Superconductivity in a two dimensional extended Hubbard model

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Abstract

The Roth’s two-pole approximation has been used by the present authors to investigate the role of $d-p$ hybridization in the superconducting properties of an extended $d-p$ Hubbard model. Superconductivity with singlet $d_{x^2-y^2}$-wave pairing is treated by following Beenen and Edwards formalism. In this work, the Coulomb interaction, the temperature and the superconductivity have been considered in the calculation of some relevant correlation functions present in the Roth’s band shift. The behavior of the order parameter associated with temperature, hybridization, Coulomb interaction and the Roth’s band shift effects on superconductivity are studied.

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1 Introduction

After almost two decades of intense research about the cuprates, there is still plenty of open questions in this problem. However, it is recognized that the electrons which move on the CuO$_2$ planes are the most relevant to describe their physical properties \cite{1}. In the undoped regime, these compounds are insulators and exhibit antiferromagnetic order at sufficient low temperatures \cite{12-1}. The physical properties of the insulating phase can be well described by the Heisenberg model \cite{2}. Upon doping, these systems suppress the antiferromagnetic order and become superconductors. In this scenario there is no doubt that the $d$-$d$ electron correlations play a fundamental role.

The study of the electronic structure near the Fermi level $\varepsilon_F$ in such strongly correlated systems is very important to understand their physical properties \cite{3}. Earlier angle-resolved photoemission experiments (ARPES) have showed the presence of flat bands close to $\varepsilon_F$ in a region centered around the point $(\pi,0)$ in the $p$-type cuprates like Bi$_2$Sr$_2$CuO$_6$ and YBa$_2$Cu$_3$O$_y$ \cite{8,9}. Due to the presence of strong correlations, to study some physical properties of these cuprate compounds, the one-band Hubbard model \cite{5} can be used. Bulut et al. \cite{6,7} have done Monte Carlo calculations in the one-band Hubbard model. Their results show bands with a flat region near $(\pi,0)$ point for a given doping which agreed with the previously mentioned ARPES results \cite{3}.

Beenen and Edwards \cite{8}, using the Roth’s two-pole approximation \cite{9} in the one-band Hubbard model, have studied the normal state of the model obtaining flat quasiparticle bands, which agree well with those found with Monte Carlo simulations \cite{6,7}. The Roth’s two-pole approximation has been proposed to improve the Hubbard-I approximation \cite{5} by considering a decoupling scheme which produces an additional energy shift (the Roth’s band shift) in the peaks of the spectral function. That result is in agreement with those obtained by Harris and Lange \cite{10}. They looked at the moments of individual peaks in the spectral function. The presence of the exchange term $\langle S_i S_j \rangle$ in the Roth’s band shift exhibits in it a spin dependence. As consequence, the Roth’s method raises the possibility of magnetic solution in the Hubbard model while this feature is not present in the Hubbard-I approximation. Recently, due to the good agreement between the Roth’s and the Monte Carlo data, Beenen and Edwards have extended the Roth’s two-pole approximation in order to investigate the superconducting properties of the one-band Hubbard model. Their main achievement has been to show the emergence of the pairing with $d_{x^2-y^2}$ symmetry in a given amount of doping. In that approach, the gap equation for $d$-wave symmetry depends on a particular four operator correlation function which, in principle, can be found extending the Roth’s formalism to obtain two particle Green’s functions. However, the authors have introduced two decoupling schemes to calculate the gap. The first one (the factorization procedure) has been formulated to treat the problem for intermediate values of $U$ (the Coulomb interaction) and it provides an upper estimate for the gap and $T_c$ (the critical temperature). The second one is adapted for very large $U$ scenario which preserves the proper limit for $U \rightarrow \infty$ where the gap function vanishes.

Nevertheless, the one-band models neglect the presence of the oxygen sites. Due to the strong correlations at the Cu-sites, the oxygen sites may be occupied by holes when the system is doped \cite{2}. For instance, the Hubbard one-band model suffers some limitations to describe the low-energy physical properties of the cuprate superconductors \cite{11}. In the doped regime, the one-band Hubbard model gives a wrong description of various properties, like, for example, the asymmetric magnetic doping-temperature phase diagram \cite{12}. Therefore, a model which take into account also the oxygen can be more adequate to treat the cuprate systems in the doped regime \cite{13}. This raises the question whether it is possible to extend the Beenen and Edwards analysis to investigate the $d$-wave symmetry superconductivity when the hybridization is present.

Recently, the present authors have used the extended Hubbard model \cite{14} with the Roth’s method to study the role of hybridization in the superconductivity following closely the approach introduced by Beenen and Edwards \cite{12}. As discussed in the references \cite{8} and \cite{15}, the flattening of the bands is directly related to the band shift. The presence of flat bands at Fermi level $\varepsilon_F$ in the $p$-type cuprates \cite{8} suggests a high density of states at the Fermi level, which can favor pair formation. Therefore, considering that the main responsible elements for the density of states at the Fermi level are the $d$-electrons, it has been assumed in Ref. \cite{14} that the $d-d$ pairs are the most relevant ones for superconductivity \cite{14}.

The band shift plays an important role in the study of the superconducting properties of the model using the Roth’s or some similar procedures. In reference \cite{14}, the factorization procedure \cite{8} has been used to investigate the effects of the hybridization on the superconductivity. It has been shown \cite{14} that the hybridization has strong effects in the shift and, therefore, in some superconducting physical properties such as the critical temperature $T_c$. However, as a first approach, in reference \cite{14}, the band shift has been evaluated taking into account the hybridization effects, but disregarding temperature effects, superconducting properties and, most important, it has been considered in the limit $U \rightarrow \infty$. As a consequence of this limit, many correlation functions, which appear in the shift, are vanished. The important point is that these correlation functions are very relevant in the sense of to
include correctly the hybridization effects. Therefore, it would be necessary to calculate the shift with the \( U \) finite in order to include the hybridization effects in a more complete way.

In this work, the superconductivity problem has been studied using the Roth’s method, following closely reference \( 8 \), but adapted to the \( d-p \) extended Hubbard model. Here, special attention is devoted to the effects of the hybridization and superconductivity in the band shift. In order to have the effects of the hybridization included properly in the superconductivity, the gap function is obtained using the factorization procedure \( 11 \) and the shift is evaluated with finite \( U \). This procedure is justified because it preserves some correlation functions present in the band shift, which are non vanishing for finite \( U \). As consequence, it captures the effects of the hybridization properly. Some preliminary results of this approach have been given in Ref. \( 17 \).

There are some shortcomings in the Beenen and Edwards approach \( 15,19 \). For instance, the \( d_x^2-y^2 \) pairing is quite dependent on the choice of the decoupling scheme for the correlation functions related to the gap. However, in the present work, the main goal is to study the effects of hybridization. Therefore, as discussed in the previous paragraph, the natural choice is the decoupling scheme for intermediated \( U \), which is also the simplest one. One is allowed to find in that procedure, at least, a better estimate for the gap (and therefore for \( T_c \)) as a function of hybridization within the same decoupling procedure.

The paper presents the following organization. In section 2 it is introduced the model and given a short introduction of the Roth’s method \( 9 \). Also, some analytic expressions for quasi-particle bands and the Green’s functions are derived. In section 3 the factorization procedure proposed by Beenen and Edwards \( 8 \) is applied for the present case. In section 4 the band shift is discussed in detail. The numerical results are showed and discussed in section 5. Finally, in section 6 a short summary and some concluding remarks are given.

