Eur. Phys. J. B **45**, 485–496 (2005)
DOI: 10.1140/epjb/e2005-00209-1

THE EUROPEAN PHYSICAL JOURNAL B

Superconductivity in a two dimensional extended Hubbard model

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Received 26 October 2004 / Received in final form 13 April 2005
Published online 13 July 2005 –

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.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 74.25.Dw Superconductivity phase diagrams

1 Introduction

After almost two decade 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 [1]. In the undoped regime, these compounds are insulators and exhibit antiferromagnetic order at sufficient low temperatures [1,2]. The physical properties of the insulating phase can be well described by the Heisenberg model [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 ε_F in such strongly correlated systems is very important to understand their physical properties [3]. Earlier angle-resolved photoemission experiments (ARPES) have showed the presence of flat bands close to ε_F in a region centered around the point $(\pi, 0)$ in the p-type cuprates like $Bi_2Sr_2CuO_6$ and $YBa_2Cu_3O_y$ [3,4]. Due to the presence of strong correlations, to study some physical properties of these cuprate compounds, the one-band Hubbard model [5] can be used. Bulut et al. [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 [3].

Beenen and Edwards [8], using the Roth's two-pole approximation [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 [6,7]. The Roth's two-pole approximation has been proposed to improve the Hubbard-I approximation [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 [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 intermediated 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

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preserves the proper limit for $U \to \infty$ 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 [2]. For instance, the Hubbard one-band model suffers some limitations to describe the low-energy physical properties of the cuprate superconductors [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 [12]. Therefore, a model which take into account also the oxygen can be more adequate to treat the cuprate systems in the doped regime [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 [13] with the Roth's method to study the role of hybridization in the superconductivity following closely the approach introduced by Beenen and Edwards [14]. As discussed in the references [8] and [15], the flattening of the bands is directly related to the band shift. The presence of flat bands at Fermi level ε_F in the p-type cuprates [3] 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 reference [14] that the $d-d$ pairs are the most relevant ones for superconductivity [16].

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 [14], the factorization procedure [8] has been used to investigate the effects of the hybridization on the superconductivity. It has been shown [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 [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 $U \to \infty$. 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 [14] 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 reference [17].

There are some shortcomings in the Beenen and Edwards approach [18,19]. 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:

$$\begin{aligned} H = & \sum_{i,\sigma}(\varepsilon_d - \mu) d^\dagger_{i\sigma} d_{i\sigma} + \sum_{i,j,\sigma} t^d_{ij} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_i n^d_{i\uparrow} n^d_{i\downarrow} \\ & + \sum_{i,\sigma}(\varepsilon_p - \mu) p^\dagger_{i\sigma} p_{i\sigma} + \sum_{i,j,\sigma} t^p_{ij} p^\dagger_{i\sigma} p_{j\sigma} \\ & + \sum_{i,j,\sigma} t^{pd}_{ij} \left(d^\dagger_{i\sigma} p_{j\sigma} + p^\dagger_{i\sigma} d_{j\sigma} \right) \end{aligned} \quad (1)$$

where μ is the chemical potential. The $d^\dagger_{i\sigma}$, $d_{i\sigma}$ and $p^\dagger_{i\sigma}$, $p_{i\sigma}$ are the creation and annihilation operators of the d- and p-electrons, respectively, with spin σ at a lattice site i. The ε_d and ε_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 equation (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 $t^p = \alpha t^d$ with $\alpha > 1$. Also, $t^d < 0$ to coincide the bottom of the d- and p-bands with the Γ 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

$$\varepsilon^d_{\boldsymbol{k}} = 2t^d(\cos(k_x a) + \cos(k_y a)) \tag{2}$$

and

$$\varepsilon^p_{\boldsymbol{k}} = 2t^p(\cos(k_x a) + \cos(k_y a)) \tag{3}$$

where a is the lattice constant.

In this work, the Hamiltonian given in equation (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:

$$[A_n, H]_{(-)} = \sum_m K_{nm} A_m. \tag{4}$$

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

$$E_{nm} = \sum_m K_{nm} N_{nm} \tag{5}$$

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

$$E_{nm} = \left\langle \left[[A_n, H]_{(-)}, A^\dagger_m \right]_{(+)} \right\rangle \tag{6}$$

and

$$N_{nm} = \langle [A_n, A^\dagger_m]_{(+)} \rangle. \tag{7}$$

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

$$G_{nm}(\omega) = \langle\langle A_n; A^\dagger_m \rangle\rangle_\omega \tag{8}$$

and the equations (4–7), it is possible to obtain the following general Green's functions

$$\langle\langle A_n; B \rangle\rangle_\omega = \sum_m \widetilde{G}_{nm}(\omega) \langle [A_m, B]_{(+)} \rangle. \tag{9}$$

In the particular case, where $B = A^\dagger_m$, the elements of the Green's function matrix $\mathbf{G}$ are given by equation (8). Thus, using the matrices $\mathbf{E}$ and $\mathbf{N}$, the matrix $\mathbf{G}$ is given by

$$\mathbf{G}(\omega) = \widetilde{\mathbf{G}}(\omega)\mathbf{N} \tag{10}$$

where

$$\widetilde{\mathbf{G}}(\omega) = \mathbf{N}(\omega\mathbf{N} - \mathbf{E})^{-1}. \tag{11}$$

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 $\{c_{i\sigma}, n_{i-\sigma}c_{i\sigma}, c^\dagger_{i-\sigma}, n_{i\sigma}c^\dagger_{i-\sigma}\}$, it has been 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

$$\left\{ d_{i\sigma}, n^d_{i-\sigma} d_{i\sigma}, d^\dagger_{i-\sigma}, n^d_{i\sigma} d^\dagger_{i-\sigma}, p_{i\sigma} \right\}. \tag{12}$$

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 $\sum_l \langle d_{i-\sigma} d_{l\sigma} \rangle = 0$, where l are the nearest neighbors of i. Using the set of operators given in equation (12), and introducing the symmetries discussed above, the elements of the energy matrix defined in equation (6) can be obtained as:

$$\mathbf{E_5} = \begin{bmatrix} & & 0 & 0 & V^{dp}_k \\ & \mathbf{E_2} & & & \\ & & 0 & \overline{\gamma}_k & n^d_{-\sigma} V^{dp}_k \\ 0 & 0 & & & 0 \\ & & -\mathbf{E_2} & & \\ 0 & \overline{\gamma}_k{}^* & & & 0 \\ V^{pd}_k & n^d_{-\sigma} V^{pd}_k & 0 & 0 & \varepsilon_p - \mu + \varepsilon^p_k \end{bmatrix} \tag{13}$$

where V^{dp}_k and V^{pd}_k are the Fourier transform of t^{dp}_{ij} and t^{pd}_{ij} respectively. The matrix $\mathbf{E_2}$ present in the energy matrix $\mathbf{E_5}$ is given by:

$$\mathbf{E_2} = \begin{bmatrix} \overline{\varepsilon}_d + \varepsilon^d_k + U n^d_{-\sigma} & (\overline{\varepsilon}_d + \varepsilon^d_k + U) n^d_{-\sigma} \\ (\overline{\varepsilon}_d + \varepsilon^d_k + U) n^d_{-\sigma} & U n^d_{-\sigma} + \Gamma_{k-\sigma} \end{bmatrix} \tag{14}$$

where $\overline{\varepsilon}_d = \varepsilon_d - \mu$. It is assumed that the system considered here is translationally invariant, then $n^d_{-\sigma} = n^d_{i-\sigma}$. The quantity $\Gamma_{k-\sigma}$ is the Fourier transform of

$$\Gamma_{ij-\sigma} = (\varepsilon_d - \mu) n^d_{-\sigma} \delta_{ij} + t^d_{ij} (n^d_{-\sigma})^2 + n^d_{-\sigma}(1 - n^d_{-\sigma}) W_{ij-\sigma}. \tag{15}$$

