



Few correlated particles in the Hubbard model

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Abstract

The ground state binding energy of few particles in an infinite one-dimensional periodic and quasiperiodic lattice is investigated rigorously in a Hubbard-like model, using a real-space method. We studied the three-body problem in the periodic lattice with correlated hoppings, for the case of non-parallel spin in an infinite linear chain, applying the generalized Hubbard Hamiltonian. The correlation is studied for different values of the hopping parameters as well as the on-site and the inter-site interactions. The results show an effect of the frustration of antibonding states on the pairing behavior. In the case of one-dimensional quasiperiodic lattice we give some preliminary results for two electrons with non-parallel spin. © 1999 Elsevier Science B.V. All rights reserved.

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The properties of correlated electron systems are usually modelled by the Hubbard Hamiltonian. The Hubbard model is one of the simplest models which considers the local interactions to be appropriate to describe the short-range electron or hole pairings. The on-site Coulomb interaction (U) is the leading term of the model, but in some circumstances other contributions of the electron–electron interactions are required, such as that for correlated hopping and for intersite interactions (V) [1,5]. The Hamiltonian which includes these terms is often called the generalized Hubbard Hamiltonian [2,6,7]. The purpose of the present work was to determine the pairing in a one-dimensional periodic lattice for three electrons or three holes and in a quasiperiodic chain for two electrons, using the Hubbard model and a real space mapping method developed previously [3,8–10].

In order to present a brief description of the mapping method, let us consider the case of two electrons with

opposite spins in an N -site chain; the number of states in this system 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. The N of these impurities, are localized along the principal diagonal of the square lattice with a self-energy U and the others, $2(N - 1)$, are localized on the two next-diagonals with a self-energy V . A simple way to obtain the solution is to take advantage of the translational symmetry of the impurities and to project the two-dimensional lattice of states onto a linear chain of effective states. In general, this method will map the original many-body problem onto a tight-binding one with some ordered impurities in a nd -dimensional lattice, n being the number of electrons and d the dimensionality of the original system.

For the three-body problem in a periodic chain, the projected lattice of effective states is a two-dimensional triangular lattice, which has been explained in detail in Refs. [4,11]. The binding energy (Δ) for both electron and hole cases with three non-parallel spin ($\uparrow\downarrow\uparrow$) as a function of the nearest-neighbor attractive interaction is shown in Fig. 1. The essential difference between these two cases is that the sign of the hopping parameter t_0 in the Hubbard model, has been taken to be equal to -1 for electrons

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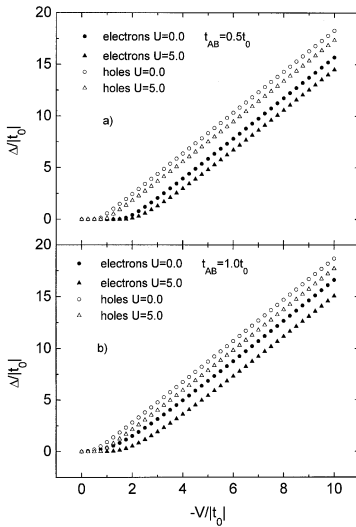


Fig. 1. Binding energy (Δ) as a function of the intersite attractive interaction (V), for three non-parallel electrons or holes in a linear chain.

and $+1$ for holes. The final numerical diagonalization were carried out for a truncated triangular lattice of 551 effective states. The matrix sizes for numerical diagonalizations have been chosen as the minimum size such that the physical quantities no longer have significant variation with increasing size. In Fig. 1, the calculations have been done 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), where t_A , t_B and t_{AB} are the hopping amplitudes from a single occupied site to an empty site, from a doubly occupied to a singly occupied site and from a doubly occupied to an empty site, respectively. In this figure, it is observed that the pairing strength between holes is always stronger than the electron case and increases as t_{AB} decreases, this asymmetry is caused by the frustration of antibonding states.

On the other hand, applying the real-space mapping method described previously to the problem of two electrons with anti-parallel spins in a Fibonacci chain, we obtain that the states configuration belongs to a two-dimensional network of states with hopping quasi-periodic symmetry in different directions. The lattice of states also has N impurities localized along the principal diagonal with a self-energy U and $2(N - 1)$ impurities localized on the two next-diagonals with a self-energy V . The numerical diagonalization was carried out in half of this two-dimensional lattice of states for a size of 630 sites. In Fig. 2, we plot the binding energy as a function of the on-site attractive interaction for the Fibonacci hopping parameters with values given by $t_a = -1.0$ and

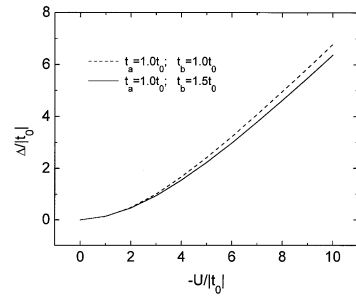


Fig. 2. Binding energy (Δ) as a function of the onsite attractive interaction (U), for two non-parallel electrons in a Fibonacci chain.

$t_b = -1.5$. It is worth mentioning that for the special case $t_a = t_b = -1.0$, our problem corresponds to the two-electron problem in a linear chain. The results for this case were previously calculated [3,8–10], and are included here for comparison with our present results.

In conclusion, we have studied the binding energy of few particles in a one-dimensional periodic and quasi-periodic lattice. The study of the periodic lattice has been done for three particles with non-parallel spins in both electron and hole cases with correlated hopping. It is observed that an asymmetry between electron and hole pairing is caused by the frustration of antibonding states. For the quasi-periodic lattice, we have studied the case of two electrons with non-parallel spin in a Fibonacci chain where we obtain the behavior of the binding energy for different values of U .

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