## 2 General formulation

The model considered here assumes overlapping bands. It is characterized by a narrow \( d \)-like band with a large density of states and a wide \( p \)-like band with low density of states. The extended Hubbard model is defined as:

\[
H = \sum_{i,\sigma} (\varepsilon_d - \mu) d_{i\sigma}^\dagger d_{i\sigma} + \sum_{i,j,\sigma} t_{ij}^d d_{i\sigma}^\dagger d_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} (\varepsilon_p - \mu) p_{i\sigma}^\dagger p_{i\sigma} + \sum_{i,j,\sigma} t_{ij}^p p_{i\sigma}^\dagger p_{j\sigma} + \sum_{i,j,\sigma} t_{ij} d_{i\sigma}^\dagger p_{j\sigma} + p_{i\sigma}^\dagger d_{j\sigma}
\]

where \( \mu \) is the chemical potential. The \( d_{i\sigma}^\dagger, d_{i\sigma} \) and \( p_{i\sigma}^\dagger, p_{i\sigma} \) are the creation and annihilation operators of the \( d \)- and \( p \)-electrons, respectively, with spin \( \sigma \) at a lattice site \( i \). The \( \varepsilon_d \) and \( \varepsilon_p \) are the centers of the on site energies of the occupied orbitals of the copper and oxygen respectively. The second term of the Hamiltonian given in Eq. \( 1 \) describes a narrow \( d \)-band with a hopping amplitude \( t^d \). The Hamiltonian \( 1 \) considers also a \( p \)-band which is wider than the \( d \)-band. The following relation between \( t^d \) and \( t^p \) can be established \( t^d = \alpha t^d \) with \( \alpha > 1 \). Also, \( t^d < 0 \) to coincide the bottom of the \( d \)- and \( p \)-bands with the \( \Gamma \) point \( k_x = k_y = 0 \) as suggested by experimental results \( 3 \). The third term corresponds to the Coulomb interaction \( U \) that represents the repulsion between two holes in the same \( d \)-orbital. The last term of the Hamiltonian \( 1 \) is the \( d-p \) hybridization and describes the nearest neighbor hopping process between the \( d \)-orbital of the Cu-atom and the \( p \)-orbital of the O-atom. Considering a rectangular two dimensional lattice, the unperturbed \( d \)- and \( p \)-energy bands are given by

\[
\varepsilon_d^d = 2t^d (\cos(ka) + \cos(kb))
\]

and

\[
\varepsilon_p^p = 2t^p (\cos(ka) + \cos(kb))
\]

where \( a \) is the lattice constant.

In this work, the Hamiltonian given in Eq. \( 1 \) has been investigated using the Roth’s two-pole approximation \( 9 \) to obtain the Green’s function in the Zubarev’s formalism. In the Roth’s procedure, a set of operators \( \{ A_n \} \) is introduced in order to describe the relevant one particle excitations of the system. These operators satisfy in some approximation the following relation:

\[
[A_n, H]_{(-)} = \sum_{m} K_{nm} A_m.
\]

Anticommuting both sides of Eq. \( 4 \) with each operator of the set \( \{ A_n \} \) and taking the thermal average, the equation \( 4 \) becomes:

\[
E_{nm} = \sum_{m} K_{nm} N_{nm}
\]

where \( E_{nm} \) and \( N_{nm} \) are the energy and normalization matrices, given by

\[
E_{nm} = \left\langle \left[ A_n, H \right]_{(-)} A_m^\dagger \right\rangle_{(+)}
\]

and

\[
N_{nm} = \langle A_n A_m^\dagger \rangle_{(+)}
\]

In matrix notation, Eq. \( 5 \) is written as \( E = K \cdot N \), where, if \( N \) is nonsingular, then the \( K \) matrix can be obtained. With the equation of motion (in the Zubarev’s formalism) of the Green’s function

\[
G_{nm}(\omega) = \langle A_n; A_m^\dagger \rangle_\omega
\]
and the Eqs. (12-17), it is possible to obtain the following general Green’s functions

\[ \langle A_n; B \rangle(\omega) = \sum_m \overline{G}_{nm}(\omega) \langle [A_m, B] \rangle(+) \].

In the particular case, where \( B = A_n \), the elements of the Green’s function matrix \( \overline{G} \) are given by Eq. (8). Thus, using the matrices \( E \) and \( N \), the matrix \( \overline{G} \) is given by

\[ \overline{G}(\omega) = \overline{G}(\omega)N \]

where

\[ \overline{G}(\omega) = N(\omega N - E)^{-1}. \]

Considering the fact that the operators of the set \( \{A_n\} \) describe the particle excitations of the system, the choice of these operators is very relevant to study the physical properties of the system. In order to discuss superconductivity, Beenen and Edwards, in their approach with the one-band Hubbard model, mixed electron and hole operators and evaluated anomalous correlation functions [8]. Therefore, using a set of four operators \( \{c_{i\sigma}, n_{i\sigma}, c^\dagger_{i\sigma}, n_{i\sigma}^\dagger\} \), it has obtained a four-pole approximation to the Green’s functions. However, in order to discuss the role of the hybridization, it is necessary to adapt the formalism to include a p-operator in the original set of operators used by Beenen and Edwards. Thus, the new set of operators is given by

\[ \{d_{i\sigma}, n_{i\sigma}^d d_{i\sigma}, d_{i\sigma}^\dagger, n_{i\sigma}^d d_{i\sigma}^\dagger, p_{i\sigma}\}. \]

In the present work, only the singlet pairing is considered, and particularly the \( d \)-wave symmetry. In this particular case, \( \langle d_{i\sigma} d_{i\sigma} \rangle = 0 \) and \( \sum_l \langle d_{i\sigma} d_{i\sigma} \rangle = 0 \), where \( l \) are the nearest neighbors of \( i \). Using the set of operators given Eq. (12), and introducing the symmetries discussed above, the elements of the energy matrix defined in Eq. (3) can be obtained as:

\[ E_5 = \begin{bmatrix} E_2 & 0 & 0 & V_{k^d}^p & 0 \\ 0 & 0 & \overline{G}_k & n_{-\sigma} d_{k^d} \\ 0 & 0 & 0 & 0 \\ 0 & \overline{G}_k^{-1} & -E_2 & 0 \\ V_{k^d}^p & n_{-\sigma} d_{k^d} & 0 & 0 & \epsilon_p - \mu + \epsilon_{k^d}^p \end{bmatrix} \]

where \( \overline{G}_k \) and \( V_{k^d}^p \) are the Fourier transform of \( t_{ij}^d \) and \( t_{ij}^p \) respectively. The matrix \( E_2 \) present in the energy matrix \( E_5 \) is given by:

\[ E_2 = \begin{bmatrix} \overline{G}_k & 0 & 0 & \overline{G}_k & 0 \\ 0 & \overline{G}_k & 0 & \overline{G}_k & 0 \\ 0 & \overline{G}_k & 0 & \overline{G}_k & 0 \\ 0 & \overline{G}_k & 0 & \overline{G}_k & 0 \\ \overline{G}_k & 0 & 0 & \overline{G}_k & 0 \end{bmatrix} \]

where \( \overline{G}_k \) = \( \varepsilon_k - \mu \). It is assumed that the system considered here is translationally invariant, then \( n_{-\sigma}^d = n_{i\sigma}^d \).

The quantity \( \Gamma_{k-\sigma} \) is the Fourier transform of

\[ \Gamma_{ij-\sigma} = (\varepsilon_d - \mu) n_{-\sigma}^d \delta_{ij} + t_{ij}^d (n_{-\sigma}^d)^2 + n_{-\sigma}^d (1 - n_{-\sigma}^d) W_{ij-\sigma}. \]

In Eq. (15), the band shift \( W_{ij-\sigma} \) is defined as:

\[ W_{ij-\sigma} = \frac{t_{ij}^d}{n_{-\sigma}^d} \left( \langle n_{i\sigma}^d n_{j\sigma}^d \rangle - \langle n_{i\sigma}^d \rangle^2 \right) + \Lambda_{ij\sigma} \]

where \( \Lambda_{ij\sigma} \) can be separated into two explicit contributions

\[ \Lambda_{ij\sigma} = \Lambda_{ij\sigma}^d + \Lambda_{ij\sigma}^{pd}. \]

The terms \( \Lambda_{ij\sigma}^d \) and \( \Lambda_{ij\sigma}^{pd} \) are associated with the hopping \( t_{ij}^d \) and the hybridization \( t_{ij}^{pd} \), respectively. The hybridized term of \( \Lambda_{ij\sigma} \) may be written as

\[ \Lambda_{ij\sigma}^{pd} = \sum_l t_{il}^{pd} \left[ \langle p_{l\sigma}^d n_{i\sigma}^d d_{i\sigma} \rangle - \langle p_{l\sigma}^d \rangle \delta_{ij} \right], \]

and the part associated to the hopping \( t_{ij}^d \) is given by

\[ \Lambda_{ij\sigma}^d = \sum_l t_{il}^d \left\{ \langle n_{i\sigma}^d d_{l\sigma}^d \rangle + \langle n_{i\sigma}^d d_{l\sigma}^d \rangle \right\} \delta_{ij} - t_{ij}^d \left\{ \langle d_{i\sigma}^d d_{i\sigma}^d \rangle + \langle d_{i\sigma}^d d_{i\sigma}^d \rangle \right\} \].

