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Non perturbative calculations for three particles in a linear chain within the generalized Hubbard model

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Abstract. A real-space method has been introduced to study the pairing problem within the generalized Hubbard Hamiltonian. This method includes the bond-charge interaction term as an extension of the previously proposed mapping method [1] for the Hubbard model. The generalization of the method is based on mapping the correlated many-body problem onto an equivalent site- and bond-impurity tight-binding one in a higher dimensional space, where the problem can be solved exactly. In a one-dimensional lattice, we analyzed the three particle correlation by calculating the binding energy at the ground state, using different values of the bond-charge, the on-site (U) and the nearest-neighbor (V) interactions. A pairing asymmetry is found between electrons and holes for the generalized hopping amplitude, where the hole pairing is not always easier than the electron case. For some special values of the hopping parameters and for all kinds of interactions in the Hubbard Hamiltonian, an analytical solution is obtained.

PACS. 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 71.10.Pm Fermions in reduced dimensions (anyons, composite fermions, Luttinger liquid, etc.) – 71.10.Li Excited states and pairing interactions in model systems

1 Introduction

Investigations of high-T_c superconductors suggest that electronic correlation may play a significant role in the formation of pairs [2]. Although the main interest is on the physics of two-dimensional highly correlated electron systems, the one-dimensional models related to high temperature superconductivity are very popular due to the conjecture [3] that properties of the one-dimensional (1D) and two-dimensional (2D) variants of certain models have common aspects. Within the models for correlated electron systems, that attempt to capture the essential physics of high-temperature superconductors and parent compounds, the simple Hubbard model [4,5] is the crudest approximation to include electronic interaction between band-electrons, by retaining only the on-site interaction U. This model also assigns the same hopping rate t to three different hopping processes regardless of the occupation of the two sites involved.

Besides the on-site interaction, other contributions of the electron-electron interaction are required [6], such as the nearest-neighbor interactions and the bond-charge interaction term. The Hamiltonian which includes these interactions is often called the generalized Hubbard Hamiltonian (GHH). It has been studied previously by several authors [7–12] and can be written as

$$H = \sum_{\langle i,j\rangle,\sigma} t^{\sigma}_{i,j} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j, \quad (1)$$

where $\langle i,j\rangle$ denotes nearest-neighbor sites, $c^{+}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma =\downarrow$ *or* $\uparrow$ at site i, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ where $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. It is worth mentioning that in principle, the parameters U and V are positive because they are direct Coulomb integrals. However, U and V could be negative if attractive indirect interaction through phonons or other bosonic excitations are included and are stronger than the direct Coulomb repulsion. In equation (1), the generalized hopping amplitude, $t^{\sigma}_{i,j}$, depends on the site occupation and is given by

$$t^{\sigma}_{i,j} = t_{\mathrm{A}}(1-n_{i,-\sigma})(1-n_{j,-\sigma}) + t_{\mathrm{B}} n_{i,-\sigma} n_{j,-\sigma} + t_{\mathrm{AB}}[n_{j,-\sigma}(1-n_{i,-\sigma}) + n_{i,-\sigma}(1-n_{j,-\sigma})]. \quad (2)$$

The three parameters t_{A}, t_{B}, and t_{AB} are the hopping amplitudes from a singly occupied to an empty site, from a doubly occupied to a singly occupied site and from a doubly occupied to an empty site, respectively. The special

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case $t_{\rm A} = t_{\rm B} = t_{\rm AB} = t$ corresponds to the $t-U-V$ extended Hubbard model, which has been studied intensively by analytical and numerical methods [4,5]. Equation (2) can also be written as

$$t_{i,j}^{\sigma} = t_{\rm A} + (t_{\rm AB} - t_{\rm A})(n_{i,-\sigma} + n_{j,-\sigma}) + (t_{\rm A} + t_{\rm B} - 2t_{\rm AB}) n_{i,-\sigma} n_{j,-\sigma}, \quad (3)$$

to emphasize the contribution from two- and four-fermion operators. These new interactions may give rise to new dynamical effects, absent in the simple Hubbard model.

When a particle-hole transformation [13] is made in the GHH, electron operators are mapped into hole's *via* $c_{i,\sigma}^{+} \rightarrow h_{i,\sigma}$, the Hamiltonian of equation (1) becomes:

$$H = (U + 2zV)\Big(N - \sum_{i,\sigma} n_{i,\sigma}^{h}\Big) - \sum_{\langle i,j\rangle,\sigma} t_{i,j}^{\sigma,h} h_{j,\sigma}^{+} h_{i,\sigma} + U \sum_{i} n_{i,\uparrow}^{h} n_{i,\downarrow}^{h} + \frac{V}{2} \sum_{\langle i,j\rangle} n_{i}^{h} n_{j}^{h}, \quad (4)$$

