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Two- and three-body correlation in dilute Hubbard systems

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Abstract

In order to find an exact solution for the Hubbard systems with few electrons, we have developed a new method, which consists of mapping the original many-body problem onto a tight-binding one in a higher-dimensional space. Applying this mapping method to a chain, a square lattice and a triangular one, the pairing problem of two electrons and two holes with anti-parallel spins has been analyzed by looking at the binding energy and the coherence length for attractive interactions. Finally, some results of the three-body correlation are also reported.

The Hubbard model has been extensively used to describe a variety of cooperative phenomena, such as, charge density wave [1], spin density wave [2], and superconductivity [3], since it is probably the *simplest* model which takes into account the many-body effects. In spite of its simplicity, rigorous results have been obtained only for one [4] and infinite [5] dimensions. Recently, the pairing problem has been studied by using k -space [3, 6]. In this paper, the mapping method developed previously [7] is applied to analyze electron and hole correlation in one- and two-dimensional low-density systems using the extended Hubbard Hamiltonian (EHH).

In order to present a brief explanation of the mapping method, let us consider the case of two electrons with opposite spins in a square lattice. There are N^2 possible states, where N is the number of sites of the lattice. These states form a hyper-cubic network in a 4-dimensional space, which can be described by a tight-binding Hamiltonian, as explained in detail in Ref. [7]. A simple way to obtain the solution is taking advantage of the translational symmetry of the network of states in two

directions and mapping this 4-dimensional network onto a 2-dimensional one, similar to that introduced by Falicov and Yndurain [8]. This mapped lattice is also a square one, which has a center “impurity” with a site-energy U , surrounded by four V -energy “impurities”, and the remainder states with null site energies, where U and V are, respectively, the on-site and the nearest-neighbor interactions in the EHH. For a triangular lattice, the mapping procedure is the same as the square lattice case explained before, except that the final mapped lattice is a triangular one, where a central U -site is surrounded by six V -sites, and the remaining states with null site energies [9]. The mapped lattices can be solved numerically, where the exact diagonalization was carried out in a truncated square lattice of 2401 effective states, and in a truncated triangular lattice of 2269 effective ones. The variations of the binding energy (Δ) and the coherence length (ξ) as functions of U are shown in Fig. 1(a) and 1(b), respectively. Notice that for triangular lattices, the holes can be paired by on-site attractions ($-U$) more easily than for the electron case. This asymmetry between electron and hole pairing is caused by the frustration of several anti-bonding states in triangular lattices. It is worth mentioning that the results of Δ for the

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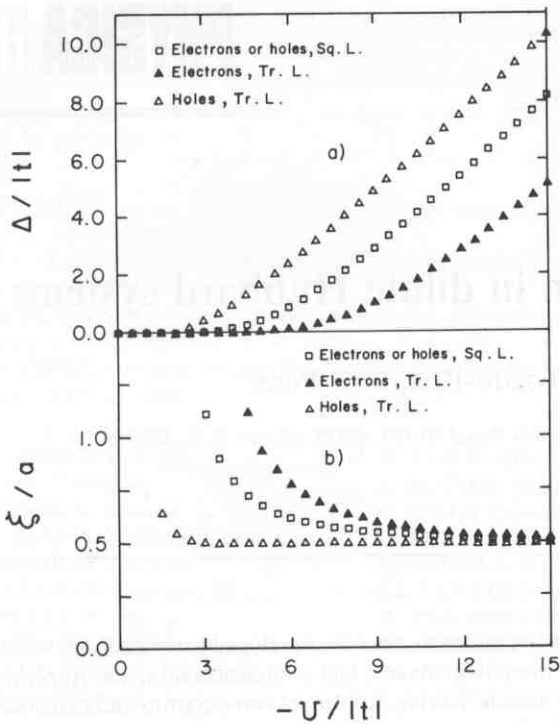


Fig. 1. Plots of (a) the binding energy (Δ) and (b) the coherence length (ξ), for electrons and holes with opposite spins with an on-site attractive interaction ($-U$) in a square and a triangular lattice.

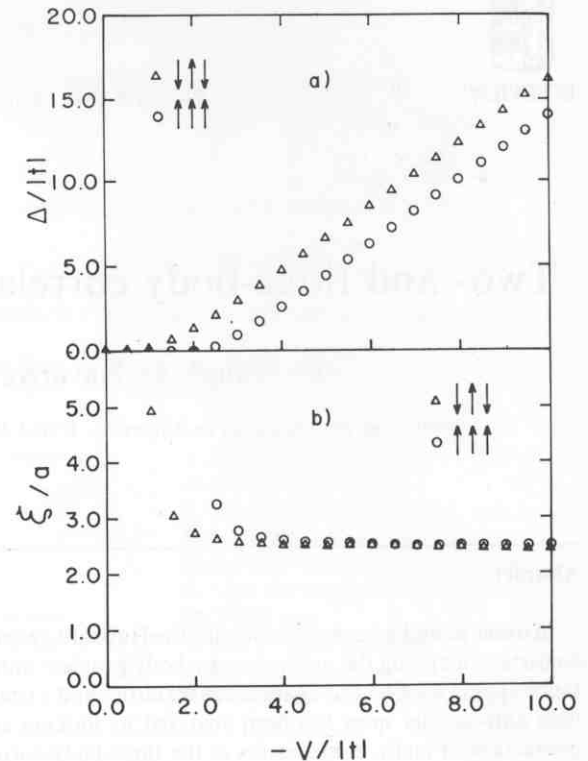


Fig. 2. A comparison of (a) the binding energy (Δ), and (b) the coherence length (ξ) between the parallel and non-parallel cases for three electrons with an inter-site attractive interaction ($-V$) in a linear chain.

square lattice coincide with those calculated by Micnas et al. [3].

For the three-body problem in a linear chain, the mapped lattice is a two-dimensional one, which has been explained in detail in Ref. [10]. The numerical calculations were carried out for a truncated lattice of 1176 and 1276 effective states for the parallel ($\uparrow\uparrow\uparrow$) and non-parallel cases ($\downarrow\uparrow\downarrow$), respectively. Figure 2 shows the results of Δ and of ξ as functions of V for the three-electron case. Δ has been calculated from the energy difference between the lowest correlated state ($K=0$) and the original lower band edge when there is no electron–electron interaction. Likewise, ξ is computed from $|\psi(r_{1,2}, r_{1,3})|^2$, where $r_{i,j}$ is the distance between electrons i and j . The results presented in Fig. 2b, were obtained from $r_{1,2} = a$ and $|\psi(a, \xi)|^2 = \max(|\psi(a, r_{1,3})|^2)/e$. In Fig. 2b, it is observed that the coherence length for the non-parallel case is always larger, and this behavior is similar to the two-body case [10].

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