The calculation of the correlation functions presented in Eqs. (18) and (19) will be discussed in detail in section 4. One of the most important elements of the matrix \( E_5 \) is \( E_{24} = \overline{\gamma}_k \), where

\[ \overline{\gamma}_k = \sum_{\langle ij \rangle} t_{il}^{pd} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \overline{\gamma}_{il} \]

and

\[ \overline{\gamma}_{il} = \langle n_{i\sigma}^d d_{il\sigma} + n_{i\sigma}^d d_{il\sigma} \rangle \].

The correlation function \( \overline{\gamma}_k \) gives the gap of the superconductor state in the \( d \)-wave case.

The elements of the normalization matrix \( N_5 \) are given from Eq. (4) as:

\[ N_{11} = N_{33} = N_{55} = 1 \]

and

\[ N_{12} = N_{21} = N_{34} = N_{43} = N_{44} = n_{-\sigma}^d. \]

The remaining elements of the normalization matrix \( N_5 \), due to the \( d \)-wave symmetry and the anticommutation rules, have been found to be zero.
Using the energy and the normalization matrices $E_5$ and $N_5$, respectively, the matrix Green’s function $G_5$ defined in Eq. (10) can be obtained. For simplicity, only the most relevant elements (for the purposes of this work) of this $(5 \times 5)$ $G_5$ matrix are shown. Following the Roth’s notation [9], the correlation function $(BA)$ is related to the Green’s function $\langle \langle A; B \rangle \rangle_\omega$ as:

$$\langle BA \rangle = \mathcal{F}_\omega \langle \langle A; B \rangle \rangle_\omega \frac{1}{2\pi i} \oint d\omega f(\omega) \langle \langle A; B \rangle \rangle_\omega,$$  \hspace{1cm} (24)

where $f(\omega)$ is the Fermi function. The chemical potential $\mu$ is obtained in the standard way, using the element $G_{5\sigma}^{11}$ of the matrix $G_5$ and the relation given in Eq. (24). The matrix element $G_{5\sigma}^{11}$ is given by

$$G_{5\sigma}^{11}(\omega) = \frac{(\omega - E_{55})[A(\omega) - (\omega + E_{11})\mathcal{U}^{-2}]}{\mathcal{D}(\omega)},$$  \hspace{1cm} (25)

where $E_{11}$ and $E_{55}$ are elements of the energy matrix $E_5$, defined in Eq. (12). In Eq. (25), it is also necessary to introduce the following definitions:

$$A(\omega) = (n^{d}_{\sigma})(1 - n^{d}_{\sigma})^2 \times (\omega^3 + \alpha(1)\omega^2 + \alpha(2)\omega + \alpha(3))$$  \hspace{1cm} (26)

with

$$\alpha(1) = E_{11},$$

$$\alpha(2) = Z_{k\sigma}^{(1)}Z_{k\sigma}^{(2)} - (Z_{k\sigma}^{(1)} + Z_{k\sigma}^{(2)})(Z_{k\sigma}^{(1)} + Z_{k\sigma}^{(2)} - E_{11}),$$

and

$$\alpha(3) = -Z_{k\sigma}^{(1)}Z_{k\sigma}^{(2)}(Z_{k\sigma}^{(1)} + Z_{k\sigma}^{(2)} - E_{11}).$$

The quantities $Z_{k\sigma}^{(1)}$ and $Z_{k\sigma}^{(2)}$ are defined as

$$Z_{k\sigma}^{(1)} = \frac{U + 2(\varepsilon_d - \mu) + \varepsilon_d^2 + W_{k-\sigma}}{2} - \Delta_{k\sigma},$$

and

$$Z_{k\sigma}^{(2)} = Z_{k\sigma}^{(1)} + \Delta_{k\sigma}.$$

In the particular case, when $\varepsilon_d$, $\gamma_k$ and $t_{ij}^{pd}$ are zero, $Z_{k\sigma}^{(1)}$ and $Z_{k\sigma}^{(2)}$ represent the quasi-particle bands in the paramagnetic normal state of the one-band Hubbard model. The term $\Delta_{k\sigma}$ is given by:

$$\Delta_{k\sigma} = \sqrt{(U + W_{k-\sigma} - \varepsilon_d^2 + 4n^{d\sigma}_{\sigma}U(\varepsilon_d - W_{k-\sigma})}$$  \hspace{1cm} (32)

where $W_{k-\sigma}$ is the Fourier transform of $W_{ij-\sigma}$ given in Eq. (10). The denominator of the Green’s function $G_{5\sigma}^{11}$ given in Eq. (24) is defined as:

$$\mathcal{D}(\omega) = (\omega - E_{55})\mathcal{D}(\omega) - V_{k\sigma}^{dpd}V_{k\sigma}^{dpd} [A(\omega) - (\omega + E_{11})\mathcal{U}^{-2}].$$  \hspace{1cm} (33)

where

$$D(\omega) = \mathcal{D}(\omega) - \gamma_k^2(\omega^2 - E_{11}^2)$$  \hspace{1cm} (34)

with

$$\mathcal{D}(\omega) = \{[\omega - E_{11}](\omega - E_{22}) - (\omega n^{d\sigma} - E_{12})^2\} \times\{[\omega + E_{11}](\omega n^{d\sigma} + E_{22}) - (\omega n^{d\sigma} + E_{12})^2\}.$$  \hspace{1cm} (35)

In Eq. (35), $E_{12}$ and $E_{22}$ are elements of the energy matrix $E_2$ given in Eq. (14). The use of a set of five operators $A_n$ results in a five-pole approximation to the Green’s functions. Then, the $\mathcal{D}(\omega)$ defined in Eq. (35) may be also written as:

$$\mathcal{D}(\omega) = (n^{d\sigma})^2(1 - n^{d\sigma})^2(\omega - E_{1k})(\omega - E_{2k})(\omega - E_{3k}) \times(\omega - E_{4k})(\omega - E_{5k})$$  \hspace{1cm} (36)

where the quasi-particle bands $E_{pk}$ (with $p = 1, \ldots, 5$) satisfy $\mathcal{D} = det(\omega N_5 - E_5) = 0$. Therefore, the resulting Green’s function can be written as a sum of five terms:

$$G_{5\sigma}^{11}(\omega) = \sum_{s=1}^{5} \frac{Z_{pk\sigma}}{\omega - E_{pk\sigma}}$$  \hspace{1cm} (37)

where $Z_{pk\sigma}$ express the spectral weights which satisfy

$$Z_{1k\sigma} + Z_{2k\sigma} + Z_{3k\sigma} + Z_{4k\sigma} + Z_{5k\sigma} = 1.$$  \hspace{1cm} (38)

3 Calculation of the gap function using the factorization procedure

In the case of $d$-wave symmetry, the traditional correlation function $\langle d_{i-\sigma}d_{i\sigma}\rangle$ is always zero. Therefore, this correlation function can not be used to determinate the pairing gap in the $d$-wave channel [8, 18]. In the factorization procedure proposed by Beenen and Edwars in Ref. 8, the correlation function given by Eq. (21) is rewritten as

$$\bar{\tau}_{il} = \frac{d_{i-\sigma}d_{i\sigma}}{\langle d_{i-\sigma}d_{i\sigma} \rangle}$$  \hspace{1cm} (39)

where the symmetry $\bar{\tau}_{il} = \bar{\tau}_{li}$ is conserved, and the products $d_{il}d_{l\sigma}$ and $d_{i\sigma}d_{il}$ are split up. It is also introduced

$$n^{d\sigma}_{01\sigma} = \langle d_{i-\sigma}d_{i\sigma} \rangle = \langle d_{i\sigma}d_{i\sigma} \rangle$$  \hspace{1cm} (40)

which allows to rewrite Eq. (39) as

$$\bar{\tau}_{il} = 2n^{d\sigma}_{01\sigma}d_{i-\sigma}d_{i\sigma}$$  \hspace{1cm} (41)

where $n^{d\sigma}_{01\sigma}$ can be calculated from $G_{k\sigma}^{11}$.