where N is the total number of sites, z is the lattice coordination number, $h_{i,\sigma}^{+}(h_{i,\sigma})$ is the hole creation (annihilation) operator and $n_{i}^{h} = n_{i,\uparrow}^{h} + n_{i,\downarrow}^{h}$ with $n_{i,\sigma}^{h} = h_{i,\sigma}^{+} h_{i,\sigma}$. The first term in equation (4) only contributes to a shift in the total energy and the second term belongs to the generalized hopping parameter for holes, $t_{i,j}^{\sigma,h}$. The expression for $t_{i,j}^{\sigma,h}$ is given as follows:

$$t_{i,j}^{\sigma,h} = t_{\rm B}(1 - n_{i,-\sigma}^{h})(1 - n_{j,-\sigma}^{h}) + t_{\rm A} n_{i,-\sigma}^{h} n_{j,-\sigma}^{h} + t_{\rm AB}[n_{j,-\sigma}^{h}(1 - n_{i,-\sigma}^{h}) + n_{i,-\sigma}^{h}(1 - n_{j,-\sigma}^{h})], \quad (5)$$

where the main difference with the electron hopping is the change of $t_{\rm A}$ by $t_{\rm B}$, and so holes also interact *via* a Hubbard model. However, there are two crucial differences between the electron and the hole cases: the density of holes is $1-n$ in terms of the electron density (n) and the signs of the hopping parameter are opposite.

For $t_{\rm A} + t_{\rm B} - 2t_{\rm AB} = 0$, the generalized hopping amplitude is reduced to the Hirsch and Marsiglio model [14], proposed as a possible mechanism for superconductivity. An occupation dependent hopping term of the form (2) arises quite naturally as the result of a trace over additional electronic degrees of freedom when mapping a multi-band Hubbard Hamiltonian onto a single-band one [15]. Recently, Hirsch [16] discussed the inapplicability of the Hubbard model for the description of strongly correlated electrons and proposed instead the generalized form (2), based on first principle calculations of the magnitude of the hopping parameters [17]. There is, however, no consensus on their amplitude in real systems [18]. So, in order to keep the model as general as possible, we will not put constraints on the values of the hopping term.

The electronic correlation for the low density limit, mainly the two particle case, has been intensively studied by analytical and numerical methods using the Hubbard model [1,4,19], including different kinds of disorder in this model [20–22] and also including the bond-charge interaction [23–26]. The next question which arises is how the behavior of the physical properties (*e.g.* the binding energy), is modified by the presence of a third electron. This kind of question is presumed helpful in the ultimate understanding of the N-body problem. The case of three correlated particles is not as widely studied as the two particle case. It was considered earlier by Mattis [27] in his study of the pair stability for the attractive-U Hubbard model and by Fabrizio *et al.* [28] for the repulsive-U case, who discussed an asymptotic behavior of the ground state.

For the two-particle case the term $(t_{\rm A} + t_{\rm B} - 2t_{\rm AB}) n_{i,-\sigma} n_{j,-\sigma}$ is ineffective. In this case, assuming that $t_{\rm A} > t_{\rm AB} > t_{\rm B}$, the hopping reduces to

$$t_{i,j}^{\sigma} = t_{\rm A} - (t_{\rm A} - t_{\rm AB})(n_{i,-\sigma} + n_{j,-\sigma}) \quad (6)$$

and

$$t_{i,j}^{\sigma,h} = t_{\rm B} + (t_{\rm AB} - t_{\rm B})(n_{i,-\sigma}^{h} + n_{j,-\sigma}^{h}) \quad (7)$$

implying that the hopping of a hole increases in the presence of another hole and can lead to pairing of holes but not of electrons [17]. The term $(t_{\rm A} + t_{\rm B} - 2t_{\rm AB}) n_{i,-\sigma} n_{j,-\sigma}$ now becomes effective for the three-particle problem and may modify the above statement as we show in the paper. In this paper, we analyzed the pairing of three electrons in a one-dimensional lattice using the generalized Hubbard Hamiltonian. The analysis has been done by extending the previously reported [1,29,30] mapping method in order to include the generalized hopping, $t_{i,j}^{\sigma}$. The paper is organized as follows: In Section 2 we introduce briefly the mapping method for the generalized Hubbard model and apply it to the problem of three electrons in a linear chain. In Section 3, analytical solutions for some special values of the Hubbard parameters as well as the numerical results are discussed. Finally, we conclude in Section 4.

2 Mapping method

In this section, we introduce an extension of the mapping method explained in detail in reference [1] for different lattice topologies. In order to present a brief explanation of the mapping method, let us consider the case of two electrons with opposite spins in an N-site chain; the number of two-electron states for this system is given by N^2. These states have a geometric representation in a square lattice, which can be described by a one-body tight-binding Hamiltonian, with $(3N-2)$ ordered site-impurities. Among these impurities, N are localized on sites along the principal diagonal of the square lattice with a self-energy U and the others, $2(N-1)$, are localized on the two next-diagonals with a self-energy V. A simple way to obtain the solution is to take advantage of the translational symmetry of the site-impurities and projecting the two-dimensional lattice of states onto a linear chain of effective states, similar to the procedure introduced by Falicov and Yndurain [31]. In general, this method will map the original many-body problem onto a tight-binding one with some ordered site-impurities in an nd-dimensional lattice, n being the number of electrons and

d the dimensionality of the original system. In this hyperspace lattice, the on-site (U) and the nearest-neighbor (V) interactions from the original Hubbard Hamiltonian become the self-energies of the site-impurities. The new effective Hamiltonian determines the density of states for the interacting n-particle system.