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

$$W_{ij-\sigma} = \frac{t^d_{ij} \left(\langle n^d_{i-\sigma} n^d_{j-\sigma} \rangle - (n^d_{-\sigma})^2 \right) + \Lambda_{ij\sigma}}{n^d_{-\sigma}(1 - n^d_{-\sigma})} \tag{16}$$

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

$$\Lambda_{ij\sigma} = \Lambda^d_{ij\sigma} + \Lambda^{pd}_{ij\sigma}. \tag{17}$$

The terms $\Lambda^d_{ij\sigma}$ and $\Lambda^{pd}_{ij\sigma}$ are associated with the hopping t^d_{ij} and the hybridization t^{pd}_{ij}, respectively. The hybridized

term of $\Lambda_{ij\sigma}$ may be written as

$$\Lambda^{pd}_{ij\sigma} = \sum_l t^{pd}_{il}[2\langle p^\dagger_{l-\sigma} n^d_{i\sigma} d_{i-\sigma}\rangle - \langle p^\dagger_{l-\sigma} d_{i-\sigma}\rangle]\delta_{ij}, \quad (18)$$

and the part associated to the hopping t^d_{ij} is given by

$$\begin{aligned}\Lambda^d_{ij\sigma} = \sum_l t^d_{il} \Big\{ &\langle n^d_{i\sigma} d^\dagger_{i-\sigma} d_{l-\sigma}\rangle + \langle n^d_{i\sigma} d^\dagger_{l-\sigma} d_{i-\sigma}\rangle \\ &+ \langle d^\dagger_{i-\sigma} d_{l-\sigma} n^d_{i-\sigma}\rangle - \langle d^\dagger_{l-\sigma} d_{i-\sigma} n^d_{i-\sigma}\rangle \Big\} \delta_{ij} \\ &- t^d_{ij}\{\langle d^\dagger_{j\sigma} d^\dagger_{j-\sigma} d_{i-\sigma} d_{i\sigma}\rangle + \langle d^\dagger_{j\sigma} d^\dagger_{i-\sigma} d_{j-\sigma} d_{i\sigma}\rangle\}. \end{aligned} \quad (19)$$

The calculation of the correlation functions presented in equations (18) and (19) will be discussed in detail in Section 4.

One of the most important elements of the matrix $\mathbf{E}_5$ is $E_{24} = \overline{\gamma}_k$, where

$$\overline{\gamma}_k = \sum_{\langle l\rangle i} t^d_{il} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_l - \boldsymbol{R}_i)} \overline{\gamma}_{il} \quad (20)$$

and

$$\overline{\gamma}_{il} = \langle n^d_{i-\sigma} d_{l\sigma} d_{l-\sigma} + n^d_{l\sigma} d_{i\sigma} d_{i-\sigma}\rangle. \quad (21)$$

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

The elements of the normalization matrix $\mathbf{N}_5$ are given from equation (7) as:

$$N_{11} = N_{33} = N_{55} = 1 \quad (22)$$

and

$$N_{12} = N_{21} = N_{22} = N_{34} = N_{43} = N_{44} = n^d_{-\sigma}. \quad (23)$$

The remaining elements of the normalization matrix $\mathbf{N}_5$, due to the d-wave symmetry and the anticommution rules, have been found to be zero.

Using the energy and the normalization matrices $\mathbf{E}_5$ and $\mathbf{N}_5$, respectively, the matrix Green's function $\mathbf{G}_5$ defined in equation (10) can be obtained. For simplicity, only the *most relevant* elements (for the purposes of this work) of this (5×5) $\mathbf{G}_5$ matrix are shown. Following the Roth's notation [9], the correlation function $\langle BA\rangle$ is related to the Green's function $\langle\langle A;B\rangle\rangle_\omega$ as:

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

where $f(\omega)$ is the Fermi function. The chemical potential μ is obtained in the standard way, using the element $G^{11}_{\boldsymbol{k}\sigma}$ of the matrix $\mathbf{G}_5$ and the relation given in equation (24). The matrix element $G^{11}_{\boldsymbol{k}\sigma}$ is given by

$$G^{11}_{k\sigma}(\omega) = \frac{(\omega - E_{55})\left[A(\omega) - (\omega + E_{11})\overline{\gamma}_k{}^2\right]}{\overline{D}(\omega)}, \quad (25)$$

where E_{11} and E_{55} are elements of the energy matrix $\mathbf{E}_5$, defined in equation (13). In equation (25), it is also necessary to introduce the following definitions:

$$\begin{aligned} A(\omega) = &(n^d_{-\sigma})^2(1-n^d_{-\sigma})^2 \\ &\times(\omega^3 + \alpha^{(1)}_{k\sigma}\omega^2 + \alpha^{(2)}_{k\sigma}\omega + \alpha^{(3)}_{k\sigma}) \end{aligned} \quad (26)$$

with

$$\alpha^{(1)}_{k\sigma} = E_{11}, \quad (27)$$

$$\alpha^{(2)}_{k\sigma} = \mathcal{Z}^{(1)}_{k\sigma}\mathcal{Z}^{(2)}_{k\sigma} - (\mathcal{Z}^{(1)}_{k\sigma} + \mathcal{Z}^{(2)}_{k\sigma})(\mathcal{Z}^{(1)}_{k\sigma} + \mathcal{Z}^{(2)}_{k\sigma} - E_{11}) \quad (28)$$

and

$$\alpha^{(3)}_{k\sigma} = -\mathcal{Z}^{(1)}_{k\sigma}\mathcal{Z}^{(2)}_{k\sigma}(\mathcal{Z}^{(1)}_{k\sigma} + \mathcal{Z}^{(2)}_{k\sigma} - E_{11}). \quad (29)$$

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

$$\mathcal{Z}^{(1)}_{k\sigma} = \frac{U + 2(\varepsilon_d - \mu) + \varepsilon^d_k + W_{k-\sigma}}{2} - \frac{\Delta_{k\sigma}}{2} \quad (30)$$

and,

$$\mathcal{Z}^{(2)}_{k\sigma} = \mathcal{Z}^{(1)}_{k\sigma} + \Delta_{k\sigma}. \quad (31)$$

In the particular case, when ε_d, $\overline{\gamma}_k$ and t^{pd}_{ij} are zero, $\mathcal{Z}^{(1)}_{k\sigma}$ and $\mathcal{Z}^{(2)}_{k\sigma}$ represent the quasi-particle bands in the paramagnetic normal state of the one-band Hubbard model. The term $\Delta_{k\sigma}$ is given by:

$$\Delta_{k\sigma} = \sqrt{(U + W_{k-\sigma} - \varepsilon^d_k)^2 + 4n^d_{-\sigma}U(\varepsilon^d_k - W_{k-\sigma})} \quad (32)$$

where $W_{k-\sigma}$ is the Fourier transform of $W_{ij-\sigma}$ given in equation (16). The denominator of the Green's function $G^{11}_{\boldsymbol{k}\sigma}$ given in equation (25) is defined as:

$$\overline{D}(\omega) = (\omega - E_{55})D(\omega) - V^{dp}_k V^{pd}_k\left[A(\omega) - (\omega + E_{11})\overline{\gamma}_k{}^2\right] \quad (33)$$

where

$$D(\omega) = \mathcal{D}(\omega) - \overline{\gamma}_k{}^2(\omega^2 - E^2_{11}) \quad (34)$$

with

$$\begin{aligned}\mathcal{D}(\omega) = &[(\omega - E_{11})(\omega n^d_{-\sigma} - E_{22}) - (\omega n^d_{-\sigma} - E_{12})^2] \\ &\times[(\omega + E_{11})(\omega n^d_{-\sigma} + E_{22}) - (\omega n^d_{-\sigma} + E_{12})^2]. \end{aligned} \quad (35)$$

