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Pairing Phase Diagram of Three Holes in the Generalized Hubbard Model

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The pairing problem of a three electrons system has been studied by using a real-space method and the generalized Hubbard Hamiltonian. This method includes the correlated hopping interactions as an extension of the previously proposed mapping method, and 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 was solved in a non-perturbative way. In a linear chain, we analyzed the pairing phase diagram of three correlated holes for different values of the Hamiltonian parameters. For some values of the hopping parameters we obtain an analytical solution for all kind of interactions.

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1. INTRODUCTION

Investigations of high-T_c superconductors suggest that the electronic correlation may play a significant role in the formation of pairs [1]. 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 [2] that properties of the 1D and 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 Hubbard model is one of the simplest.

In this study, we will use the generalized Hubbard Hamiltonian (GHH)

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$$H = \sum_{<i,j>,\sigma} t^{\sigma}_{i,j} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{<i,j>} n_i n_j, \tag{1}$$

where U and V are the on-site and the inter-site interaction respectively. The generalized hopping amplitude for electrons, $t^{\sigma}_{i,j}$, is given by

$$\begin{aligned} t^{\sigma}_{i,j} &= t_A(1-n_{i,-\sigma})(1-n_{j,-\sigma}) + t_B n_{i,-\sigma} n_{j,-\sigma} + \\ & \quad t_{AB}[n_{j,-\sigma}(1-n_{i,-\sigma}) + n_{i,-\sigma}(1-n_{j,-\sigma})]. \end{aligned} \tag{2}$$

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 site and from a doubly occupied to an empty site, respectively. The special case $t_A = t_B = t_{AB} = t$ corresponds to the $t - U - V$ model.

When a particle-hole transformation is made in the GHH, i.e. electron operators are mapped into hole's via $c^{+}_{i,\sigma} \rightarrow h_{i,\sigma}$, the Hamiltonian becomes:

$$H = (U + 2ZV)(N - \sum_{i,\sigma} n^{h}_{i,\sigma}) - \sum_{<i,j>,\sigma} t^{\sigma,h}_{i,j} h^{+}_{j,\sigma} h_{i,\sigma}$$

$$+U \sum_{i} n^{h}_{i,\uparrow} n^{h}_{i,\downarrow} + \frac{V}{2} \sum_{<i,j>} n^{h}_{i} n^{h}_{j}, \tag{3}$$

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 $n^{h}_{i} = n^{h}_{i,\uparrow} + n^{h}_{i,\downarrow}$ with $n^{h}_{i,\sigma} = h^{+}_{i,\sigma} h_{i,\sigma}$. The first term in equation (3) only contributes to a shift in the total energy and the second term belongs to the generalized hopping parameter for holes ($t^{\sigma,h}_{i,j}$). The expression for $t^{\sigma,h}_{i,j}$ is the following:

$$\begin{aligned} t^{\sigma,h}_{i,j} &= t_B(1-n^{h}_{i,-\sigma})(1-n^{h}_{j,-\sigma}) + t_A n^{h}_{i,-\sigma} n^{h}_{j,-\sigma} + \\ & \quad t_{AB}[n^{h}_{j,-\sigma}(1-n^{h}_{i,-\sigma}) + n^{h}_{i,-\sigma}(1-n^{h}_{j,-\sigma})]. \end{aligned} \tag{4}$$

The main differences with the electron hopping are the change of t_A by t_B and the minus sign. In this paper, we analyzed the paring of three electrons in a one-dimensional lattice using the GHH. The analysis has been done by extending the mapping method previously reported [3] in order to include the bond-charge interaction.