When the bond-charge interaction is included, the mapping method showed above should be modified. Let us see how this modification takes place for the problem of three electrons, two with up-spin and one with down-spin in an infinite linear chain. In this case, the network of three-electron states belongs to a three-dimensional lattice with site- and bond-impurities. For illustration of the mapping method, let us consider below the configuration of states for three electrons in a 4-site chain. It is worth mentioning that both the numerical and analytical calculations will be done in an infinite chain. For our example, the different states are:

$$\begin{array}{lll}
|1\rangle = |\pm +00\rangle, & |2\rangle = |\pm 0+0\rangle, & |3\rangle = |\pm 00+\rangle, \\
|4\rangle = |-++0\rangle, & |5\rangle = |-+0+\rangle, & |6\rangle = |-0++\rangle, \\
|7\rangle = |+\pm 00\rangle, & |8\rangle = |+-+0\rangle, & |9\rangle = |+-0+\rangle, \\
|10\rangle = |0\pm +0\rangle, & |11\rangle = |0\pm 0+\rangle, & |12\rangle = |0-++\rangle, \\
|13\rangle = |++-0\rangle, & |14\rangle = |+0\pm 0\rangle, & |15\rangle = |+0-+\rangle, \\
|16\rangle = |0+\pm 0\rangle, & |17\rangle = |0+-+\rangle, & |18\rangle = |00\pm +\rangle, \\
|19\rangle = |++0-\rangle, & |20\rangle = |+0+-\rangle, & |21\rangle = |+00\pm\rangle, \\
|22\rangle = |0++-\rangle, & |23\rangle = |0+0\pm\rangle, & |24\rangle = |00+\pm\rangle.
\end{array} \tag{8}$$

Electrons with spin up and spin down are denoted by + and − respectively, a doubly-occupied site is indicated by ± and 0 represents an empty site. In the generalized Hubbard Hamiltonian, a state with a site occupied by two electrons requires an energy U and a state in which two electrons are situated on nearest-neighbor sites, requires an energy V. States with a site occupied by two electrons and an electron situated on a nearest-neighbor site requires an energy $U + 2V$, the remaining states with electrons placed at distant sites do not require any energy (see Eq. (8)). Finally, the amplitudes of the transition probability between nearest-neighbor states will depend on the site occupation and are given by $t_{\rm A}$, $t_{\rm B}$ and $t_{\rm AB}$. In Figure 1, we show a three-dimensional geometric representation of our previous 24 states, where the circles represent the states with their self-energy indicated inside and the number levels of the states are as given in equation (8). As already mentioned, the hopping between these states depends on the site occupation but it is important to remark that the difference of two connected states is only the hopping of one electron. For instance in Figure 1, the hopping amplitude from state 1 ($|1\rangle$) to state 2 ($|2\rangle$) is $t_{\rm A}$, the hopping amplitude from state 2 ($|2\rangle$) to state 4 ($|4\rangle$) is $t_{\rm AB}$ and the hopping amplitude from state 1 ($|1\rangle$) to state 7 ($|7\rangle$) is given by $t_{\rm B}$, etc. Therefore, the network of states in Figure 1 can be described by a site- and bond-impurities tight-binding Hamiltonian.

For the case of three electrons in an infinite periodic chain, the network of states corresponds to an infinite

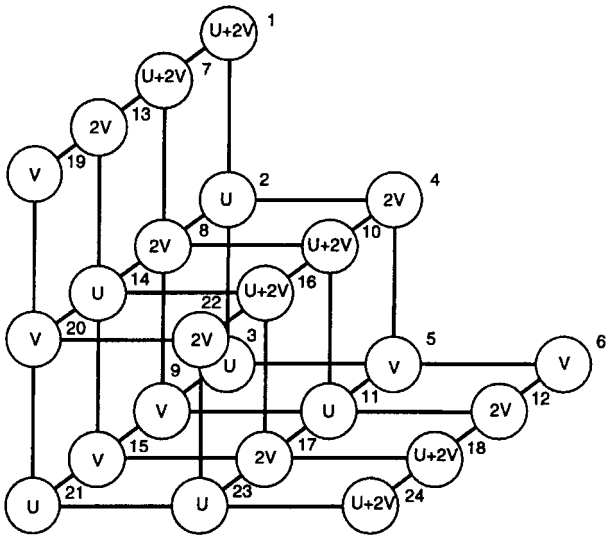

Fig. 1. Geometrical representation of the three-electron states for a chain of four sites. The states are represented by circles with self-energy indicated inside, and the numeration of states is according to equation (8). Details of the hopping parameters and the symmetry of the lattice are discussed in the text.