In equation (35), E_{12} and E_{22} are elements of the energy matrix $\mathbf{E}_2$ given in equation (14). The use of a set of five operators A_n results in a five-pole approximation to the Green's functions. Then, the $\overline{D}(\omega)$ defined in equation (33) may be also written as:

$$\begin{aligned}\overline{D}(\omega) = &(n^d_{-\sigma})^2(1-n^d_{-\sigma})^2(\omega - E_{1k})(\omega - E_{2k})(\omega - E_{3k}) \\ &\times(\omega - E_{4k})(\omega - E_{5k}) \end{aligned} \quad (36)$$

where the quasi-particle bands E_{pk} (with $p = 1,..,5$) satisfy $\overline{D} = \det(\omega\mathbf{N}_5 - \mathbf{E}_5) = 0$. Therefore, the resulting Green's function can be written as a sum of five terms:

$$G^{11}_{k\sigma}(\omega) = \sum_{p=1}^{5} \frac{Z_{p\boldsymbol{k}\sigma}}{\omega - E_{p\boldsymbol{k}\sigma}} \quad (37)$$

where $Z_{p\boldsymbol{k}\sigma}$ express the spectral weights which satisfy

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

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 Edwards in reference [8], the correlation function given by equation (21) is rewritten as

$$\overline{\gamma}_{il} = [\langle d^{\dagger}_{i-\sigma} d_{l-\sigma}\rangle + \langle d^{\dagger}_{l\sigma} d_{i\sigma}\rangle]\langle d_{i-\sigma} d_{l\sigma}\rangle \tag{39}$$

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

$$n^{d}_{01\sigma} = \langle d^{\dagger}_{i-\sigma} d_{l-\sigma}\rangle = \langle d^{\dagger}_{l\sigma} d_{i\sigma}\rangle \tag{40}$$

which allows to rewrite equation (39) as

$$\overline{\gamma}_{il} = 2 n^{d}_{01\sigma}\langle d_{i-\sigma} d_{l\sigma}\rangle \tag{41}$$

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

Considering the d-wave symmetry, the Fourier transform of $\overline{\gamma}_{il}$ given by equation (20) becomes

$$\overline{\gamma}_{k} = \overline{g}\,[\cos(k_x a) - \cos(k_y a)] \tag{42}$$

where

$$\overline{g} = 2 t^{d}\overline{\gamma} \tag{43}$$

is the gap-function amplitude. Due to the d-wave symmetry, $\overline{\gamma}_{il} = +\overline{\gamma}$ for $\boldsymbol{R}_i - \boldsymbol{R}_l$ in the x direction and $\overline{\gamma}_{il} = -\overline{\gamma}$ when $\boldsymbol{R}_i - \boldsymbol{R}_l$ is in the y direction. The Fourier transform of the correlation function $\langle d_{i-\sigma} d_{l\sigma}\rangle$ is given by

$$\langle d_{i-\sigma} d_{l\sigma}\rangle = \frac{1}{L}\sum_{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_l - \boldsymbol{R}_i)}\langle d_{k-\sigma} d_{k\sigma}\rangle \tag{44}$$

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 $G^{13}_{k\sigma}$ and the relation given by equation (24). The Green's function $G^{13}_{k\sigma}$ can be rewritten as:

$$G^{13}_{k\sigma}(\omega) = -\overline{\gamma}_{k} U^{2} F^{13}_{k\sigma} \tag{45}$$

where

$$F^{13}_{k\sigma}(\omega) = \frac{(n^{d}_{-\sigma})^{2}(1 - n^{d}_{-\sigma})^{2}(\omega - E_{55})}{\overline{D}\,(\omega)} \tag{46}$$

and $\overline{D}(\omega)$ is defined in equation (33).

Combining the equation (20) with the equations (41) to (45), the gap equation can be written as:

$$\overline{\gamma}_{k} = -\overline{\gamma}_{k} 2 n^{d}_{01\sigma} t^{d} U^{2} I_{\sigma} \tag{47}$$

where

$$I_{\sigma} = \frac{1}{2\pi i}\oint f(\omega) F_{\sigma}(\omega) d\omega \tag{48}$$

with

$$F_{\sigma}(\omega) = \frac{1}{L}\sum_{\boldsymbol{q}} [\cos(\boldsymbol{q}_x a) - \cos(\boldsymbol{q}_y a)]^{2} F^{13}_{q\sigma}(\omega). \tag{49}$$

4 Definition and calculation of the band shifts

Using the definition (17) in equation (16), the band shift $W_{ij-\sigma}$ can be written as:

$$W_{ij-\sigma} = W^{d}_{ij-\sigma} + W^{pd}_{ij-\sigma} \tag{50}$$

where

$$W^{d}_{ij-\sigma} = \frac{t^{d}_{ij}[\langle n^{d}_{i-\sigma} n^{d}_{j-\sigma}\rangle - (n^{d}_{-\sigma})^{2}] + \Lambda^{d}_{ij\sigma}}{n^{d}_{-\sigma}(1 - n^{d}_{-\sigma})} \tag{51}$$

and

$$W^{pd}_{ij-\sigma} = \frac{\Lambda^{pd}_{ij\sigma}}{n^{d}_{-\sigma}(1 - n^{d}_{-\sigma})}. \tag{52}$$

The quantity $\Lambda^{pd}_{ij\sigma}$ is given by equation (18). The correlation function $\langle p^{\dagger}_{l-\sigma} d_{i-\sigma}\rangle$ present in $\Lambda^{pd}_{ij\sigma}$ can be obtained from de Green's function

$$G^{15}_{k\sigma}(\omega) = \frac{\left[A(\omega) - (\omega + E_{11})\overline{\gamma}_{k}{}^{2}\right] V^{pd}_{k}}{\overline{D}\,(\omega)}. \tag{53}$$

The remaining correlation function $\langle p^{\dagger}_{l-\sigma} n^{d}_{i\sigma} d_{i-\sigma}\rangle$ present in $\Lambda^{pd}_{ij\sigma}$ is calculated from the Green's function

$$G^{25}_{k\sigma}(\omega) = \frac{n^{d}_{-\sigma}\left[B(\omega) - (\omega + E_{11})\overline{\gamma}_{k}{}^{2}\right] V^{dp}_{k}}{\overline{D}\,(\omega)}, \tag{54}$$

where

$$B(\omega) = A(\omega) + n^{d}_{-\sigma}(1 - n^{d}_{-\sigma})^{2} U \mathcal{D}_{1}(\omega) \tag{55}$$

with $A(\omega)$ defined in equation (26). The quantity $\mathcal{D}_1(\omega)$, in terms of the elements of the energy matrix (13), is given by:

$$\mathcal{D}_{1}(\omega) = (\omega - E_{11})(\omega n^{d}_{-\sigma} - E_{22}) - (\omega n^{d}_{-\sigma} - E_{12})^{2}. \tag{56}$$

The Green's function $G^{25}_{k\sigma}$ tends to zero as $U \to \infty$, consequently, the correlation function $\langle p^{\dagger}_{l-\sigma} n^{d}_{i\sigma} d_{i-\sigma}\rangle$ also vanishes recovering the result of reference [14] for $\Lambda^{pd}_{ij\sigma}$.