Considering the $d$-wave symmetry, the Fourier transform of $\bar{\tau}_{il}$ given by Eq. (21) becomes

$$\bar{\tau}_k = \bar{\tau} \cos(k_xa) - \cos(k_ya).$$  \hspace{1cm} (42)
where
\[ \gamma = 2 \nu \bar{\gamma} \] (43)
is the gap-function amplitude. Due to the \( d \)-wave symmetry, \( \bar{\gamma}_t = +\bar{\gamma} \) for \( \vec{R}_t - \vec{R}_0 \) in the \( x \) direction and \( \bar{\gamma}_y = -\bar{\gamma} \) when \( \vec{R}_y - \vec{R}_0 \) is in the \( y \) direction. The Fourier transform of the correlation function \( \langle d_{i\sigma}d_{j\sigma} \rangle \) is given by
\[ \langle d_{i\sigma}d_{j\sigma} \rangle = \frac{1}{L} \sum_k c e^{i\vec{k} \cdot \vec{R}_0} \langle d_{k\sigma}d_{k\sigma} \rangle \] (44)
where \( L \) is the number of sites in the system. The correlation function \( \langle d_{k\sigma}d_{k\sigma} \rangle \) can be evaluated using the Green’s function \( G_{k\sigma}^{13} \) and the relation given by Eq. (44).

The Green’s function \( G_{k\sigma}^{13} \) can be rewritten as:
\[ G_{k\sigma}^{13}(\omega) = -\bar{\gamma}_k U^2 F_{k\sigma}^{13} \] (45)
where
\[ F_{k\sigma}^{13}(\omega) = (n_{d,\sigma}^d)^2 (1 - n_{d,\sigma}^d)^2 (\omega - E_{55}) B(\omega) D(\omega) \] (46)
and \( B(\omega) \) is defined in Eq. (33).

Combining the equation (20) with the Eqs. (34) to (36), the gap equation can be written as:
\[ \bar{\gamma}_k = -\bar{\gamma}_k 2n_{d,\sigma}^d U^2 I_\sigma \] (47)
where
\[ I_\sigma = \frac{1}{2\pi i} \int \phi(\omega) F_{\sigma}(\omega) d\omega \] (48)
with
\[ F_{\sigma}(\omega) = \frac{1}{L} \sum_q \left[ \cos (\bar{q}_\sigma a) - \cos (\bar{q}_\sigma a) \right] F_{\sigma}^{13}(\omega) \] (49)

4 Definition and calculation of the band shifts

Using the definition (17) in Eq. (18), the band shift \( W_{ij\sigma} \) can be written as:
\[ W_{ij\sigma} = W_{ij\sigma}^d + W_{ij\sigma}^{pd} \] (50)
where
\[ W_{ij\sigma}^d = \frac{t_{ij}^d (n_{i-\sigma}^d n_{j\sigma}^d) - (n_{d,\sigma}^d)^2}{n_{d,\sigma}^d (1 - n_{d,\sigma}^d)} \] (51)
and
\[ W_{ij\sigma}^{pd} = \frac{\Lambda_{ij\sigma}^{pd}}{n_{d,\sigma}^d (1 - n_{d,\sigma}^d)}. \] (52)
The quantity \( \Lambda_{ij\sigma}^{pd} \) is given by Eq. (15). The correlation function \( \langle p_{i-\sigma}^d d_{j\sigma} \rangle \) present in \( \Lambda_{ij\sigma}^{pd} \) can be obtained from de Green’s function
\[ G_{k\sigma}^{15}(\omega) = \left[ A(\omega) - (\omega + E_{11}) \bar{\gamma}_k^2 \right] V_{k\sigma}^{pd} \frac{1}{D(\omega)}. \] (53)
The remaining correlation function \( \langle p_{i-\sigma}^d n_{i\sigma}^d d_{i-\sigma} \rangle \) present in \( \Lambda_{ij\sigma}^{pd} \) is calculated from the Green’s function
\[ G_{k\sigma}^{25}(\omega) = \frac{n_{d,\sigma}^d B(\omega) - (\omega + E_{11}) \bar{\gamma}_k^2 V_{k\sigma}^{pd}}{D(\omega)}. \] (54)
where
\[ B(\omega) = A(\omega) + n_{d,\sigma}^d (1 - n_{d,\sigma}^d)^2 U D_1(\omega) \] (55)
with \( A(\omega) \) defined in Eq. (20). The quantity \( D_1(\omega) \), in terms of the elements of the energy matrix (43), is given by:
\[ D_1(\omega) = (\omega - E_{11})(\omega n_{d,\sigma}^d - E_{22}) - (\omega n_{d,\sigma}^d - E_{12})^2. \] (56)

The Green’s function \( G_{k\sigma}^{25} \) tends to zero as \( U \to \infty \), consequently, the correlation function \( \langle p_{i-\sigma}^d n_{i\sigma}^d d_{i-\sigma} \rangle \) also vanishes recovering the result of Ref. [3] for \( \Lambda_{ij\sigma}^{pd} \). The quantity \( \Lambda_{ij\sigma} \) present in Eq. (51) is given by Eq. (15). The Fourier transform of \( W_{ij\sigma}^d \) is given by:
\[ W_{k\sigma}^d = \sum_{(j)} e^{i\vec{k} \cdot \vec{R}_0} W_{ij\sigma}^d. \] (57)
Substituting Eq. (15) into Eq. (57) and then putting the result into Eq. (57), the Fourier transform of \( W_{ij\sigma}^d \) can be written as:
\[ W_{k\sigma}^d = -\frac{1}{n_{d,\sigma}^d (1 - n_{d,\sigma}^d)} \sum_{j \neq 0} t_{ij}^d (n_{j-\sigma}^d n_{0\sigma}^d - (1 - n_{d,\sigma}^d) (1 - n_{d,\sigma}^d) (1 - n_{d,\sigma}^d) (1 - n_{d,\sigma}^d) \sum_{j \neq 0} t_{ij}^d e^{i\vec{k} \cdot \vec{R}_0} \left[ (n_{j-\sigma}^d n_{0\sigma}^d) - (n_{0\sigma}^d)^2 \right] \right. \]
\[ + \left. (n_{j-\sigma}^d n_{0\sigma}^d - (n_{0\sigma}^d)^2) \right) \] (58)