three-dimensional lattice with an infinite number of site- and bond-impurities ordered along the principal diagonals of each cube in the lattice. The network of states has an exact solution, since the Hamiltonian is a tight-binding type. A simple way to obtain the solution is to take advantage of the translational symmetry of the impurities and to project the network of states onto a two-dimensional triangular lattice of effective states, as it is shown in Figure 2. This figure represents the projection of states for an original system with three electrons in a five-site chain, where the effective projected hopping parameters $\beta_{\rm A}^{+}$, $\beta_{\rm A}^{-}$, $\beta_{\rm B}^{+}$, $\beta_{\rm B}^{-}$, $\beta_{\rm AB}^{+}$, and $\beta_{\rm AB}^{-}$ are given by

$$\begin{array}{ll}
\beta_{\rm A}^{+} = t_{\rm A}{\rm e}^{{\rm i}Ka/\sqrt{3}}, & \beta_{\rm A}^{-} = t_{\rm A}{\rm e}^{-{\rm i}Ka/\sqrt{3}}, \\
\beta_{\rm B}^{+} = t_{\rm B}{\rm e}^{{\rm i}Ka/\sqrt{3}}, & \beta_{\rm B}^{-} = t_{\rm B}{\rm e}^{-{\rm i}Ka/\sqrt{3}}, \\
\beta_{\rm AB}^{+} = t_{\rm AB}{\rm e}^{{\rm i}Ka/\sqrt{3}}, & \beta_{\rm AB}^{-} = t_{\rm AB}{\rm e}^{-{\rm i}Ka/\sqrt{3}}.
\end{array} \tag{9}$$

Here, K is the wave vector in the projection direction and $a = 1$ is the lattice parameter. The effective hopping parameters satisfy the following relation $\beta^{+} = (\beta^{-})^{*}$. Finally, the two-dimensional results must be integrated with respect to K within the first Brillouin zone.

3 Results and discussion

3.1 Analytical solutions

In this subsection we will study the analytical solution for some particular cases of the ground state for three electrons ($K = 0$) in a linear chain, therefore using equation (9)

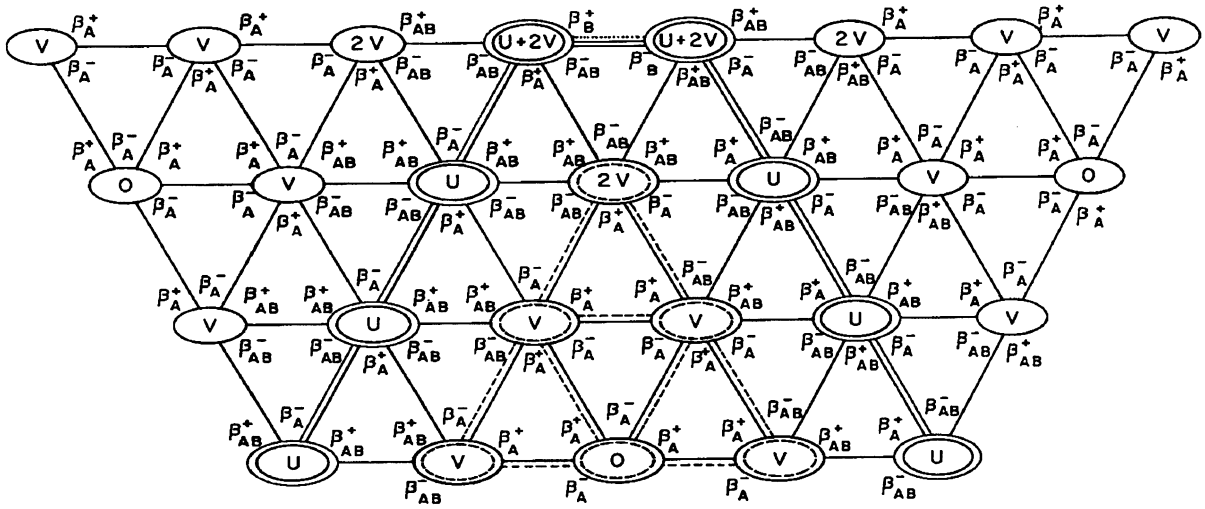

Fig. 2. Lattice of effective states for three electrons in a linear chain. The effective states are represented by ellipses and the self-energy for each of them is indicated inside. There are six different effective-hopping parameters $\beta_{\rm A}^{+}$, $\beta_{\rm A}^{-}$, $\beta_{\rm B}^{+}$, $\beta_{\rm B}^{-}$, $\beta_{\rm AB}^{+}$, and $\beta_{\rm AB}^{-}$, with values given in the text. The full-line and dash-line represent the non-parallel ($\uparrow\downarrow\uparrow$) and parallel ($\uparrow\uparrow\uparrow$) cases respectively. The double lines show a linear chain of effective states with two nearest-neighbor site impurities ($2V$) and the dotted lines represent the single bond-impurity.

we have: $\beta_{\rm A}^{+} = \beta_{\rm A}^{-} = t_{\rm A}$, $\beta_{\rm B}^{+} = \beta_{\rm B}^{-} = t_{\rm B}$ and $\beta_{\rm AB}^{+} = \beta_{\rm AB}^{-} = t_{\rm AB}$. The analytical solutions were obtained using these new values for the effective hopping parameters and analyzing the network of states given in Figure 2, where we observed two important limits; the first limit is when the hopping amplitude from a doubly occupied to an empty site is forbidden $t_{\rm AB} = 0$ but the hopping amplitudes $t_{\rm A} \neq 0$ and $t_{\rm B} \neq 0$, and the second limit is when both $t_{\rm AB} = 0$ and $t_{\rm B} = 0$ are forbidden but $t_{\rm A} \neq 0$.