The quantity $\Lambda^{d}_{ij\sigma}$ present in equation (51) is given by equation (19). The Fourier transform of $W^{d}_{ij\sigma}$ is given by:

$$W^{d}_{k\sigma} = \sum_{\langle j\rangle i} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_i)} W^{d}_{ij\sigma}. \tag{57}$$

Substituting equation (19) into equation (51) and then putting the result into equation (57), the Fourier transform of $W^{d}_{ij\sigma}$ can be written as:

$$\begin{aligned} W^{d}_{k\sigma} = & -\frac{1}{n^{d}_{\sigma}(1 - n^{d}_{\sigma})}\sum_{j\neq 0} t^{d}_{0j}\langle d^{\dagger}_{0\sigma} d_{j\sigma}(1 - n^{d}_{0-\sigma} - n^{d}_{j-\sigma})\rangle \\ & + \sum_{j\neq 0} t^{d}_{0j} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}\left\{\langle n^{d}_{j\sigma} n^{d}_{0\sigma}\rangle - \langle n^{d}_{0\sigma}\rangle^{2}\right. \\ & \left. + \langle d^{\dagger}_{j\sigma} d_{j-\sigma} d^{\dagger}_{0-\sigma} d_{0\sigma}\rangle - \langle d^{\dagger}_{j\sigma} d^{\dagger}_{j-\sigma} d_{0-\sigma} d_{0\sigma}\rangle\right\}. \end{aligned} \tag{58}$$

The correlation functions present in $W^d_{k\sigma}$ are evaluated following the original Roth's procedure [9]. Introducing extra operators $B_{i\sigma}$, the correlation functions of the form $\langle A_n B_{i\sigma}\rangle$ can be calculated by using equations (9) and (24). In references [8,14], the sum present in equation (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, $W^d_{k\sigma}$ is given by:

$$n^d_\sigma(1-n^d_\sigma)W^d_{\boldsymbol{k}\sigma} = h_{1\sigma} + \sum_{j\neq 0} t^d_{0j} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}(h_{2j\sigma} + h_{3j\sigma}) \quad (59)$$

where the term $h_{3j\sigma}$ is directly related to the gap function $\overline{\gamma}_{\boldsymbol{k}}$ through the Green's functions $G^{13}_{\boldsymbol{k}\sigma}$ and $G^{14}_{\boldsymbol{k}\sigma}$ (see Appendix A). The quantities $h_{1\sigma}$, $h_{2j\sigma}$ and $h_{3j\sigma}$ are given in Appendix A.

5 Results

In this section, the numerical results obtained in this work are presented. One of the most important parameters of the model given in equation (1) is the $d-p$ hybridization [14,20], which is defined as

$$V^{dp}_{\boldsymbol{k}} = -iV^{dp}_0[\sin(k_x a) - \sin(k_y a)]. \quad (60)$$

In this work, as in reference [20], the hybridization has been assumed $\boldsymbol{k}$-independent $(V^{dp}_0)^2 \equiv \langle V^{dp}_{\boldsymbol{k}} V^{pd}_{\boldsymbol{k}}\rangle$, where $\langle ...\rangle$ is the average over the Brillouin zone. In reference [21] Sengupta and Ghatak have also used a $\boldsymbol{k}$-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 $n_T = n^d_\sigma + n^d_{-\sigma}$, where n^d_σ is obtained combining $G^{11}_{k\sigma}$ (Eq. (25)) and the relation given in equation (24). The charge transfer energy $\Delta = \varepsilon_p - \varepsilon_d$ is positive. This means that the first hole added to the system will energetically prefer to occupy the d-orbital of the copper ions [1]. All results presented in this section are obtained with $\varepsilon_d = 0$ and $\varepsilon_p = 3.6$ eV. Consequently, $\Delta = 3.6$ eV, as estimated in reference [22].

As discussed in references [8,9], the band shift $W_{\boldsymbol{k}\sigma}$ (see Eq. (50)) can be evaluated considering different approximations. In the limit $U\to\infty$, some terms of the band shift vanish (see Ref. [9]). In reference [14], the present authors estimate $W_{\boldsymbol{k}\sigma}$ in the limit of $U\to\infty$, but with finite U in other parts of the problem. In reference [8], Beenen and Edwards evaluated $W_{\boldsymbol{k}\sigma}$ in the normal state (where $\overline{\gamma}_{\boldsymbol{k}} = 0$) 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 $W_{\boldsymbol{k}\sigma}$ given in equation (58) are evaluated following closely the procedure used by Roth in reference [9]. Nevertheless, here, also the hole operators given in the set of equation (12) are used to evaluate the correlation functions. As consequence, a new term $(h_{3j\sigma})$ appears in $W_{\boldsymbol{k}\sigma}$ (see Eq. (59)). The approximations used to evaluate $W_{\boldsymbol{k}\sigma}$ are shown in Table 1. In Figure 1a, the quasi-particle bands E_{pk}, with $p = 1..5$ (see Eq. (36)), are plotted along the symmetry lines $(0,0)-(\pi,\pi)-(\pi,0)-(0,0)$, in the two-dimensional Brillouin zone. The quasi-particle energies E_{pk}, in the superconducting state, are relative to the chemical potential μ. The circles show the $\varepsilon^p_{\boldsymbol{k}}$ band, where the center of $\varepsilon^p_{\boldsymbol{k}}$ is shifted by $\varepsilon_p = 3.6$ eV relative to the zero of energy. All results shown in this paper are obtained with $t^p = 2t^d$. The dashed line corresponds to the noninteracting ($U=0$) band $\varepsilon^d_{\boldsymbol{k}}$ relative to the noninteracting chemical potential. Figure 1b 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. 1a) 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 1c, the region near to the (π,π) point shows the gaps produced

Table 1. The different approaches considered for evaluate the band shift $W_{\boldsymbol{k}\sigma}$.

	U	$\overline{\gamma}_{\boldsymbol{k}}$	T	V^{pd}_0	$h_{3j\sigma}$
Beenen and Edwards [8]	*finite*	0	0	0	0
Ref. [14]	∞	0	0	*finite*	0
Present work	*finite*	*finite*	*finite*	*finite*	*finite*

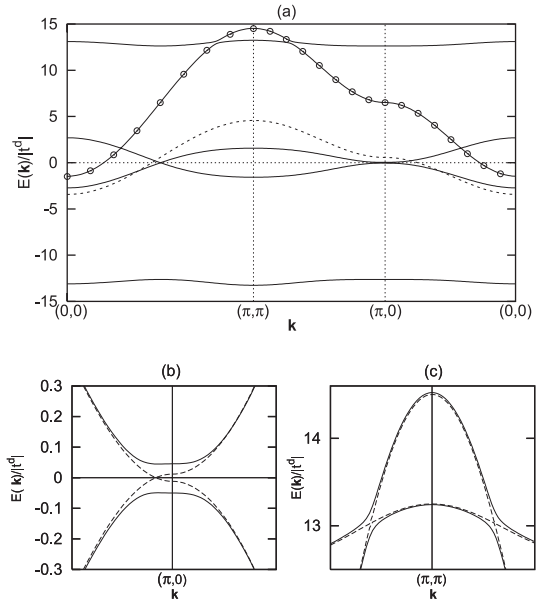

Fig. 1. (a) The quasi-particle bands for $U = 12|t^d|$, $V^{pd}_0 = 0.2|t^d|$ and $n_T = 0.76$. (b) The electron and hole bands in the neighborhood of the $(\pi,0)$ point where the gap structure is relevant. The dashed lines show the result for $V^{pd}_0 = 0.0$ while the solid lines correspond to $V^{pd}_0 = 0.2|t^d|$. (c) shows the hybridization (V^{pd}_0) gap near the point (π,π).