The correlation functions present in \( W_{ij\sigma}^d \) are evaluated following the original Roth’s procedure [3]. Introducing extra operators \( B_{ij\sigma} \), the correlation functions of the form \( \langle B_{ij\sigma} \rangle \) can be calculated by using Eqs. (9) and (24). In Refs. [3,4], the sum present in Eq. (9) has been considered only over the operators which describe the normal state of the system. In the present work, the sum includes also the hole operators which describe the superconducting properties of the system. Thus, \( W_{k\sigma}^{pd} \) is given by:
\[ n_{d,\sigma}^d (1 - n_{d,\sigma}^d) W_{k\sigma}^{pd} = h_{1\sigma} + \sum_{j \neq 0} t_{ij}^d e^{i\vec{k} \cdot \vec{R}_0} (h_{2\sigma} + h_{3\sigma} - (h_{2\sigma} + h_{3\sigma}) \] (59)
where the term \( h_{3\sigma} \) is directly related to the gap function \( \bar{\gamma}_k \) through the Green’s functions \( G_{k\sigma}^{13} \) and \( G_{k\sigma}^{14} \) (see Appendix A). The quantities \( h_{1\sigma}, h_{2\sigma}, h_{3\sigma} \) and \( h_{3\sigma} \) are given in Appendix A.
In this section, the numerical results obtained in this work are presented. One of the most important parameters of the model given in Eq. (14) is the $d-p$ hybridization $\Gamma_{k}$, which is defined as

$$W_{d}^{dp} = -iV_{d}^{dp}[\sin(k_{x}a) - \sin(k_{y}a)].$$  \hspace{1cm} (60)

In this work, as in Ref. [20], the hybridization has been assumed $\vec{k}$-independent $(V_{d}^{dp})^{2} = (\langle V_{d}^{dp} \rangle)^{2}$, where $\langle \cdots \rangle$ is the average over the Brillouin zone. The quasi-particle bands are presented. One of the most important parameters of $\vec{k}$-independent hybridization due to the fact that the pairs occur within a small energy interval around the Fermi level, therefore the dispersion of the hybridization can be neglected.

The total occupation number is given by $n_{T} = n_{d}^{d} + n_{-d}$, where $n_{d}^{d}$ is obtained combining $G_{k\sigma}^{14}$ (Eq. (24)) and the relation given in Ref. [21]. The charge transfer energy $\Delta = \epsilon_{d} - \epsilon_{d}$ is positive. This means that the first hole added to the system will energetically prefer to occupy the $d$-orbital of the copper ions $\bar{H}$. All results presented in this section are obtained with $\epsilon_{d} = 0$ and $\epsilon_{p} = 3.6eV$. Consequently, $\Delta = 3.6eV$, as estimated in Ref. [21].

As discussed in Refs. [8, 9], the band shift $W_{k\sigma}$ (see Eq. (59)) can be evaluated considering different approximations. In the limit $U \rightarrow \infty$, some terms of the band shift vanish (see Ref. [9]). In Ref. [14], the present authors estimate $W_{k\sigma}$ in the limit of $U \rightarrow \infty$, but with finite $U$ in other parts of the problem. In Ref. [8], Beenen and Edwards evaluated $W_{k\sigma}$ in the normal state (where $\tau_{k} = 0$) and considering $T$ equal to zero and finite $U$ using the one-band Hubbard model (hybridization null). In the present work, the correlation functions present in $W_{k\sigma}$ given in Eq. (55) are evaluated following closely the procedure used by Roth in Ref. [9]. Nevertheless, here, also the hole operators given in the set of Eq. (12) are used to evaluate the correlation functions. As consequence, a new term $(h_{3j}\sigma)$ appears in $W_{k\sigma}$ (see Eq. (55)). The approximations used to evaluate $W_{k\sigma}$ are shown in Table I. In figure (a), the quasi-particle bands $E_{pk}$, with $p = 1.5$ (see Eq. (36)), are plotted along the symmetry lines $(0,0) - (\pi,0) - (\pi,\pi) - (0,0)$, in the two-dimensional Brillouin zone. The quasi-particle energies $E_{pk}$, in the superconducting state, are relative to the chemical potential $\mu$. The circles $bf$ show the $\epsilon_{k}^{p}$ band, where the center of $\epsilon_{k}^{p}$ is shifted by $\epsilon_{p} = 3.6eV$ relative to the zero of energy. All results shown in this paper are obtained with $_p = 2t_{d}^{\prime}$. The dashed line corresponds to the noninteracting $(U = 0)$ band $\epsilon_{k}^{d}$ relative to the noninteracting chemical potential. The figure (b) shows the superconducting gap between the electron and hole bands in the neighborhood of the $(\pi,0)$ point, while on the $k_{x} = k_{y}$ diagonal (Fig. (a)) the gap is zero. This fact reflects the $d$-wave symmetry proposed in this work. The dashed lines show the absence of the gap in the normal state. In figure (c), the region near to the $(\pi,\pi)$ point shows the gaps produced by the $d-p$ hybridization $V_{d}^{pp}$. The dashed lines show the result for $V_{d}^{pp} = 0$. In figure (d) the electron and hole quasi-particle bands are shown for two different values of hybridization. As can be observed, the hybridization shifts the quasi-particle bands to lower energy by breaking the symmetry.
Figure 2: The electron and hole bands in the region close to the \((\pi, 0)\) point for \(U = 12|t^d|\) and \(n_T = 0.76\). The solid lines correspond to \(V_0^{pd} = 0.0\), while the dashed lines show the result for \(V_0^{pd} = 0.3|t^d|\), in relation to the \(\vec{k}\) axis.

The figure 3 shows the spectral weights \(Z_{p\vec{k}\sigma}\) for two different hybridizations. The dashed line corresponds to the sum of the five spectral weights which is equal to one (see Eq. \ref{eq:Zp}). In figure 3(b), the effects of the hybridization on the spectral weights are shown. Such effects cause a small change in the chemical potential and consequently in the superconductivity.

The figure 4 shows the behavior of gap function amplitude \(\mathcal{F}\) as a function of the hybridization \(V_0^{pd}\). It is clear that there is a decreasing of \(\mathcal{F}\) with increasing \(V_0^{pd}\).

The analysis of the function \(F_\sigma(\omega)\) introduced in Eq. \ref{eq:Fsigma} and defined in Eq. \ref{eq:FsigmaDef} is important to understand the behavior of the gap function amplitude showed in figure 4. The figure 5 shows the function \(F_\sigma(\omega)\) for \(T = 0\) and two different values of hybridization. As can be seen in the dashed line, the magnitude of the function \(F_\sigma(\omega)\) decreases when the hybridization is enhanced. Moreover, the function is shifted to lower energy, breaking the symmetry with respect to \(\omega = 0\). The symmetry break has been also observed in figure 2 for the electron and hole quasi-particle bands. For \(T = 0\), the product \(f(\omega)F_\sigma(\omega)\) given in Eq. \ref{eq:Fsigma} vanishes when \(\omega > 0\). That is because the Fermi function \(f(\omega)\) is zero for that range of \(\omega\). As consequence of the shift and the suppression of \(F_\sigma(\omega)\), the value of \(I_\sigma\), which is given by the integral in Eq. \ref{eq:ISigma}, decreases when the hybridization increase. However, from Eq. \ref{eq:ISigma}, it is necessary a minimum value for \(I_\sigma\) to obtain a nonzero solution for \(\mathcal{F}\). But, for very strong values of hybridization, the minimum value for \(I_\sigma\) is not reached and only the zero solution exists.

According to this analysis, there is a critical value of hybridization \((V_0^{pd})\), above which, the superconductivity is suppressed. Similar results, which show a critical value for the hybridization, were also obtained in Ref. \ref{ref:20}, for a \(\vec{k}\)-dependent hybridization and using the Hartree-Fock approximation for the electron-electron interaction. In Refs. \ref{ref:16, 21}, although the high \(T_c\) was not considered, the hybridization effects play an important role for resonant states. The discussion above is also valid if the values of the temperature \(T\) are raised with \(V_0^{pd}\) constant. The only difference is that in this case the Fermi function becomes sloping smoothly, changing the product \(f(\omega)F_\sigma(\omega)\). The effect of the temperature in the Fermi function causes a decreasing of \(I_\sigma\) and consequently of \(T_c\).