Let us analyze the first case ($t_{\rm AB} = 0$, $t_{\rm A} \neq 0$ and $t_{\rm B} \neq 0$), it shows that there is a competition between the linear chain of effective states with two site-impurities (shown in Fig. 2 by double lines) and the triangular lattice of effective states (shown in Fig. 2 by dashed lines). The latter one is in fact the network of effective states associated to the problem of three electrons with parallel spin ($\uparrow\uparrow\uparrow$) in a linear chain for the Hubbard model [32]. It is important to mention that for the special case $t_{\rm A} = t_{\rm B} = t$, the linear chain of effective states (having two equal nearest-neighbor site-impurities with self-energy $2V$), has an analytical solution for the ground state energy. In order to obtain the solution, let us consider the problem of two substitutional impurities introduced at two nearest-neighbor sites in a periodic linear chain described by a tight-binding Hamiltonian. The solution for the ground-state energy can be found using the Green's function technique. In the linear chain, the Green's function for two impurities is given by [33]

$$G(n,l;E) = \langle n|G_{0p}|l\rangle + \frac{\epsilon_2\langle n|G_{0p}|m\rangle\langle m|G_{0p}|l\rangle}{1-\epsilon_2 G_{0p}(m,m;E)}, \quad (10)$$

where ϵ_2 is the site energy of the second impurity at site m and G_{0p} is the Green's function for a single impurity with site energy ϵ_1. For a linear chain with one impurity localized at the central site ($p = 0$), the Green's function G_{0p} evaluated at the energy of the second impurity ($m = 1$) is given by

$$G_{0p}(1,1;E_{\rm imp}) = \frac{D^2 + 2\epsilon_1\sqrt{E_{\rm imp}^2 - D^2} - 2\epsilon_1 E_{\rm imp}}{D^2(\sqrt{E_{\rm imp}^2 - D^2} - \epsilon_1)}, \quad (11)$$

where $D = |zt_{\rm A}|$ is equal to half the bandwidth within the independent particle approximation and z is the number of nearest-neighbors. In the present case of two impurities, the poles of $G(n,l;E)$ in equation (10) are given by

$$G_{0p}(m,m;E_{\rm imp}) = \frac{1}{\epsilon_2}\cdot \quad (12)$$

When the second impurity is localized on site 1 ($m = 1$), we obtain

$$G_{0p}(1,1;E_{\rm imp}) = \frac{1}{\epsilon_2} = \frac{D^2 + 2\epsilon_1\sqrt{E_{\rm imp}^2 - D^2} - 2\epsilon_1 E_{\rm imp}}{D^2(\sqrt{E_{\rm imp}^2 - D^2} - \epsilon_1)}\cdot \quad (13)$$

Therefore, the ground state energy is given by

$$E_{\rm imp} = \frac{-2\epsilon_1\epsilon_2(\epsilon_1+\epsilon_2) \pm (2\epsilon_1\epsilon_2 - D^2)\sqrt{(\epsilon_1-\epsilon_2)^2 + D^2}}{D^2 - 4\epsilon_1\epsilon_2}\cdot \quad (14)$$

Finally, for the special case $\epsilon_1 = \epsilon_2 = 2V$, the solution is given as follows:

$$E_{\rm imp} = \frac{1}{D^2 - 16V^2}\left[-32V^3 \pm D(8V^2 - D^2)\right]. \quad (15)$$

In equation (15), $E_{\rm imp}$ gives the energies of the two localized states for the two equal site-impurities. Since the linear chain is a bipartite lattice and the hopping between two nearest-neighbor sites is the same all along the chain, there is a symmetry of these localized states. This means for repulsive potentials ($V > 0$) the states are opposite to those for attractive potentials ($V < 0$). The binding energy is given by $\Delta \equiv \max(|E_{\rm imp}|) - D$.

For the second limit ($t_{\rm AB} = 0$, $t_{\rm B} = 0$ and $t_{\rm A} \neq 0$), the competition (see Fig. 2) is between the semi-infinite linear chain of effective states with a site-impurity of self-energy $2V$ located at the surface and the triangular lattice of effective states. The semi-infinite linear chain with a surface site-impurity has an analytical solution [34] given by:

$$E_{\rm imp} = 2V + \frac{t_{\rm A}^2}{2V} \cdot \tag{16}$$

Such a solution is only valid for $|2V| > |t_{\rm A}|$ which leads to $|E_{\rm imp}| > 2|t_{\rm A}|$, so that this solution corresponds to a localized state lying outside the band. For $V > 0$ (repulsive potentials) the state is above the band, the reverse being true for attractive potentials ($V < 0$).