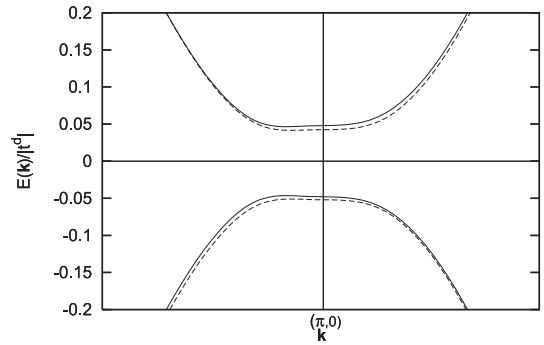

Fig. 2. The electron and hole bands in the region close to the $(\pi, 0)$ point for $U = 12|t^d|$ and $n_T = 0.76$. The solid lines correspond to $V_0^{pd} = 0.0$, while the dashed lines show the result for $V_0^{pd} = 0.3|t^d|$.

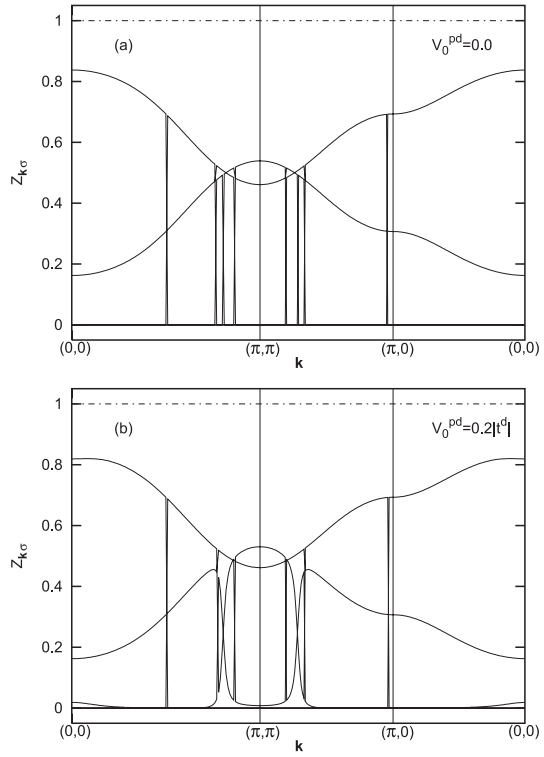

Fig. 3. The spectral weights $Z_{p\boldsymbol{k}\sigma}$ for $U = 12|t^d|$, $n_T = 0.76$, $T = 0$ and two different values of hybridization.

by the $d - p$ hybridization V_0^{pd}. The dashed lines show the result for $V_0^{pd} = 0$. In Figure 2, 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 in relation to the $\boldsymbol{k}$ axis.

Figure 3 shows the spectral weights $Z_{p\boldsymbol{k}\sigma}$ for two different hybridization. The dashed line corresponds to the sum of the five spectral weights which is equal to one (see Eq. (38)). In Figure 3b, 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.

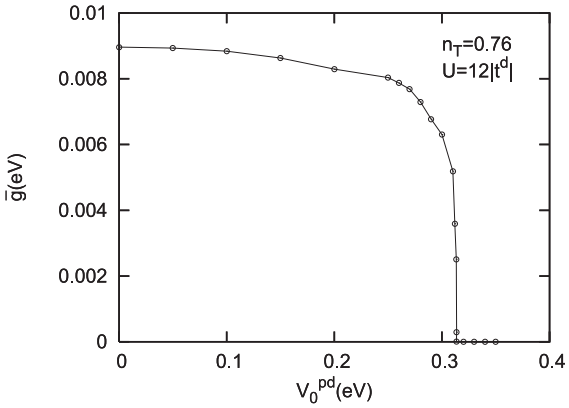

Fig. 4. Behavior of the gap function amplitude $\overline{g}$ as a function of the hybridization V_0^{pd} for $T = 0.004$ eV.

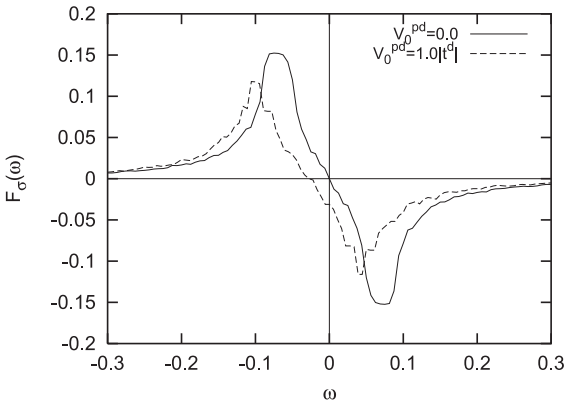

Fig. 5. Function $F_\sigma(\omega)$ (defined in Eq. (49)) for $U = 12|t^d|$, $n_T = 0.76$, $T = 0$ and two different hybridization.

Figure 4 shows the behavior of gap function amplitude $\overline{g}$ as a function of the hybridization V_0^{pd}. It is clear that there is a decreasing of $\overline{g}$ with increasing V_0^{pd}.

The analysis of the function $F_\sigma(\omega)$ introduced in equation (48) and defined in equation (49) is important to understand the behavior of the gap function amplitude showed in Figure 4. 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 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 equation (48) vanishes when $\omega > 0$. That is because the Fermi function $f(\omega)$ is zero for that range of ω. As consequence of the shift and the suppression of $F_\sigma(\omega)$, the value of I_σ, which is given by the integral in equation (48), decreases when the hybridization increase. However, from equation (47), it is necessary a minimum value for I_σ to obtain a nonzero solution for $\overline{\gamma}$. But, for very strong values of hybridization, the minimum value for I_σ is not reached and only the zero solution exists.

According to this analysis, there is a critical value of hybridization (V_{0c}^{pd}), above which, the superconductivity

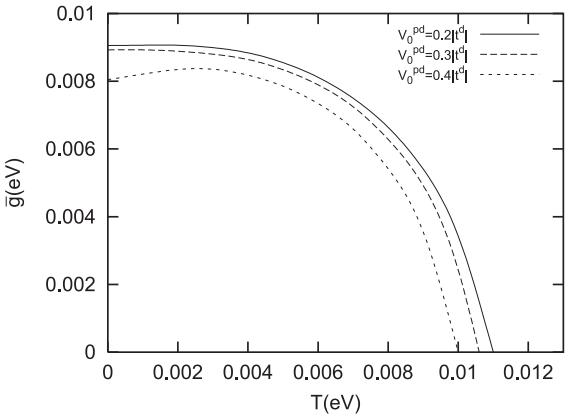

Fig. 6. The gap function amplitude $\overline{g}$, as a function of temperature T, for $U = 12|t^d|$, $n_T = 0.76$ and several values of hybridization. ($t^d = -0.5$ eV.)

