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The generalized Hubbard model: a solution for the binding of three particles in a linear chain

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Abstract

The binding problem is studied within the generalized Hubbard Hamiltonian by using a real-space method. This method is an extension of the previously proposed mapping method for the simple Hubbard model in order to include the bond–charge interaction term. 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. The three particles correlation in a linear chain has been analyzed by calculating the binding energy using different values of the bond–charge, the on-site (U) and the nearest-neighbor (V) interactions. A bound state asymmetry between electrons and holes was found for bond–charge interactions. Also, an analytical solution is obtained for some special values of the hopping parameters and for all kind of interactions in the Hubbard Hamiltonian.

Keywords: Hubbard model; Three particles bound states; Fermions in reduced dimensions

The simple Hubbard model [1], 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 [2], 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 is 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

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

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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.

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

The special case $t_A = t_B = t_{AB} = t$ corresponds to the t–U–V extended Hubbard model. For $t_A + t_B - 2t_{AB} = 0$, the generalized hopping amplitude is reduced to the Hirsch and Marsiglio model [4], proposed as a possible mechanism for superconductivity. An occupation dependent hopping term of the form (2) arise 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 [5]. There is, however, no consensus on the hopping amplitude in real systems [6]. So, in order to keep the model as general as possible, we will not put constraints in the values of the hopping term.

The electronic correlation for the low density limit, mainly the two particles case, has been intensively studied by analytical and numerical methods using the Hubbard model [1,7,8]. 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 questions are 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 particles case. It was considered earlier by Mattis [9] in his study of the bound state stability for the attractive-U Hubbard model and by Fabrizio et al. [10] for the repulsive-U case, who discussed an asymptotic behavior of the ground state.

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

$$t^{\sigma}_{i,j} = t_A - (t_A - t_{AB})(n_{i,-\sigma} + n_{j,-\sigma}) \tag{3}$$

and

$$t^{\sigma,h}_{i,j} = t_B + (t_{AB} - t_B)(n^h_{i,-\sigma} + n^h_{j,-\sigma}) \tag{4}$$

implying that the hopping of a hole increase in the presence of another hole and can lead to pairing of holes but not of electrons. The term $(t_A + t_B - 2t_{AB})n_{i,-\sigma}n_{j,-\sigma}$ now becomes effective for the three-particles problem and may modify the above statement as we show in the paper.

In this paper, we analyzed the bound state 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 [7], in order to include the generalized hopping. The discussion is done following the paper by Espinosa et al. [3]. Let us see how this modification take 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 ($\beta^{\pm}_A$, $\beta^{\pm}_B$ and $\beta^{\pm}_{AB}$) [3].

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:

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

where $D = |zt_A|$. The binding energy (gap) is given by $\Delta = \max(|E_{\mathrm{imp}}|) - D$.

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.

In Fig. 1, we show the ground-state phase diagram for both electron-singlet and hole-singlet in a

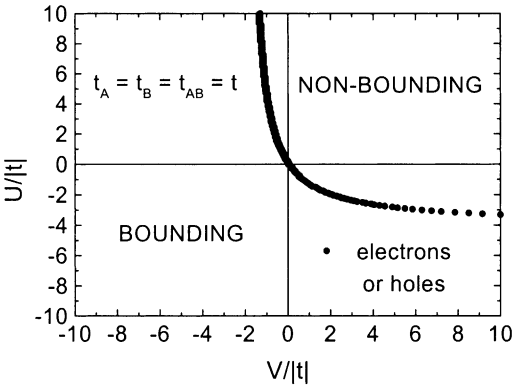

Fig. 1. Bounding phase diagram for the case of three electrons or three holes in an infinite linear chain within the extended Hubbard model ($t_A = t_B = t_{AB} = t$).

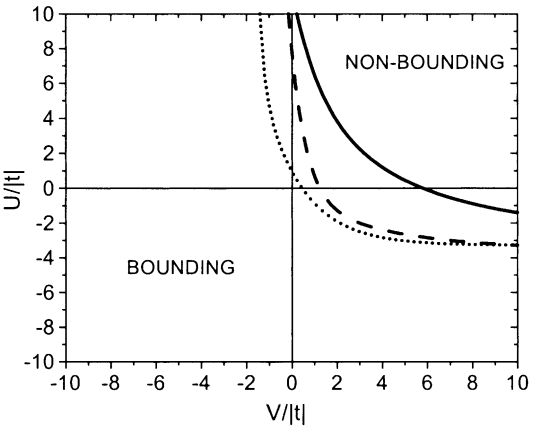

Fig. 2. Bounding phase diagram for three electrons: dash line gives the results for $t_A = -1.02$, $t_B = t_{AB} = -1.0$; dot line for the case $t_B = -6.0$, $t_A = t_{AB} = -1.0$ and solid line for $t_{AB} = -2.0$, $t_A = t_B = -1.0$.

linear chain for the Hubbard model $t_A = t_B = t_{AB} = t$. In this figure, we can notice the electron–hole symmetry and the absence of bound states for U and V positives which is very well established.

In Fig. 2, we present the numerical calculations for the phase diagram of the electron binding energy: dash line gives the results for $t_A = -1.02$, $t_B = t_{AB} = -1.0$; dot line for the case $t_B = -6.0$, $t_A = t_{AB} = -1.0$ and solid line for $t_{AB} = -2.0$, $t_A = t_B = -1.0$. From Fig. 2, it is clear that with a very small increase of the t_A hopping parameter, 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 (solid line in Fig. 2) has higher probability, this favors bound states, and the electron–hole symmetry is preserved since $t_A = t_B$.

As we mentioned above the results for holes are simply obtained from electrons by interchanging t_A and t_B. Thus, from Fig. 2 we can observe clearly the electron- and hole-asymmetry, where bounding holes is not always easier than bounding electrons.

In conclusion, we did non-perturbative calculation to study the correlation of three electrons in an infinite linear chain. This study was done, using the GHH and extending the real space mapping method to include the bond–charge interaction term. We observed clearly an asymmetry between electron and holes, this asymmetry being due to the bond–charge interaction.

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