3.2 Numerical solutions

Here we will present the numerical solution, for variations of the hopping parameters and of the interaction terms, for the case of three non-parallel ($\uparrow\downarrow\uparrow$) electrons and for the case of three non-parallel ($\uparrow\downarrow\uparrow$) holes in an infinite one-dimensional lattice, within a generalized Hubbard model.

In order to analyze the pairing state we look at the binding energy (Δ) for both cases of electrons and holes. The binding energy has been calculated from the energy difference between the lowest correlated state and the lowest non-correlated state localized at the lower non-interacting ($U = V = 0$ and $t_{\rm A} = t_{\rm B} = t_{\rm AB} = t$) three-particle band edge. The lowest correlated state energy is obtained for $K = 0$ in the case of electrons and for $K/\sqrt{3} = \pi$ for the hole case, which corresponds to eliminating the change of sign of the effective hopping parameters similar to a gauge transformation in a bipartite lattice. As we already mentioned, the essential difference between holes and electrons within the generalized Hubbard Hamiltonian is that the hopping amplitude $t_{\rm A}$ for electrons should be changed to $t_{\rm B}$ for holes. Results for holes are simply obtained from electrons by interchanging $t_{\rm A}$ and $t_{\rm B}$. This produces an asymmetry between electron- and hole-pairing. The final numerical diagonalization was carried out for a truncated two-dimensional triangular lattice of 551 effective states. The matrix sizes for numerical diagonalizations were chosen as the minimum size so that the physical quantities do not vary significantly with the matrix size.

In Figure 3, we show the ground-state phase diagram for both electron-singlet and hole-singlet in a linear chain for the Hubbard model $t_{\rm A} = t_{\rm B} = t_{\rm AB} = t$. In this figure, we can notice the electron-hole symmetry and the absence of pairing for U and V positives which is very well established.

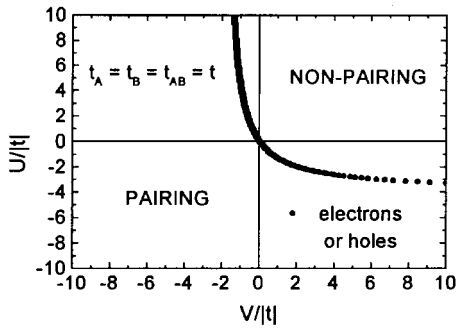

Fig. 3. Singlet-pairing phase diagram for both cases of three-electrons or three-holes in an infinite linear chain within the extended Hubbard Hamiltonian, it means, when $t_{\rm A} = t_{\rm B} = t_{\rm AB} = t$.

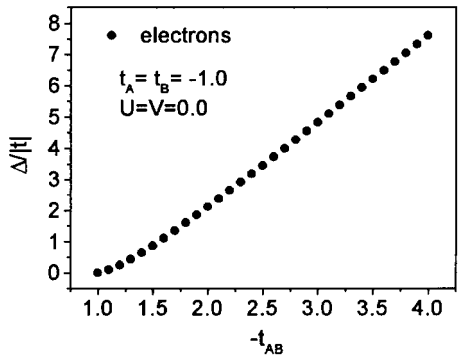

Fig. 4. Numerical results of the binding energy for three electrons or three holes with antiparallel spin in a linear chain as a function of the $t_{\rm AB}$ parameter and without on-site and nearest-neighbor interaction.

In Figure 4, we present the numerical calculations of the electron-binding energy for $t_{\rm A} = t_{\rm B} = -1$ and $|t_{\rm AB}| > |t_{\rm A}|, |t_{\rm B}|$. The calculations have been done when the hopping $t_{\rm AB}$ from a doubly occupied site to an empty site (or, hopping from a single occupied site to a single occupied site) has higher probability, this favoring pairing. Here, we put $U = V = 0$ in order to observe only the effects of the bond-charge interaction term on Δ. In this figure the electron-hole symmetry is preserved since $t_{\rm A} = t_{\rm B}$ and the $t_{\rm AB}$ term in equation (5) did not change after the transformation.

The effect of $t_{\rm A}$ and $t_{\rm B}$ on the binding energy is shown in Figure 5 (for $t_{\rm B} = t_{\rm AB} = -1$) and in Figure 6 (for $t_{\rm A} = t_{\rm AB} = -1$) respectively. From Figure 5, it is clear that increasing $t_{\rm A}$ favors pairing of electrons although $t_{\rm A} > t_{\rm AB}$, in contrast with the two-particle case. This shows the strong effect of the additional term $(t_{\rm A} - t_{\rm AB}) n_{i,-\sigma} n_{j,-\sigma}$. The effect of $t_{\rm B}$ is much weaker as compared to $t_{\rm A}$, since the number of possibilities of hopping from a doubly occupied site to a singly occupied one is much smaller than hopping from a singly occupied site to an empty one. Therefore pairing electrons requires larger values of $t_{\rm B}$.