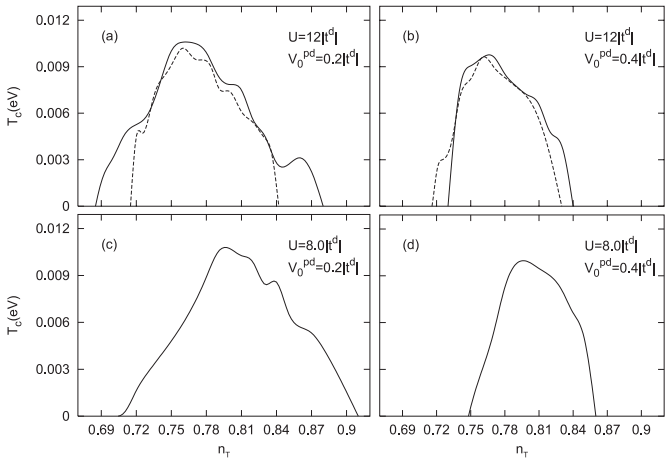

Fig. 7. T_c as a function of the total occupation number n_T. In (a) and (b), the dotted lines show the previous results from reference [14] for $U = 12|t^d|$. The solid lines show the behavior of T_c in the present approach. The figures (c) and (d) show the present results for $U = 8|t^d|$. ($t^d = -0.5$ eV.)

is suppressed. Similar results, which show a critical value for the hybridization, were also obtained in reference [23], for a $\boldsymbol{k}$-dependent hybridization and using the Hartree-Fock approximation for the electron-electron interaction. In references [16,23], 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_σ and consequently of T_c.

Since the hybridization is directly related to the applied pressure [16], 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 reference [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. Figure 6 shows the function amplitude $\overline{g}$, as a function of temperature T for several values of hybridization. If the hybridization is enhanced, the critical temperature T_c decreases. Therefore, the present results agree with the discussion above in the scenario where the electronic effects dominate. This behavior for T_c is also shown in Figure 7, in phase diagrams displaying T_c versus the total occupation number n_T. The numerical results obtained show that there is a critical value of hybridization where the superconducting phase vanishes. These results agree with the ones obtained by the authors of reference [24] for heavy-fermion superconductivity with an X-boson treatment.

The solid lines in Figures 7a–b show the present result for T_c, where the effects of the temperature, the superconductivity and the Coulomb interaction have been included in the calculation of the band shift $W_{\boldsymbol{k}\sigma}$. The dashed lines correspond to the results obtained in reference [14], where the band shift has been evaluated considering $T = 0$, $\overline{\gamma}_{\boldsymbol{k}} = 0$ and $U \to \infty$ (see Tab. 1). The difference between the results can be explained by the analysis of equation (18) where some of the correlation functions present in the band shift vanish in the $U \to \infty$ limit. In equation (18), the correlation function $\langle p^\dagger_{l-\sigma} n^d_{i\sigma} d_{i-\sigma}\rangle$, 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 equation (18) are both negative. Therefore, for large U, the correlation function $\langle p^\dagger_{l-\sigma} n^d_{i\sigma} d_{i-\sigma}\rangle$ decreases and the hybridized shift W^{pd}_σ 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 7c–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 reference [8].

In Figure 8a, the chemical potential is show as a function of the total occupation number n_T for $U = 12|t^d|$ and three different hybridizations. In reference [19], the authors criticized the Roth's method because the compressibility $k = \frac{\partial n_T}{\partial \mu}$ is negative in the vicinity of half-filling in the Beenen and Edwards result. In reference [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 important contribution to provide negative compressibility

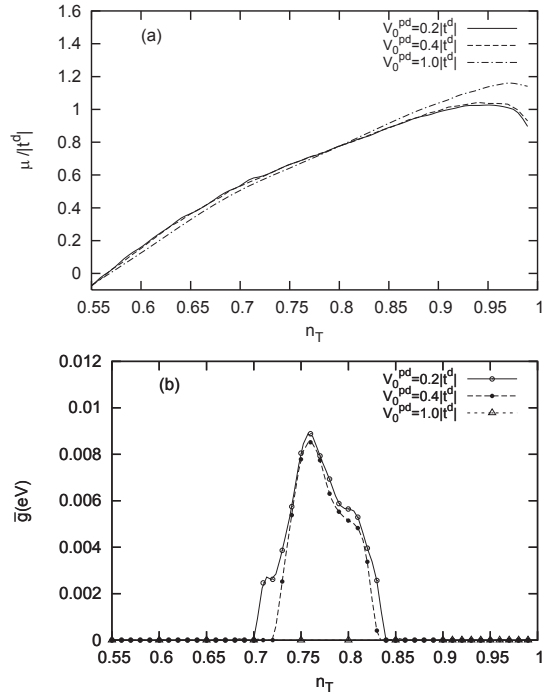

Fig. 8. (a) The chemical potential as a function of the total occupation number for $U = 12|t^d|$, $T = 0.004$ eV and different values of hybridization. (b) The gap function amplitude, as a function of the total occupation number, with U and V_0^{pd} identical to (a).

comes from the spin-term $\langle S_j S_i \rangle$ present in the d-part $W^d_{\boldsymbol{k}\sigma}$ of the Roth's band shift $W_{\boldsymbol{k}\sigma}$ (see Eqs. (58) and (A.34). 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 $\boldsymbol{k}$-independent [20], the hybridization term W^{pd}_{σ} 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 8a, it is clear that the effect of the hybridization in the chemical potential decreases the negative compressibility.

Figure 8b shows the gap function amplitude $\overline{g}$ as a function of the total occupation number. This result agrees with those obtained in Figure 4, where $\overline{g}$ decreases with increasing of V_0^{pd}.

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 equation (1). The quality of the Roth's two-pole approximation had been investigated in a previous work by Beenen and Edwards [8]. 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 [3] 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 [25].

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 properties of the model has been studied. This work has been carried out following the factorization procedure proposed by Beenen 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 reference [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 $V_0^{pd} = 0$ in the present work. The hybridization V_0^{pd} breaks the symmetry between the electron and hole quasi-particle bands, respect to $\boldsymbol{k}$ axis. Also, the gap amplitude function $\overline{g}$ and the critical temperature T_c are suppressed with increasing the hybridization V_0^{pd}. 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_0^{pd}. The correlation functions present in the d-part of the band shift $W_{\boldsymbol{k}\sigma}$ 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 $W_{\boldsymbol{k}\sigma}$. 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.

The authors are grateful to the Grupo de Física Estatística-IFM, Universidade Federal de Pelotas where part of numerical calculations were performed. This work was partially supported by the Brazilian agencies CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior) and FAPERGS (Fundação de Amparo à Pesquisa do Rio Grande do Sul).

Appendix A

The correlation functions present in the band shift $W^d_{\boldsymbol{k}\sigma}$ can be evaluated by introducing extra B operators, as in the original Roth's procedure. Combining the equation (9) and the relation given in equation (24), it is possible to write

$$\langle BA_n\rangle = \mathcal{F}_\omega \sum_m \widetilde{G}_{nm}(\omega)\langle[A_m, B]_{(+)}\rangle, \tag{A.1}$$

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

$$B^{(1)}_{\boldsymbol{k}j\sigma} = \frac{1}{\sqrt{L}}\sum_i e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} n^d_{i+j\sigma} d^\dagger_{i\sigma} \tag{A.2}$$

and

$$B^{(2)}_{\boldsymbol{k}j\sigma} = \frac{1}{\sqrt{L}}\sum_i e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} n^d_{i+j-\sigma} d^\dagger_{i\sigma}. \tag{A.3}$$

By considering the operator given in the equation (A.2), the correlation function $\langle n^d_{j\sigma} n^d_{0\sigma}\rangle$ can be written as:

$$\langle n^d_{j\sigma} n^d_{0\sigma}\rangle = \frac{1}{L}\sum_{\boldsymbol{k}} \langle B^{(1)}_{\boldsymbol{k}j\sigma} d_{\boldsymbol{k}\sigma}\rangle \tag{A.4}$$