Since the hybridization is directly related to the applied pressure \(\Pi\), the transition temperature \(T_c\) may have a dependence on pressure through the hybridization. However, the pressure dependence of \(T_c\) is very complicated in high temperature superconductors. As discussed in Ref. \ref{ref:16}, at least, in conventional superconductivity where the electron pairing is mediated by phonons, two effects are responsible for the pressure dependence of \(T_c\). The first one is related to the lattice vibrations, while the second one comes from the electronic contribution. As long the pressure is increased, the lattice vibrations tend to increase \(T_c\), whereas the effects of the electronic contribution associated with the hybridization cause a decreases of \(T_c\).
The figure 6 shows the function amplitude $\mathcal{F}$ as a function of temperature $T$, for $U = 12|t^d|$, $n_T = 0.76$ and several values of hybridization. ($t^p = -0.5eV$.) The dashed lines correspond to the results obtained in Ref. [12], where the band shift has been evaluated considering $T = 0$, $\mathcal{T}_k = 0$ and $U \to \infty$ (see table 1). The difference between the results can be explained by the analysis of the Eq. [15], where some of the correlation functions present in the band shift vanish in the $U \to \infty$ limit. In Eq. [18], the correlation function $\langle \hat{p}^\dagger_{\vec{k},\sigma} n^d_{\sigma\sigma} \hat{d}^\dagger_{\vec{k},-\sigma} \rangle$, which is directly related to the hybridization effects in the band shift, vanishes for $U \to \infty$. It is important to highlight that the correlation functions in Eq. [15] are both negative. Therefore, for large $U$, the correlation function $\langle \hat{p}^\dagger_{\vec{k},\sigma} n^d_{\sigma\sigma} \hat{d}^\dagger_{\vec{k},-\sigma} \rangle$ decreases and the hybridized shift $W^d_{\vec{k},\sigma}$ is enhanced. However, for intermediate values of $U$, both correlation functions remain finite. As consequence, the hybridization effects in the band shift and, therefore, in the superconductivity, are weakened. The figures [7] (c)-(d) show the present results when the value of $U$ is increased.

The main consequence is, within the factorization procedure, to shift the window of doping where superconductivity is found, as in Ref. [8].

In figure 8(a), the chemical potential is show as a function of the total occupation number $n_T$ for $U = 12|t^d|$ and two different hybridizations. In Ref. [21], the authors criticized the Roth’s method because the compressibility $k = \frac{\partial \mu}{\partial n}$ is negative in the vicinity of half-filling in the Beenen and Edwards result. In Ref. [18], by using a composite operator approach and imposing the Pauli principle, the authors have showed that the compressibility remains negative. However, they also showed that the pairing decreases the strength of the negative compressibility.

In the present work, a careful study about the nature of the negative compressibility and the effect of the hybridization near half-filling in Roth’s approximation has been carried out. It has been verified that the most im-
important contribution to provide negative compressibility comes from the spin-term \( \langle S_j S_i \rangle \) present in the \( d \)-part \( W_{d}^\mu \) of the Roth’s band shift \( W_{k\sigma} \) (see Eqs. A.34 and A.35). In reference [8], it has been showed that the correlation function \( \langle S_j S_i \rangle \) plays an important role on the flattening of the quasi-particle bands. The correlation function \( \langle S_j S_i \rangle \) increases with occupation and its effect is pronounced near half-filling. Nevertheless, when the hybridization is present, the numerical results show that it acts in the sense of suppressing the negative compressibility near half-filling. Because the hybridization considered here is \( k \)-independent [20], the hybridization term \( W_{\sigma}^{d} \) of the band shift is constant within the Brillouin zone. Its main effect is to shift the poles of the Green’s functions and consequently to change the value of the chemical potential suppressing the negative compressibility. In figure 6(a), it is clear that the effect of the hybridization in the chemical potential decreases the negative compressibility.

The figure 6(b) shows the gap function amplitude \( \bar{\gamma} \) as a function of the total occupation number. This result agrees with those obtained in figure 4 where \( \bar{\gamma} \) decreases with increasing of \( V_{0}^{d} \).

6 Conclusions

In this work, the Roth’s two-pole approximation is extended to study the superconducting properties of the extended Hubbard model given in Eq. (11). The quality of the Roth’s two-pole approximation had been investigated in a previous work by Beenen and Edwards [5]. In their work, they showed the remarkable agreement between the Roth’s and the Monte Carlo results [6, 7] for the one-band Hubbard model in the paramagnetic normal state. Moreover, the flat bands obtained with Roth’s procedure show a qualitative agreement with the ARPES experiment data [9] in cuprates. It is important to point out that the flattening observed in the quasi-particle bands which produces a peak in the density of states, can be connected with the Van Hove scenario. In cuprate systems the Van Hove singularity is present in the vicinity of the Fermi energy. Therefore, it is believed that the Van Hove scenario play a fundamental role in order to clarify the mechanism which drives the transition to superconductivity in these interesting materials [23].

The accuracy of the Roth’s results is very related to the adequate evaluation of the band shift. Therefore, the focus of the present work has been to evaluate the Roth’s band shift taking into account relevant effects as Coulomb interaction, temperature, superconductivity and hybridization. Also, the effect of the hybridization in the superconducting of the model has been studied. This work has been carried...
out following the factorization procedure proposed by Beenens and Edwards [8]. In order to study superconductivity, Beenen and Edwards proposed to include hole operators in the original set of operators that describes the normal state of the system. These operators can introduce the pairing formation in the d-band. The factorization procedure proposed by Beenen and Edwards [8] and the d-wave symmetry are considered to obtain the gap function amplitude. The hybridization effects are considered by also including a $p$-operator. Thus, the set of operators is enlarged to five, which results in a five-pole approximation to the Green’s functions.

The hybridization effects present in the band shift come from some correlation functions. The important point is that part of them vanish when $U \to \infty$, as it have been done in Ref. [14]. In order to consider properly the hybridization effects, the band shift should be obtained for finite $U$. In fact, the obtained phase diagrams show that the presence of superconducting order exists in a larger range of doping when compared with the $U \to \infty$ limit [14], for the same hybridization. Therefore, this result suggests that, in the $U \to \infty$ limit, the hybridization effects are overestimated. That is the ultimate justification for the use of the factorization procedure [8], which is valid for intermediated values of $U$ for the gap function.

The Beenen and Edwards’s [8] results are recovered taking $V_{pd}^0 = 0$ in the present work. The hybridization $V_{pd}^0$ breaks the symmetry between the electron and hole quasi-particle bands, respect to $\vec{k}$ axis. Also, the gap amplitude function $\overline{g}$ and the critical temperature $T_c$ are suppressed with increasing the hybridization $V_{pd}^0$. The results show that the chemical potential does not change significantly away the half-filling. However, near half-filling, it is showed that the negative compressibility decreases with increasing $V_{pd}^0$. The correlation functions present in the $d$-part of the band shift $W_{d\sigma}$ were discussed in detail. When the hole operators are also considered to obtain this correlation functions, a new term appears in the $d$-part of the band shift $W_{d\sigma}$. The new term is directly associated with the superconducting properties of the system. Nevertheless, this term is quite small and therefore may be disregarding in the calculation of the band shift.