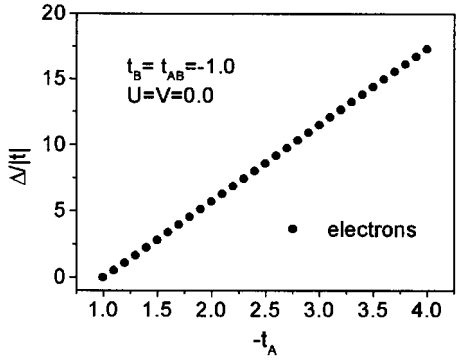

Fig. 5. Binding energy for the case of three electrons in a chain as a function of the $t_{\rm A}$ parameter and with $U = V = 0$.

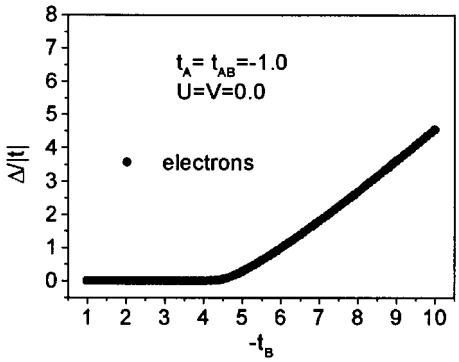

Fig. 6. Singlet-binding energy of three electrons in a linear chain *versus* the $t_{\rm B}$ parameter, and without on-site and nearest-neighbor interaction.

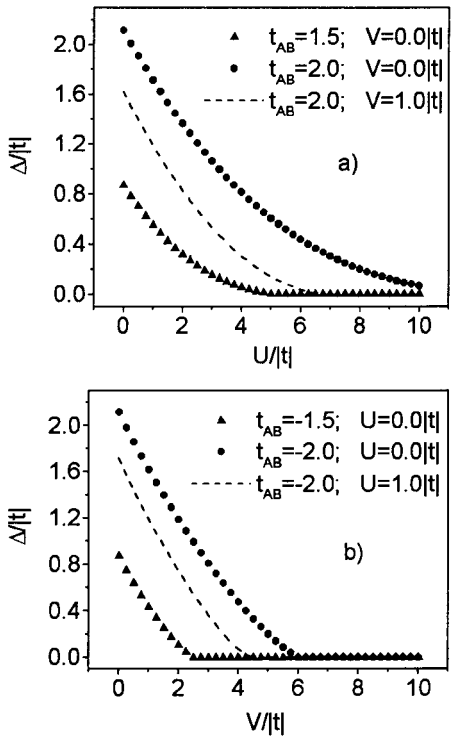

Fig. 7. In (a), the binding energy is shown for electrons or holes as a function of the repulsive on-site interaction U for two values of the repulsive nearest-neighbor interaction, $V = 0$ and $V = 1.0|t|$, and also for two values of the $t_{\rm AB}$ hopping parameter $t_{\rm AB} = 1.5|t|$ and $t_{\rm AB} = 2.0|t|$. In (b) we show the binding energy as a function of V for the same hopping parameters but for two on-site interaction, $U = 0$ and $U = 1.0|t|$.

In fact, the effect of the parameter $t_{\rm B}$ results from a single band-impurity in the tight-binding Hamiltonian (see dotted line in Fig. 2), while $t_{\rm A}$ provides a large number of band-impurities as can be seen in Figure 2.

As already mentioned the results for holes are simply obtained from electrons by interchanging $t_{\rm A}$ and $t_{\rm B}$. For example, the behavior of the hole-binding energy as a function of the $t_{\rm B}$ parameter is the same as that given in Figure 5 for electrons and the corresponding results for the $t_{\rm A}$ parameter are those of Figure 6. Thus, from Figures 5 and 6 we can observe clearly the electron- and hole-pairing asymmetry, where pairing holes is not always easier than pairing electrons.

Let us now consider the behavior of Δ as a function of U (Fig. 7a) and as a function of V (Fig. 7b) for electrons, with two different values of the $t_{\rm AB}$ parameter and with $t_{\rm A} = t_{\rm B} = -1$. Here, the nearest-neighbor interaction has the values $V = 0$ and $V = 1.0|t|$ in Figure 7a, and the on-site interaction has the values $U = 0$ and $U = 1.0|t|$ in Figure 7b. Both U and V reduces the pairing, but as a result of the increased $t_{\rm AB}$, we can obtain a binding energy even when both interactions are positive. U and V tend to reduce pairing in doubly occupied sites and nearest-neighbor single occupied sites, thus weakening the role of the $t_{\rm AB}$ hopping processes. However, in the case considered ($t_{\rm AB} > t_{\rm A}, t_{\rm B}$), V appears to be more efficient than U in breaking electrons or hole paring. The results correspond to a phase diagram similar to Figure 3, but with the boundary between pairing and non-pairing region eventually pushed toward positive U and V.