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

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

$$A_{2\boldsymbol{k}\sigma} = \frac{1}{\sqrt{L}}\sum_l e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l} n^d_{l-\sigma} d_{l\sigma}, \tag{A.6}$$

$$A_{3\boldsymbol{k}\sigma} = \frac{1}{\sqrt{L}}\sum_l e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l} d^\dagger_{l-\sigma}, \tag{A.7}$$

$$A_{4\boldsymbol{k}\sigma} = \frac{1}{\sqrt{L}}\sum_l e^{i\boldsymbol{k}\cdot\boldsymbol{R}_l} n^d_{l\sigma} d^\dagger_{l-\sigma} \tag{A.8}$$

and

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

Thus, the following results have been obtained

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

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

$$\langle[A_{3\boldsymbol{k}\sigma}, B^{(1)}_{\boldsymbol{k}j\sigma}]_{(+)}\rangle = 0, \tag{A.12}$$

$$\langle[A_{4\boldsymbol{k}\sigma}, B^{(1)}_{\boldsymbol{k}j\sigma}]_{(+)}\rangle = -\langle n^d_{j\sigma} d^\dagger_{0\sigma} d^\dagger_{0-\sigma}\rangle, \tag{A.13}$$

$$\langle[A_{5\boldsymbol{k}\sigma}, B^{(1)}_{\boldsymbol{k}j\sigma}]_{(+)}\rangle = 0 \tag{A.14}$$

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, $n^d_{0\sigma} = n^d_{j\sigma}$. Considering the relations given by equations (A.1) and (A.4) with the results from equation (A.10) to equation (A.14), the correlation function $\langle n^d_{j\sigma} n^d_{0\sigma}\rangle$ can be written as:

$$\langle n^d_{l\sigma} n^d_{0\sigma}\rangle = \alpha_\sigma n^d_\sigma - \alpha_{j\sigma} n^d_{0j\sigma} + \beta_\sigma\langle n^d_{0-\sigma} n^d_{j\sigma}\rangle - \beta_{j\sigma} m_{j\sigma} + \beta^{(1)}_\sigma\langle n^d_{j\sigma} d^\dagger_{0-\sigma} d^\dagger_{0\sigma}\rangle \tag{A.15}$$

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

$$n^d_{0j\sigma} = \langle d^\dagger_{0\sigma} d_{j\sigma}\rangle = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega G^{11}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}, \tag{A.16}$$

$$m_{j\sigma} = \langle d^\dagger_{0\sigma} n^d_{j-\sigma} d_{j\sigma}\rangle = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega G^{12}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}, \tag{A.17}$$

$$\alpha_{j\sigma} = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega \widetilde{G}^{11}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}, \tag{A.18}$$

$$\beta_{j\sigma} = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega \widetilde{G}^{12}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j} \tag{A.19}$$

and

$$\beta^{(1)}_{j\sigma} = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega \widetilde{G}^{14}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j} \tag{A.20}$$

where $G^{11}_{\boldsymbol{k}\sigma}$ is given in equation (25). The remaining Green's functions $G^{12}_{\boldsymbol{k}\sigma}$ and $G^{14}_{\boldsymbol{k}\sigma}$ are given respectively by

$$G^{12}_{k\sigma}(\omega) = \frac{n^d_{-\sigma}(\omega - E_{55})\left[B(\omega) - (\omega + E_{11})\overline{\gamma}_k{}^2\right]}{\overline{D}(\omega)} \tag{A.21}$$

and

$$G^{14}_{k\sigma}(\omega) = (n^d_{-\sigma})^2(1 - n^d_{-\sigma})^2 U\overline{\gamma}_k \times \frac{(\omega - E_{55})(\omega + E_{11} - Un^d_{-\sigma})}{\overline{D}(\omega)} \tag{A.22}$$

where $B(\omega)$ is defined in equation (55) and $\overline{D}(\omega)$ in equation (36). It is also necessary to define

$$\widetilde{G}^{11}_{\boldsymbol{k}\sigma}(\omega) = \frac{G^{11}_{\boldsymbol{k}\sigma}(\omega) - G^{12}_{\boldsymbol{k}\sigma}(\omega)}{1 - n^d_{-\sigma}}, \tag{A.23}$$

$$\widetilde{G}^{12}_{\boldsymbol{k}\sigma}(\omega) = \frac{G^{12}_{\boldsymbol{k}\sigma}(\omega) - n^d_{-\sigma} G^{11}_{\boldsymbol{k}\sigma}(\omega)}{n^d_{-\sigma}(1-n^d_{-\sigma})} \tag{A.24}$$

and

$$\widetilde{G}^{14}_{\boldsymbol{k}\sigma}(\omega) = \frac{G^{14}_{\boldsymbol{k}\sigma}(\omega) - n^d_{-\sigma} G^{13}_{\boldsymbol{k}\sigma}(\omega)}{n^d_{-\sigma}(1-n^d_{-\sigma})} \tag{A.25}$$

where $G^{13}_{\boldsymbol{k}\sigma}$ is given in equation (45).

The correlation function $\langle n^d_{0-\sigma} n^d_{j\sigma}\rangle$ present in equation (A.15), can be obtained by repeating the procedure above using the operator $B^{(2)}_{\boldsymbol{k}j\sigma}$ (given by Eq (A.3)). Thus,

$$\langle n^d_{j-\sigma} n^d_{0\sigma}\rangle = \alpha_\sigma n^d_{-\sigma} + \beta_\sigma \langle n^d_{0-\sigma} n^d_{j-\sigma}\rangle + \alpha^{(1)}_{j\sigma} n^{(1)}_{0j\sigma} + \beta^{(1)}_{j\sigma} m^{(1)}_{j\sigma} - \beta^{(1)}_{\sigma} \langle n^d_{j-\sigma} d^\dagger_{0\sigma} d^\dagger_{0-\sigma}\rangle \tag{A.26}$$

where

$$n^{(1)}_{0j\sigma} = \langle d_{j-\sigma} d_{0\sigma}\rangle = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega G^{13}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}, \tag{A.27}$$

$$m^{(1)}_{j\sigma} = \langle d_{j-\sigma} n^d_{j\sigma} d_{0\sigma}\rangle = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega G^{14}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}, \tag{A.28}$$

and

$$\alpha^{(1)}_{j\sigma} = \frac{1}{L}\sum_{\boldsymbol{k}} \mathcal{F}_\omega \widetilde{G}^{13}_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j} \tag{A.29}$$

with

$$\widetilde{G}^{13}_{\boldsymbol{k}\sigma}(\omega) = \frac{G^{13}_{\boldsymbol{k}\sigma}(\omega) - G^{14}_{\boldsymbol{k}\sigma}(\omega)}{1-n^d_{-\sigma}}. \tag{A.30}$$

Reversing the spin labels i.e., $\sigma \rightarrow -\sigma$ in equation (A.26) and substituting the result into equation (A.15), then

$$\langle n^d_{j\sigma} n^d_{0\sigma}\rangle = \frac{\alpha_\sigma n^d_\sigma - \alpha_{j\sigma} n^d_{0j\sigma} + \beta_\sigma \alpha_{-\sigma} n^d_\sigma - \beta_{j\sigma} m_{j\sigma}}{1-\beta_\sigma\beta_{-\sigma}} + \frac{1}{1-\beta_\sigma\beta_{-\sigma}}\Big[\beta_\sigma(\alpha^{(1)}_{j-\sigma} n^{(1)}_{0j-\sigma} + \beta^{(1)}_{j-\sigma} m^{(1)}_{j-\sigma}) + (\beta_\sigma\beta^{(1)}_{-\sigma} + \beta^{(1)}_\sigma)\langle n^d_{j\sigma} d^\dagger_{0-\sigma} d^\dagger_{0\sigma}\rangle\Big]. \tag{A.31}$$

