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Electronic correlation in the generalized Hubbard model: the diluted case

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We have solved the generalized Hubbard Hamiltonian for a system with few correlated electrons, using a real-space method. This method is based on mapping the many-body Hubbard problem onto an equivalent tight-binding problem in a higher dimensional space, where the problem can be solved in an exact way. We have obtained a solution for three non-parallel electrons in a linear chain. The correlation is studied by examining the ground state binding energy, for different values of the hopping parameters as well as the on-site and the inter-site interactions.

Keywords: Hubbard model; narrow band systems; many electrons systems

Se resuelve el hamiltoniano de Hubbard generalizado para un sistema de pocos electrones que estan correlacionados, usando un método en el espacio real. Este método se basa en mapear el problema de Hubbard de muchos cuerpos, hacia un problema equivalente de amarre fuerte en un espacio de mayor dimensión, donde el problema puede resolverse en forma exacta. Hemos obtenido una solución para un problema de tres electrones con espines anti-paralelos en una cadena lineal. La correlación se estudia examinando la energía de amarre del estado base para diferentes valores de los parámetros de salto, asi como de los parámetros de interacción tanto en el mismo sitio como en sitios distintos.

Descriptores: Modelo de Hubbard; sistemas de banda angosta; sistemas de muchos electrones

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1. Introduction

Within the models for correlated electron systems that attempt to capture the essential physics of high-T_c superconductors [1], the Hubbard model [2] is certainly one of the simplest models that include electronic interactions 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 [3], such as the nearest-neighbor interactions and the bond-charge interaction term. The Hamiltonian that includes these interactions is often called the generalized Hubbard Hamiltonian and has been studied previously by several authors [4-7]. This Hamiltonian can be written as

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

where $< i,j >$ denotes nearest-neighbor sites, $c^{+}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ where $n_{i,\sigma} = c^{+}_{i,\sigma}c_{i,\sigma}$, and the occupation-dependent hopping amplitude, $t^{\sigma}_{i,j}$, is given by

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

The 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 extended Hubbard model. 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 following a mapping method previously reported [8].

In Sect. II we introduce briefly the mapping method and we present an analyze of the results. Finally, in Sect. III a summary is presented.

2. Results and discusion

In this section, we study the correlation of three electrons by using the mapping method explained in Ref. 8 for different lattices topologies. In order to present a brief explanation of this mapping method, let us consider the case of two electrons with opposite spins in an N-site chain; the number of states is given by N^2. These states form a square lattice with $(3N-2)$ "impurities", which can be described by a single-body tight-binding Hamiltonian. N of these impurities, are localized along the principal diagonal of the square lattice with a self-energy U and the other $2(N-1)$, are localized on the two next-diagonals with a self-energy V. A simple way to obtain the solution is taking advantage of the translational symmetry of the impurities and projecting the two-dimensional lattice of states onto a linear chain of effective

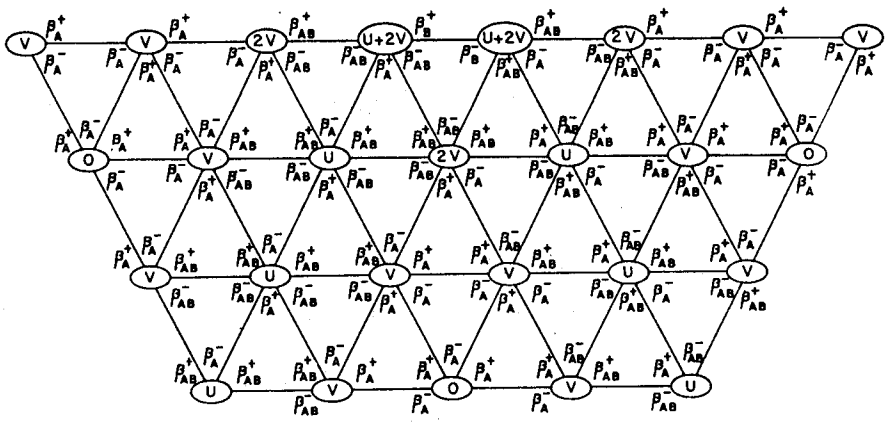

FIGURE 1. Lattice of effective states for three electrons with non-parallel spin in a linear chain. This effective states are represented by a ellipses and the self-energy for each of them is indicated inside. There are six different effective-hopping parameters β_A^+, β_A^-, β_B^+, β_B^-, β_{AB}^+, and β_{AB}^-, with values given in the text.

states, similar to the procedure introduced by Falicov and Yndurain [9]. In general, this method will map the original many-body problem onto a tight-binding one with some ordered impurities in an nd-dimensional lattice, being n the number of electrons and d the dimensionality of the original system. In this hyper-space lattice, the on-site (U) and the nearest-neighbor (V) interactions from the original Hubbard Hamiltonian become the self-energies of the impurities.