In Figures 8a, b, we show the electron-binding energy as a function of U and V respectively for two different values of $t_{\rm A}$ and with $t_{\rm AB} = t_{\rm B} = -1$. In order to see the behavior of the hole-binding energy for the $t_{\rm A}$ parameter we should take Figures 9a, b but changing $t_{\rm B}$ by $t_{\rm A}$. From all these figures, we can observe clearly the electron-hole asymmetry and also that the pairing strength between electrons is stronger than for the hole case. The latter happens because the large number of $t_{\rm A}$ bond-impurities for the electron case dominates over the single $t_{\rm A}$ bond-impurity for the hole case. We can also see the hyperbolic behavior of Δ for the electron case, which show us the strong dependence on the correlated hopping.

In Figures 9a, b, we show the evolution of the electron-binding energy as a function of the on-site and the nearest-neighbor interaction respectively, using two values of the parameter $t_{\rm B}$ and with $t_{\rm A} = t_{\rm AB} = -1$. The behavior of the hole-binding energy is the same as in Figure 8 but changing $t_{\rm A}$ by $t_{\rm B}$. From all these figures we can see that the pairing strength between holes is stronger than in the electron case. The reason is similar to that given in the previous paragraph, for the electron case the effect

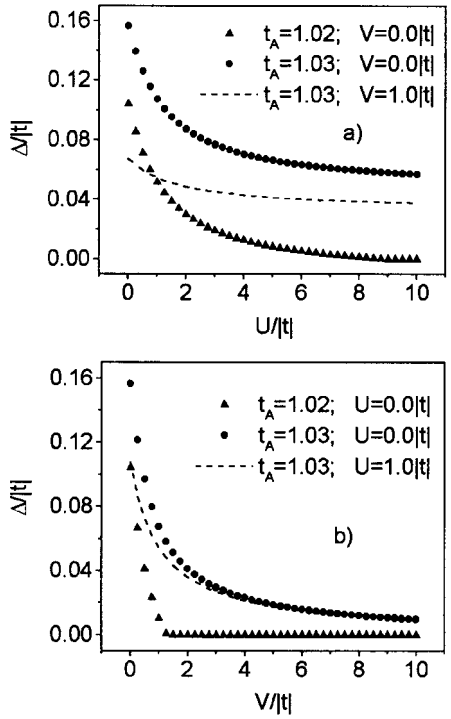

Fig. 8. In this figure, the electron binding energy is shown for two different values of the $t_{\rm A}$ parameter as a function of the repulsive on-site interaction U (a) and as a function of the repulsive nearest-neighbor interaction V (b). This figure also gives the behavior of the hole binding energy but for the case of two different values of the $t_{\rm B}$ parameter, it means, we should simply change $t_{\rm A}$ by $t_{\rm B}$.

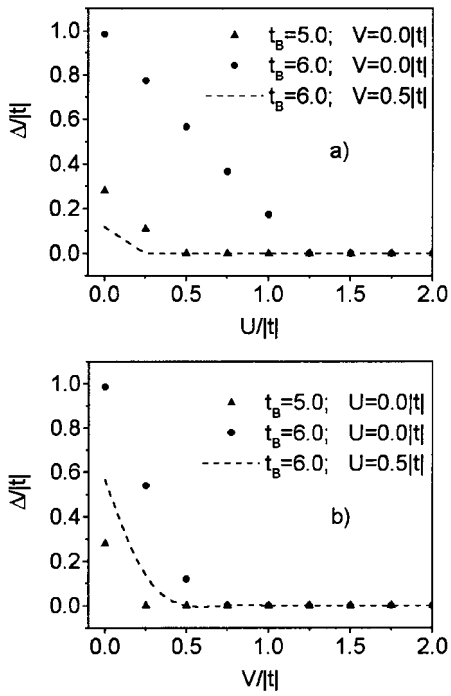

Fig. 9. Here, the electron binding energy is shown for two different values of the $t_{\rm B}$ parameter as a function of the repulsive on-site interaction U (a) and as a function of the repulsive nearest-neighbor interaction V (b). This figure also gives the behavior of the hole binding energy but for the case of the $t_{\rm A}$ parameter, it means, we should simply change $t_{\rm B}$ by $t_{\rm A}$.

on the binding energy results from only one bond-impurity (see dotted line in Fig. 2) while for the hole case we have a large number of $t_{\rm B}$ bond-impurities.

4 Conclusions

We have studied the electronic correlation within the generalized Hubbard model, by extending the previously introduced real-space mapping method to include the bond-charge interaction term. The original correlated many-body problem has been mapped onto an equivalent site- and bond-impurity tight-binding one in a higher dimensional space, where the problem was solved exactly. The bond-charge interaction appears as bond-impurities and the on-site and nearest-neighbor interactions as site-impurities in the network of states. This study has been carried out for a system with three-correlated electrons in an infinite one-dimensional lattice, where an analytical solution has been obtained for some special values of the hopping parameters and all kind of interactions. A clear pairing asymmetry between electrons and holes is observed. It is found that the effects of a strong competition between the bond-charge interaction and the on-site and nearest-neighbor interaction in the three-body problems are definitely relevant for the behavior of the binding energy, in particular we established that the pairing strength for holes or for electrons depends strongly on the parameters of the bond-charge interactions.

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