2. RESULTS AND DISCUSSION

When the correlation hopping interaction is included, the previously reported mapping method [3] is modified. Let us see how this modification

takes place in the problem of three electrons, two with up-spin and one with down-spin in a linear chain. In this case, the network of three-electron states belongs to a three-dimensional lattice with site- and bond-impurities. For example, let us consider the three electrons in a 4-site chain. The state configuration is:

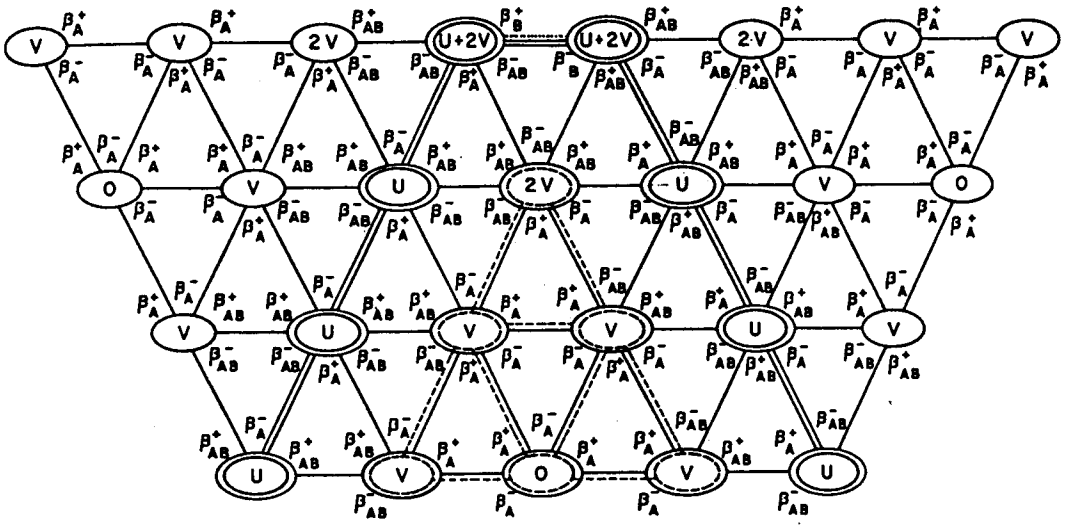

Fig. 1. Lattice of effective states for three electrons in a linear chain

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

Electrons with spin up and spin down are denoted by $+$ and $-$, respectively, a doubly-occupied site is indicated by $\pm$, and 0 represents an empty site. In the GHH, a state with a site occupied by two electrons requires an energy U and a state in which two electrons are situated in nearest-neighbor sites, requires an energy V. Finally, states with a site occupied by two electrons and an electron situated in a nearest-neighbor site requires an energy $U + 2V$, the remaining states with electrons placed at distant sites do not requires any energy. The amplitudes of the transition probability between nearest-neighbor states will depend on the site occupation and are given by t_A, t_B and t_{AB}. As we already mentioned, the geometric representation of the states belongs to a three-dimensional lattice, where taking advantage of the translational symmetry in this network of states, it can be projected onto a two-dimensional lattice of effective states.

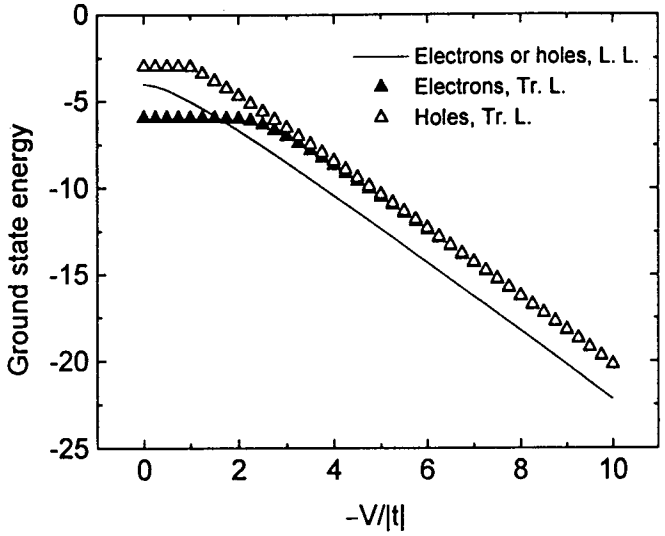

Fig. 2. Ground state energy versus V for $U = 0$. For V values larger than $-1.7|t|$ the linear chain has a dominant behavior.