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A Appendix

The correlation functions present in the band shift $W_{k\sigma}^d$ can be evaluated by introducing extra $B$ operators, as in the original Roth’s procedure. Combining the Eq. (2) and the relation given in Eq. (24), it is possible to write

$$\langle BA_n \rangle = F_\omega \sum_m \bar{G}_{nm}(\omega) \langle [A_m, B]_{(+)} \rangle,$$  \hspace{1cm} (A.1)

where $A_n$ and $A_m$ are members of the set of operators given in Eq. (12). For evaluate $\langle n_{d\sigma}^d n_{0\sigma}^\dagger \rangle - \langle n_{0\sigma}^d \rangle^2$, it has been necessary to introduce the following $B$ operators:

$$B_{k\sigma}^{(1)} = \frac{1}{\sqrt{L}} \sum_{l} e^{-i\vec{k} \cdot \vec{R}_l} n_{l+\sigma}^d a_{l\sigma}^d$$  \hspace{1cm} (A.2)

and

$$B_{k\sigma}^{(2)} = \frac{1}{\sqrt{L}} \sum_{l} e^{-i\vec{k} \cdot \vec{R}_l} n_{l+\sigma}^d a_{l\sigma}.$$  \hspace{1cm} (A.3)

By considering the operator given in the Eq. (A.2), the correlation function $\langle n_{d\sigma}^d n_{0\sigma}^\dagger \rangle$ can be written as:

$$\langle n_{d\sigma}^d n_{0\sigma}^\dagger \rangle = \frac{1}{L} \sum_k \langle B_{k\sigma}^{(1)} d_{k\sigma}^d \rangle \tag{A.4}$$

where the right side of Eq. (A.4) may be obtained using the relation given by Eq. (A.1). Therefore, it is necessary to evaluate the anticommutators $[A_m, B_{k\sigma}^{(1)}_{(+)}]$ for the set of operators $A_m$ given in Eq. (12). For $m = 1..5$, the $A$ operators are given by:

$$A_{1k\sigma} = \frac{1}{\sqrt{L}} \sum_{l} e^{i\vec{k} \cdot \vec{R}_l} d_{l\sigma}, \tag{A.5}$$

$$A_{2k\sigma} = \frac{1}{\sqrt{L}} \sum_{l} e^{i\vec{k} \cdot \vec{R}_l} n_{l-\sigma}^d d_{l\sigma}, \tag{A.6}$$

$$A_{3k\sigma} = \frac{1}{\sqrt{L}} \sum_{l} e^{i\vec{k} \cdot \vec{R}_l} d_{l-\sigma}, \tag{A.7}$$

$$A_{4k\sigma} = \frac{1}{\sqrt{L}} \sum_{l} e^{i\vec{k} \cdot \vec{R}_l} n_{l+\sigma}^d d_{l-\sigma}, \tag{A.8}$$

and

$$A_{5k\sigma} = \frac{1}{\sqrt{L}} \sum_{l} e^{i\vec{k} \cdot \vec{R}_l} p_{l\sigma}. \tag{A.9}$$

Thus, the following results have been obtained

$$\langle [A_{1k\sigma}, B_{k\sigma}^{(1)}_{(+)}] \rangle = n_{0\sigma}^d - e^{i\vec{k} \cdot \vec{R}_j} \langle d_{j\sigma}^d d_{j\sigma} \rangle, \tag{A.10}$$

$$\langle [A_{2k\sigma}, B_{k\sigma}^{(1)}_{(+)}] \rangle = (n_{0-\sigma}^d n_{0+\sigma}^d) - e^{i\vec{k} \cdot \vec{R}_j} \langle d_{0\sigma}^d n_{j-\sigma}^d d_{j\sigma}^d \rangle, \tag{A.11}$$

$$\langle [A_{3k\sigma}, B_{k\sigma}^{(1)}_{(+)}] \rangle = 0. \tag{A.12}$$
\begin{align}
\langle A_{4\tilde{\kappa}, \sigma} B_{k\sigma}^{(1)} \rangle &= -\langle n^d_{0\sigma} d_{0\sigma} d_{0\sigma} \rangle, \quad \text{(A.13)} \\
\langle A_{4\tilde{\kappa}, \sigma} B_{k\sigma}^{(1)} \rangle &= 0 \quad \text{(A.14)}
\end{align}

where, it has been assumed that the brackets are real and unchanged when the indices 0 and \( j \) are interchanged. Also, due to translational invariance of the system, \( n^0_{0\sigma} = n^d_{0\sigma} \). Considering the relations given by Eqs. (A.1) and (A.4) with the results from Eq. (A.10) to Eq. (A.14), the correlation function \( \langle n^d_{0\sigma} n^d_{0\sigma} \rangle \) can be written as:

\begin{equation}
\langle n^d_{0\sigma} n^d_{0\sigma} \rangle = \alpha_\sigma n^d_{0\sigma} - \beta_\sigma n^d_{0\sigma} + \alpha_\sigma n^d_{0\sigma} - \beta_\sigma m_{j\sigma} + \beta_\sigma (n^d_{0\sigma} d_{0\sigma} d_{0\sigma}) \quad \text{(A.15)}
\end{equation}

where \( n^0_{0\sigma} = n^d_{0\sigma} \). In Eq. (A.15), it has been introduced the following definitions:

\begin{equation}
n^d_{0j\sigma} = \langle d_{0\sigma}^d d_{0\sigma} \rangle = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{11}^{12} \mathcal{R}_j, \quad \text{(A.16)}
\end{equation}

\begin{equation}
m_{j\sigma} = \langle d_{0\sigma}^d d_{0\sigma} d_{0\sigma} \rangle = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{12}^{12} \mathcal{R}_j, \quad \text{(A.17)}
\end{equation}

\begin{equation}
\alpha_\sigma = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{11}^{12} \mathcal{R}_j, \quad \text{(A.18)}
\end{equation}

\begin{equation}
\beta_\sigma = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{12}^{12} \mathcal{R}_j, \quad \text{(A.19)}
\end{equation}

and

\begin{equation}
\beta^{(1)}_\sigma = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{0}^{14} \mathcal{R}_j, \quad \text{(A.20)}
\end{equation}

where \( G_{11}^{12} \) is given in Eq. (20). The remaining Green’s functions \( G_{12}^{12} \) and \( G_{14}^{14} \) are given respectively by

\begin{equation}
G_{12}^{12}(\omega) = \frac{n^d_{0\sigma} (\omega - E_{55}) [B(\omega) - (\omega + E_{11}) \mathcal{T}']}{\mathcal{D}(\omega)}, \quad \text{(A.21)}
\end{equation}

and

\begin{equation}
G_{14}^{14}(\omega) = \langle n^d_{0\sigma} (1 - n^d_{0\sigma})^2 U \mathcal{T} \rangle_k \times \frac{(\omega - E_{55}) (\omega + E_{11} - U n^d_{0\sigma})}{\mathcal{D}(\omega)}, \quad \text{(A.22)}
\end{equation}

where \( B(\omega) \) is defined in Eq. (55) and \( \mathcal{D}(\omega) \) in Eq. (30). It is also necessary to define

\begin{equation}
\tilde{G}_{12}^{12}(\omega) = \frac{G_{11}^{12}(\omega) - G_{12}^{12}(\omega)}{1 - n^d_{0\sigma}}, \quad \text{(A.23)}
\end{equation}

\begin{equation}
\tilde{G}_{14}^{12}(\omega) = \frac{G_{12}^{12}(\omega) - n^d_{0\sigma} G_{11}^{12}(\omega)}{n^d_{0\sigma} (1 - n^d_{0\sigma})}, \quad \text{(A.24)}
\end{equation}

and

\begin{equation}
\tilde{G}_{14}^{14}(\omega) = \frac{G_{14}^{14}(\omega) - n^d_{0\sigma} G_{12}^{14}(\omega)}{n^d_{0\sigma} (1 - n^d_{0\sigma})}. \quad \text{(A.25)}
\end{equation}

where \( G_{12}^{13} \) is given in Eq. (15).

