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Exact results for three electrons in a linear chain within the Hubbard model

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Abstract

In this work we analyzed the ground-state symmetry for the cases of three particles in a linear chain, using the generalized Hubbard Hamiltonian and a previously developed real-space mapping method. The method is based on mapping the correlated many-body problem onto an equivalent site- and bond-impurity one-body problem in a higher dimensional space, where the problem can be solved exactly. For the case of three particles, it is obtained a ground-state when the correlated hopping interactions are included. A clear asymmetry between electrons and holes is observed due to the bond–charge interactions. The three-particle problem is analyzed by looking at the phase diagram for the bound state.

Keywords: Hubbard model; Bound states; Fermions in reduced dimensions

The electronic correlation has considerable interest due to its significant role in the formation of pairs suggested by investigations in superconductivity, especially those ones coming from high-T_c superconductors [1]. Although the main study concern to the physics of two-dimensional correlated electron system, the one-dimensional models related to high-temperature superconductivity are very popular due to the conjecture [2] that properties of the one- and two-dimensional variants of certain models have common aspects. Within the models that attempt to capture the essential physics from correlated electrons systems, the simple Hubbard model is the crudest approximation to include electronic interaction between band-electrons. A generalization of this model that include also the nearest-neighbor interactions and the bond–charge interactions is called the generalized Hubbard Hamiltonian (GHH), which can be written as

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

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 $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. The parameters U and V are the Coulomb integrals. In Eq. (1), the generalized hopping amplitude, $t^{\sigma}_{i,j}$, is given by

$$t^{\sigma}_{i,j} = t_A + (t_{AB} - t_A)(n_{i,-\sigma} + n_{j,-\sigma}) + (t_A + t_B - 2t_{AB}) n_{i,-\sigma} n_{j,-\sigma}, \tag{2}$$

written in this form to emphasize the contribution from two- and four-fermion operators. These new interactions may give arise to new dynamical effects, absent in the simple Hubbard model. For the two-particles problem the term $(t_A + t_B - 2t_{AB}) n_{i,-\sigma} n_{j,-\sigma}$ in Eq. (2) is ineffective. In this two-particles case, assuming that $t_A > t_{AB} > t_B$, the hopping parameter reduces to $t^{\sigma}_{i,j} = t_A - (t_A - t_{AB})(n_{i,-\sigma} + n_{j,-\sigma})$.

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 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

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electrons should be changed by t_B for the case of holes in Eq. (2) [3].

In this paper, we analyzed the bound states of three non-parallel ($\uparrow\downarrow\uparrow$) electrons and also the case of three non-parallel ($\uparrow\downarrow\uparrow$) holes in a one-dimensional lattice using the GHH. The bound-state is the lowest correlated state and its energy is obtained for $K = 0$ in the case of electrons and for $K/\sqrt{3} = \pi$ for the hole case. The analysis has been done by extending the mapping method previously reported [4], in order to include the bond–charge interactions. The discussion is done following the paper by Espinosa et al. [3]. Let us see how this modification takes place in our problem of three electrons. 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 $\beta_{AB}^{\pm}$) [3].

In Fig. 1, the ground-state phase diagram for both electron-singlet and hole-singlet is shown. In this figure, we show the phase diagrams for different values of the hopping parameters; once the hopping parameter is chosen in each plot the other two parameters are equal to -1. From Fig. 1, it is clear that with a very small increase of t_A, the bound states of electrons are favored although $t_A > t_{AB}$, in contrast with the two-particles case. This shows the strong effect of the additional term $(t_A - t_{AB})n_{i,-\sigma}n_{j,-\sigma}$. The effect of t_B is much weaker as compared to t_A, since in this case we need larger values of t_B hopping parameter. When the hopping t_{AB} from a doubly occupied site to an empty site has higher probability, this favors bound states, and the electron–hole symmetry is preserved since $t_A = t_B$ for this case.

As we have mentioned above the results for holes are simply obtained from electrons by interchanging t_A and t_B. Thus, from Fig. 1 we can observe clearly the electron- and hole-asymmetry, where bounding holes are not always easier than bounding electrons.

In conclusion, we have analyzed the bound states of three electrons in an infinite linear chain. The analysis

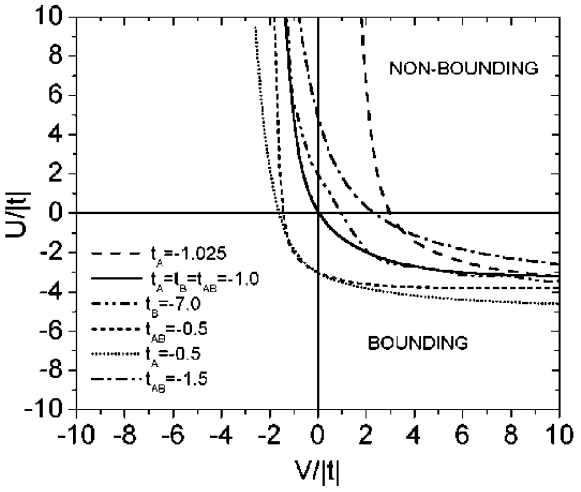

Fig. 1. Bounding phase diagrams for three electron in a linear chain. When one of the hopping parameter is chosen the other two are equal to -1.

was done, using the generalized Hubbard Hamiltonian and extending the real space mapping method to include the bond–charge interaction term. We observed clearly an asymmetry between electron and holes bound states, this asymmetry being due to the bond–charge interaction.

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