a forthcoming paper.

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