For the case of three electrons [10], two with up-spin and one with down-spin in a linear chain, the network of states belongs to a three-dimensional state lattice. For example, let us consider these three electrons in a 4-site chain. The state configuration is:

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

Spin up and down are denoted by $+$ and $-$, respectively, a doubly-occupied site by $\pm$, and a hole by 0. A site occupied by two electrons requires an energy U, and the amplitudes of the transition probability for nearest-neighbor states will be t_A, t_B and t_{AB}. As we already mentioned, the geometric representation of these 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.

In Fig. 1 we show the two-dimensional lattice of effective states for an original system with three electrons in a five-site chain, where the hopping parameters β_A^+, β_A^-, β_B^+, β_B^-, β_{AB}^+, and β_{AB}^- are given by

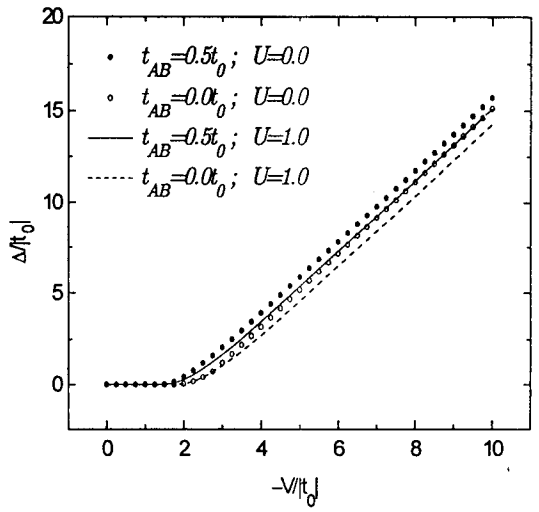

FIGURE 2. Binding energy (Δ) as a function of the nearest-neighbor atractive interaction ($-V$), for three non-parallel electrons in a linear chain. In this plot we made some variations of the t_{AB} hopping parameter for differents values of the on-site repulsion interaction term (U).

$$\beta_A^+ = t_A e^{iKa/\sqrt{3}}, \qquad \beta_A^- = t_A e^{-iKa/\sqrt{3}},$$
$$\beta_B^+ = t_B e^{iKa/\sqrt{3}}, \qquad \beta_B^- = t_B e^{-iKa/\sqrt{3}},$$
$$\beta_{AB}^+ = t_{AB} e^{iKa/\sqrt{3}}, \qquad \beta_{AB}^- = t_{AB} e^{-iKa/\sqrt{3}}.$$

Here, K is the wave vector and a is the lattice parameter. The two-dimensional results must also be integrated with respect to K within the first Brillouin zone.

The binding energy (Δ) as a function of the nearest-neighbor attractive interaction, is shown in Fig. 2 for the case of three non-parallel electrons ($\uparrow\downarrow\uparrow$) on a one-dimensional

infinite lattice. The binding energy has been calculated from the energy difference between the lowest correlated state ($K = 0$), and the original lower band edge when there is not an electron-electron interaction. The final numerical diagonalization were carried out for a truncated triangular lattice of 551 effective states. The matrix sizes for numerical diagonalizations were chosen as the minimum size so that the physical quantities, such as the binding energy, have not an important variation with the matrix size.

In Fig. 2, the binding energy was calculated for the case $t_A = t_B = t_0$, using different values of the hopping parameter t_{AB} and the on-site repulsive interaction (U). In this figure, we observed that the on-site interactions change the slope of Δ and that the variations of the t_{AB} parameter shift the binding energy. A linear behavior of Δ, for large values of the nearest-neighbor interaction, can also be observed.

3. Summary

We have studied a generalized Hubbard model with hopping depending on the occupation, using a simple mapping method. This study has been carried out in a real space for a system with three-correlated electrons in a one-dimensional lattice, where an exact solution has been obtained for this problem. In particular, we got the behavior of the binding energy for three non-parallel electrons with different values of U and t_{AB}.

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