The correlation function \( \langle n^d_{0\sigma} n^d_{0\sigma} \rangle \) present in Eq. (A.16), can be obtained by repeating the procedure above using the operator \( B_{k\sigma}^{(2)} \) (given by Eq. (A.3)). Thus,

\begin{equation}
\langle n^d_{0\sigma} n^d_{0\sigma} \rangle = \alpha_\sigma n^d_{0\sigma} + \beta_\sigma n^d_{0\sigma} + \alpha_\sigma n^d_{0\sigma} - \beta_\sigma m_{j\sigma} + \beta^{(1)}_\sigma (n^d_{0\sigma} d_{0\sigma} d_{0\sigma}) \quad \text{(A.26)}
\end{equation}

where

\begin{equation}
\langle n^d_{0\sigma} \rangle = \langle d_{0\sigma} d_{0\sigma} \rangle = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{13}^{13} \mathcal{R}_j, \quad \text{(A.27)}
\end{equation}

\begin{equation}
m_{j\sigma} = \langle d_{0\sigma} d_{0\sigma} d_{0\sigma} \rangle = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{14}^{14} \mathcal{R}_j, \quad \text{(A.28)}
\end{equation}

and

\begin{equation}
\alpha^{(1)}_\sigma = \frac{1}{L} \sum_k \mathcal{F}_\omega G_{13}^{12} \mathcal{R}_j \quad \text{(A.29)}
\end{equation}

with

\begin{equation}
\tilde{G}_{12}^{13}(\omega) = \frac{G_{12}^{13}(\omega) - G_{14}^{14}(\omega)}{1 - n^d_{0\sigma}}. \quad \text{(A.30)}
\end{equation}

Reversing the spin labels i.e., \( \sigma \rightarrow -\sigma \) in Eq. (A.26) and substituting the result into Eq. (A.18), then

\begin{equation}
\langle n^d_{j\sigma} n^d_{0\sigma} \rangle = \alpha_\sigma n^d_{0\sigma} - \alpha_\sigma n^d_{j\sigma} + \beta_\sigma \alpha_\sigma n^d_{0\sigma} - \beta_\sigma m_{j\sigma} + \beta^{(1)}_\sigma (n^d_{j\sigma} d_{0\sigma} d_{0\sigma}) \quad \text{(A.31)}
\end{equation}

For the evaluation of the last two correlation functions present in Eq. (38), the following operators have been introduced

\begin{equation}
B_{k\sigma}^{(3)} = \frac{1}{\sqrt{L}} \sum_i e^{-i \mathcal{R}_i} \mathcal{R}_i^{t_{i+j\sigma}} d^{t_{i+j\sigma}} d^{t_{i-j\sigma}} d^{t_{i-j\sigma}} \quad \text{(A.32)}
\end{equation}

and

\begin{equation}
B_{k\sigma}^{(4)} = \frac{1}{\sqrt{L}} \sum_i e^{-i \mathcal{R}_i} \mathcal{R}_i^{t_{i+j\sigma}} d^{t_{i+j\sigma}} d^{t_{i-j\sigma}} d^{t_{i-j\sigma}} \quad \text{(A.33)}
\end{equation}

Using \( B_3 \), and following the procedure outlined above, the correlation function \( \langle d_{0\sigma}^t d_{0\sigma} d_{0\sigma} \rangle \) is given by

\begin{equation}
\langle S_j S_0 \rangle = \langle d_{0\sigma}^t d_{0\sigma} d_{0\sigma} \rangle = \frac{1}{1 + \beta_{j\sigma}} [\alpha_{j\sigma} n^d_{0\sigma} - \alpha_{j\sigma} m_{j\sigma}]. \quad \text{(A.34)}
\end{equation}

Similarly, using \( B_4 \)

\begin{equation}
\langle d_{0\sigma}^t d_{0\sigma} d_{0\sigma} d_{0\sigma} \rangle = \frac{\alpha_{j\sigma} n^d_{0\sigma} + \beta_{j\sigma} (n^d_{0\sigma} - m_{j\sigma})}{1 - \beta^{(1)}_{j\sigma}} \quad \text{(A.35)}
\end{equation}
where the $d$-wave symmetry has been considered, therefore, $\langle d^1_{j\sigma} d^d_{-j-\sigma} \rangle = 0$.

The four $B^{(p)}$ operators introduced up to now are exactly the same operators used by Roth in Ref. [9] to obtain the band shift $W_{k\sigma}$ in the normal state and without hybridization. However, in the present work, due to the presence of the hole operators (see Eq. (12)), a new $B$ operator, which is given by

$$
B^{(5)}_{k\sigma} = \frac{1}{\sqrt{L}} \sum_i e^{-i\vec{k}\cdot\vec{R}_i} d^d_{i\sigma} d^1_{i+j\sigma} d^1_{i+j-\sigma},
$$

(A.36)

has been introduced. With this operator, the correlation function $\langle n_{0\sigma} d^d_{j\sigma} d^1_{j-\sigma} \rangle$ present in Eq. (A.33) may be evaluated. Thus,

$$
\langle d^d_{0\sigma} d^1_{j-\sigma} d^1_{j\sigma} d^d_{0\sigma} \rangle = \frac{\alpha_{j\sigma} n_{0\sigma}^d + \beta_{j\sigma} (n_{0\sigma}^d - m_{j\sigma})}{1 - \beta_{j\sigma}}.
$$

(A.37)

Substituting the result into Eq. (A.36), the correlation function $\langle d^d_{j\sigma} d^1_{j-\sigma} d^d_{0\sigma} d^d_{0\sigma} \rangle$ can be rewritten as:

$$
\langle d^d_{j\sigma} d^1_{j-\sigma} d^d_{0\sigma} d^d_{0\sigma} \rangle = \frac{\alpha_{j\sigma} n_{0\sigma}^d + \beta_{j\sigma} (n_{0\sigma}^d - m_{j\sigma})}{1 - \beta_{j\sigma}} \left[ 1 + \frac{1}{1 - \beta_{j\sigma}} \left( \frac{\alpha_{j\sigma} n_{0\sigma}^d}{\beta_{j\sigma}^2} + \frac{\beta_{j\sigma} (n_{0\sigma}^d - m_{j\sigma})}{\beta_{j\sigma}^2} \right) \right].
$$

(A.38)

The result given in Eq. (A.37) can be used in Eq. (A.31) to obtain

$$
\langle n_{j\sigma} d^d_{n\sigma} \rangle = (n_{0\sigma}^d)^2 - \frac{\alpha_{j\sigma} n_{0\sigma}^d + \beta_{j\sigma} m_{j\sigma}}{1 - \beta_{j\sigma}} \left[ 1 + \frac{1}{1 - \beta_{j\sigma}} \left( \frac{\alpha_{j\sigma} n_{0\sigma}^d}{\beta_{j\sigma}^2} + \frac{\beta_{j\sigma} (n_{0\sigma}^d - m_{j\sigma})}{\beta_{j\sigma}^2} \right) \right].
$$

(A.39)

Finally, with the results (A.37), (A.38) and (A.39) into Eq. (50), the following result has been obtained

$$
n_{j\sigma}^d (1 - n_{j\sigma}^d) W_{k\sigma}^d = h_{1\sigma} + \sum_{j \neq \delta} n_{\delta j\sigma}^d e^{i\vec{k}\cdot\vec{R}_j} (h_{2\sigma} + h_{3\sigma}^j)
$$

(A.40)

where

$$
h_{1\sigma} = - \sum_{j \neq 0} n_{\delta j\sigma}^d (n_{\delta j\sigma}^d - 2 m_{j\sigma}).
$$

(A.41)

$$
h_{2\sigma} = - \left\{ \frac{\alpha_{j\sigma} n_{0\sigma}^d + \beta_{j\sigma} m_{j\sigma}}{1 - \beta_{j\sigma}^2} + \frac{\alpha_{j\sigma} n_{0\sigma}^d + \beta_{j\sigma} m_{j\sigma}}{1 + \beta_{j\sigma}} \right\},
$$

(A.42)

$$
h_{3\sigma} = \phi_{j\sigma} \left\{ \frac{\alpha_{j\sigma} n_{0\sigma}^d + \beta_{j\sigma} m_{j\sigma}}{1 - \beta_{j\sigma}^2} - \frac{\beta_{j\sigma} (n_{0\sigma}^d - m_{j\sigma})}{1 - \beta_{j\sigma}} \right\},
$$

(A.43)

with

$$
\phi_{j\sigma} = \frac{\beta_{j\sigma}^2}{1 - \beta_{j\sigma}^2} + \frac{\beta_{j\sigma}^2}{1 - \beta_{j\sigma}^2}.
$$

(A.44)

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