The Fig. 1 shows the two-dimensional lattice of effective states for an original system with three electrons in a five-site chain, where the effective projected hopping parameters are: $\beta_A^+ = t_A e^{iKa/\sqrt{3}}$, $\beta_A^- = t_A e^{-iKa/\sqrt{3}}$, $\beta_B^+ = t_B e^{iKa/\sqrt{3}}$, $\beta_B^- = t_B e^{-iKa/\sqrt{3}}$, $\beta_{AB}^+ = t_{AB} e^{iKa/\sqrt{3}}$ and $\beta_{AB}^- = t_{AB} e^{-iKa/\sqrt{3}}$. Here, K is the wave vector and a is the lattice parameter.

Analyzing the network of states given in Fig. 1, one important limit is observed; when the hopping amplitude from a doubly occupied to an empty site is forbidden $\beta_{AB} = 0$. In this case, we can see that there is a competition between the linear chain of effective states with two site-impurities (shown in Fig. 1 by double lines) and the triangular lattice of effective states (shown in Fig. 1 by dash lines). The latter one is in fact the projected network of states for the problem of three electrons with parallel spin ($\uparrow\uparrow\uparrow$) in a linear chain. For $\beta_A = \beta_B$ the linear chain of effective states with two equal nearest-neighbors site-impurities with energy $2V$, has an analytical solution for the ground state energy given as follows:

$$E_{imp} = \frac{1}{D^2 - 16V^2}\left\{-32V^3 \pm D(8V^2 - D^2)\right\}, \tag{5}$$

where $D = |2zt|$. In Eq. (5), E_{imp} gives the two energies of the localized states for the two equal site-impurities. Using Eq. (5) the binding energy is given by $\Delta \equiv \max(|E_{imp}|) - D$.

In Fig. 2, numerical results of the ground state energy versus V ($U = 0$) are shown for the linear chain (double lines in Fig. 1) and the triangular

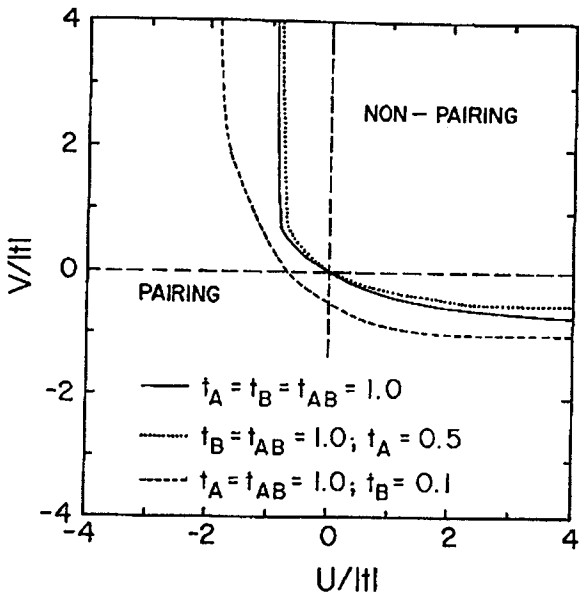

Fig. 3. Hole-singlet pairing phase diagram for three holes in a linear chain

lattice (dash lines in Fig. 1) for electrons and for holes. As we can see in this figure, for V values between 0.0 and $-1.7|t|$ the dominant behavior is the one for the triangular lattice associated to electrons, after those values the linear chain has a dominant behavior, the parameter t was equal 1. It is worth mentioning that the energy of holes in the triangular lattices never predominates. The peculiar behavior of the ground state energy for electrons and for holes in the triangular lattices come because of the nonbipartite nature of this lattice.

The essential difference between holes and electrons without electron-electron interaction is that the hopping amplitude is tA for electrons and $-tB$ for holes in the GHH.

Preliminary results of the hole-singlet phase diagram for different values of the hopping parameters and the on-site and inter-site interaction are shown in Fig. 3.

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