For evaluate the two last correlation functions present in equation (58), the following operators have been introduced

$$B^{(3)}_{\boldsymbol{k}j\sigma} = \frac{1}{\sqrt{L}}\sum_i e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} d^\dagger_{i+j\sigma} d_{i+j-\sigma} d^\dagger_{i-\sigma} \tag{A.32}$$

and

$$B^{(4)}_{\boldsymbol{k}j\sigma} = \frac{1}{\sqrt{L}}\sum_i e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} d^\dagger_{i+j\sigma} d^\dagger_{i+j-\sigma} d_{i-\sigma}. \tag{A.33}$$

Using B_3, and following the procedure outlined above, the correlation function $\langle d^\dagger_{j\sigma} d_{j-\sigma} d^\dagger_{0-\sigma} d_{0\sigma}\rangle$ is given by

$$\langle S_j S_0\rangle = \langle d^\dagger_{j\sigma} d_{j-\sigma} d^\dagger_{0-\sigma} d_{0\sigma}\rangle = -\frac{1}{1+\beta_\sigma}\left[\alpha_{j\sigma} n^d_{0j-\sigma} + \beta_{j\sigma} m_{j-\sigma} - \alpha^{(1)}_{j\sigma} n^{(1)}_{0j-\sigma} - \beta^{(1)}_{j\sigma} m^{(1)}_{j-\sigma}\right]. \tag{A.34}$$

Similarly, using B_4

$$\langle d^\dagger_{j\sigma} d^\dagger_{j-\sigma} d_{0-\sigma} d_{0\sigma}\rangle = \frac{\alpha_{j\sigma} n^d_{0j-\sigma} + \beta_{j\sigma}(n^d_{0j-\sigma} - m_{j-\sigma})}{1-\beta_\sigma} + \frac{\beta^{(1)}_\sigma \langle n^d_{0\sigma} d^\dagger_{j\sigma} d^\dagger_{j-\sigma}\rangle}{1-\beta_\sigma} \tag{A.35}$$

where the d-wave symmetry has been considered, therefore, $\langle d^\dagger_{j\sigma} d^\dagger_{j-\sigma}\rangle = 0$.

The four $B^{(p)}$ operators introduced up to now are exactly the same operators used by Roth in reference [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

$$B^{(5)}_{\boldsymbol{k}j\sigma} = \frac{1}{\sqrt{L}}\sum_i e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} d^\dagger_{i\sigma} d_{i+j\sigma} d_{i+j-\sigma}, \tag{A.36}$$

has been introduced. With this operator, the correlation function $\langle n^d_{0\sigma} d^\dagger_{j\sigma} d^\dagger_{j-\sigma}\rangle$ present in equation (A.35) may be evaluated. Thus,

$$\langle d^\dagger_{0\sigma} d_{j-\sigma} d_{j\sigma} d_{0\sigma}\rangle = \frac{\alpha^{(1)}_{j\sigma} n^d_{0j\sigma} + \beta^{(1)}_{j\sigma}(n^d_{0j\sigma} - m_{j\sigma})}{1-\beta_\sigma}. \tag{A.37}$$

Substituting the result (A.37) into equation (A.35), the correlation function $\langle d^\dagger_{j\sigma} d^\dagger_{j-\sigma} d_{0-\sigma} d_{0\sigma}\rangle$ can be rewritten as:

$$\langle d^\dagger_{j\sigma} d^\dagger_{j-\sigma} d_{0-\sigma} d_{0\sigma}\rangle = \frac{\alpha_{j\sigma} n^d_{0j-\sigma} + \beta_{j\sigma}(n^d_{0j-\sigma} - m_{j-\sigma})}{1-\beta_\sigma} + \frac{\beta^{(1)}_\sigma[\alpha^{(1)}_{j\sigma} n^d_{0j\sigma} + \beta^{(1)}_{j\sigma}(n^d_{0j\sigma} - m_{j\sigma})]}{(1-\beta_\sigma)^2}. \tag{A.38}$$

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

$$\langle n^d_{j\sigma} n^d_{0\sigma}\rangle = (n^d_{0j\sigma})^2 - \frac{\alpha_{j\sigma} n^d_{0j\sigma} + \beta_{j\sigma} m_{j\sigma}}{1-\beta_\sigma\beta_{-\sigma}} + \frac{1}{1-\beta_\sigma\beta_{-\sigma}}\Big[\beta_\sigma(\alpha^{(1)}_{-\sigma} n^{(1)}_{0j-\sigma} + \beta^{(1)}_{j-\sigma} m^{(1)}_{j-\sigma}) - \frac{\alpha^{(1)}_{j\sigma} n^d_{0j\sigma}(\beta_\sigma\beta^{(1)}_{-\sigma} + \beta^{(1)}_\sigma)}{1-\beta_\sigma} - \frac{\beta^{(1)}_{j\sigma}(n^d_{0j\sigma} - m_{j\sigma})(\beta_\sigma\beta^{(1)}_{-\sigma} + \beta^{(1)}_\sigma)}{1-\beta_\sigma}\Big]. \tag{A.39}$$

Finally, with the results (A.37), (A.38) and (A.39) into equation (59), the following result has been obtained

$$n^d_{-\sigma}(1-n^d_{-\sigma}) W^d_{\boldsymbol{k}\sigma} = h_{1\sigma} + \sum_{j\neq 0} t^d_{0j} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j}(h_{2j\sigma} + h_{3j\sigma}) \tag{A.40}$$

where

$$h_{1\sigma} = -\sum_{j\neq 0} t^d_{0j}(n^d_{j0\sigma} - 2m_{j\sigma}), \tag{A.41}$$

$$h_{2j\sigma} = -\left\{ \frac{\alpha_{j\sigma} n^d_{0j\sigma} + \beta_{j\sigma} m_{j\sigma}}{1-\beta_\sigma \beta_{-\sigma}} + \frac{\alpha_{j\sigma} n^d_{0j-\sigma} + \beta_{j\sigma} m_{j-\sigma}}{1+\beta_\sigma} + \frac{\alpha_{j\sigma} n^d_{0j-\sigma} + \beta_{j\sigma}(n^d_{0j-\sigma} - m_{j-\sigma})}{1-\beta_\sigma} \right\}, \tag{A.42}$$

$$h_{3j\sigma} = \phi_{j\sigma} \left\{ \frac{\alpha^{(1)}_{j\sigma} n^d_{0j\sigma} + \beta^{(1)}_{j\sigma}(n^d_{0j\sigma} - m_{j\sigma})}{1-\beta_\sigma} \right\} - \frac{\beta_\sigma[\alpha^{(1)}_{j-\sigma} n^{(1)}_{0j-\sigma} + \beta^{(1)}_{j-\sigma} m_{j-\sigma}]}{1-\beta_\sigma\beta_{-\sigma}} - \frac{\alpha^{(1)}_{j\sigma} n^{(1)}_{0j-\sigma} + \beta^{(1)}_{j\sigma} m^{(1)}_{j-\sigma}}{1+\beta_\sigma} \tag{A.43}$$

with

$$\phi_{j\sigma} = \frac{(\beta^{(1)}_\sigma}{1-\beta_\sigma} + \frac{\beta_\sigma \beta^{(1)}_{-\sigma} + \beta^{(1)}_\sigma}{1-\beta_\sigma\beta_{-\sigma}}. \tag{A.44}$$

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