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Physica C 341–348 (2000) 241–242

PHYSICA C

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Pairing of three holes in a one-dimensional lattice within the generalized Hubbard model

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Within the generalized Hubbard model, the pairing problem of a system of three correlated holes in a one-dimensional lattice is studied. This study has been done by extending the previously reported real-space mapping method [1], in order to incorporate the bond-charge interactions. The system is solved in a non-perturbative way for different values of the hopping parameters as well as the on-site (U) and nearest-neighbor (V) interaction. It is found an electron-hole pairing asymmetry, contrary to that for a bipartite lattice We also obtained, for some values of the Hubbard parameters, that the hole-singlet pairing is not always stronger than the electron case, in contrast with that for a non-bipartite lattice like the triangular one.

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 [2], 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 [3], 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) and has been studied previously by several authors [4–7]. This Hamiltonian is

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

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, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ where $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. The parameters U and V are the Coulomb integrals. In Eq. (1), the generalized 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 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 $t - U - V$ extended Hubbard model, which has been studied intensively by analytical and numerical methods [2]. The essential difference between electrons and holes within the GHH, besides a minus sign in the generalized hopping term, is that the hopping amplitude t_A for electrons should be changed by t_B for the case of holes in Eq. (2).

In this paper, we analyzed the paring of three non-parallel ($\uparrow\downarrow\uparrow$) holes and also the case of three non-parallel ($\uparrow\downarrow\uparrow$) electrons in a one-dimensional lattice using the GHH. The analysis has been done by extending the mapping method previously reported [1] in order to include the generalized hopping. Let us see how this modification take place in the problem of three electrons, two with up-spin and one with down-spin in a lin-

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PII S0921-4534(00)00460-3

ear chain. In this case, the network of the three-electron states belongs to a three-dimensional lattice with site- and bond-impurities, where taking advantage of the translational symmetry of this network of states, it can be projected onto a two-dimensional triangular lattice of effective states and effective hopping ($\beta_A^{\pm}$, $\beta_B^{\pm}$ and $\beta_{AB}^{\pm}$) [7].

For the ground state we have that: $\beta_A^{+} = \beta_A^{-} = t_A$, $\beta_B^{+} = \beta_B^{-} = t_B$ and $\beta_{AB}^{+} = \beta_{AB}^{-} = t_{AB}$. With these new values, analytical solutions can be obtained for some particular cases; for example, when the hopping amplitude from a doubly occupied to an empty site is forbidden ($t_{AB} = 0$), the solution is:

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

where $D = |2zt|$. In Eq. (3), E_{imp} gives the energies of the localized states. The binding energy (gap) is given by $\Delta = \max(|E_{imp}|) - D$.

Below, we show numerical solutions for variations of the hopping parameters and of the interaction terms. The numerical diagonalization were done in 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 have not an important variation with the matrix size.

The numerical calculation for Δ versus U for two different values of the t_{AB} parameter are shown in Fig. 1, a) for holes and b) for electrons. Here the nearest-neighbor interaction has the values $V = 0$ and $V = 1.0|t|$. In this figure, it can be observed an electron-hole pairing asymmetry caused by the frustration in our triangular lattice of effective states. It is also obtained, for different values of the t_{AB} hopping parameter, that the pairing strength between electrons is stronger than the hole case. It happen because the great number of bond-impurities dominates over the frustration in the triangular lattice of effective states. We can also see the hyperbolic behavior of the gap which show us the strong dependence on the correlated hopping.

Therefore, the effects of a strong competition between the bond-charge interaction and the frustration of antibonding states in the three-body problem are definitely relevant on the binding energy. Particularly, we obtained that the hole pairing is not always stronger than the electron case, in contrast with that for a triangular lattice in the Hubbard model [8].

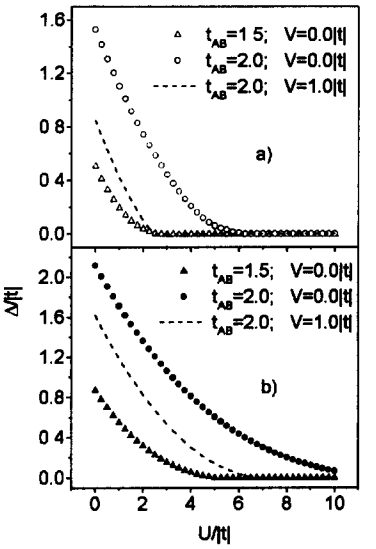

Fig. 1. Binding energy vs. the repulsive interaction U for holes a) and for electrons b).

Acknowledgment: This work was partially supported by grants from DGAPA-UNAM IN109998 and by CONACyT 25582-E.

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