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Few particles correlation in a one-dimensional quasiperiodic lattice

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During the last two decades, two of the most important discoveries in condensed matter physics have been the discovery of quasicrystals and the discovery of high-Tc ceramic superconductors. These topics have generated a large number of experimental and theoretical studies in the physics of low dimension. They have also modified some of the concepts in solid state physics. For instance, it was believed that the five-fold symmetry was incompatible with a long-range order and it was not expected that ceramic materials with a high-Tc and a short coherence length exhibit superconductivity. Therefore, it is important to revise both the spatial symmetry and the electronic correlation to identify how they affect the physical properties of materials. The study of these subjects is complex since we cannot use the reciprocal space to study quasicrystals and the electronic correlation in many-body systems has not entirely been solved. Even in one-dimensional quasiperiodic structures, the interactions between electrons have often been neglected and only few results have been obtained. In this work, we solved the cases of two and three interacting particles in a Fibonacci lattice using a real-space method, the Green function technique, the renormalized perturbation expansion method and the Hubbard model. For the case of two interacting particles an analytical solution for the pairing phase diagram was obtained using the extended Hubbard Hamiltonian. For the case of three interacting particles the binding energy was numerically calculated. The results present here are compared with those obtained for the periodic and binary lattices.

1 Introduction

Quasicrystals constitute a class of solids different from both crystals and glasses, since they simultaneously exhibit sharp diffraction peaks and an icosahedral point-group symmetry. The former showed long-range order, whereas the latter is incompatible with lattice periodicity. Since the discovery of quasicrystals [1], significant progress has been made in determined their structural, static, and dynamic properties [2]. Perhaps the most widely studied one-dimension model is based on the Fibonacci sequence which draws attention after two interesting papers by Kohmoto et al. [3] and Ostlund et al. [4]. The spectral properties of the Fibonacci chain are exotic, the single-particle eigenstates are neither extended nor localized but critical and the spectrum is a Cantor set [3, 4]. A Fibonacci sequence consists of two letters, A and B, and the entire sequence is generated by successive application of the substitution rule. The first few generations are $G_0 = B$, $G_1 = A$, $G_2 = AB$, $G_3 = ABA$, $G_4 = ABAAB$, …, $G_i = G_{i-1}G_{i-2}$ for $i \geq 2$, where G_i indicates the i-th generation. In a Fibonacci chain, the letters A and B from the Fibonacci sequence may denote two different atoms (site model) or two different bonds separating identical atoms (transfer

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model). In this work, the transfer model will be studied, where the hopping integrals take two values, t_A and t_B, that correspond to a short bond and a large bond respectively. In the transfer model the number of short bonds is $N_A(n)$ and the number of large bonds is $N_B(n)$. The total number of bonds in a generation n is represented by $N(n)$, $N(0) = N(1) = 1$. These numbers relate as follow:

$$N(n) = N(n-1) + N(n-2), \qquad N_A(n) = N(n-1), \qquad N_B(n) = N(n-2). \tag{1}$$

In the quasiperiodic limit $(n \to \infty)$, the ratio $N_A(n)/N_B(n)$ converges toward the golden mean $\sigma = \left(\sqrt{5}+1\right)/2$.

The Hubbard model [5] is the simplest one used to describe correlations in narrow-band systems and has been extensively studied. However, even when the Hubbard model is conceptually very simple, it is very difficult to solve it in general. It has been solved exactly only in one-dimension for a periodic system [6] where the ground state has proved to be antiferromagnetic and insulating for $U > 0$ at half-filled band. The extended Hubbard Hamiltonian may be written in real space as [7]:

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

where $\langle i, j\rangle$ denotes nearest-neighbor sites, $c^{+}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin $\sigma = \uparrow$ or $\downarrow$ at site i, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ with $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. The parameters of the Hamiltonian are: $t_{i,j}$ the hopping integral, U the on-site Coulomb interaction and V the nearest-neighbor Coulomb interaction. It is worth mentioning that in principle, the parameters U and V are positive because they are direct Coulomb integrals. However, U and V could be negative if attractive indirect interaction through phonons or other bosonic excitations are included and are stronger than the direct Coulomb repulsion.

In this paper, we wish to address the low-density limit, the case of two and three interacting particles in a one-dimensional quasiperiodic empty lattice. Within the extended Hubbard Hamiltonian we presented, for the two-particles case, the analytical solution for the full pairing phase diagram, and for the three-particles case we calculated numerically the binding energy for different values of the interaction.

2 Results and discussion

The Hamiltonian in Eq. (2) is analyzed by using the mapping method previously reported [7]. This method maps the original many-body problem onto a one-body one with some ordered site-impurities in a nd-dimensional lattice, n being the number of particles and d the dimensionality of the original system. Usually, the nd-dimensional lattice (lattice of states) has a translational symmetry which can be used to project the configurational space to a $(n-1)d$-dimensional lattice of effective states.

For the case of two-particles with non-parallel spins in a Fibonacci lattice, the mapping method and the projection technique can be applied. We should finally solve a one-dimensional lattice of effective states with effective hopping between these states given by [8]:

$$\beta = 2t_B \left(\frac{\sigma f + 1}{\sigma + 1} \right), \tag{3}$$

where $t_A = f t_B$. Using the Renormalized Perturbation Expansion [8] and the one-body Hamiltonian associated to the new lattice of effective states, we find that the condition for pairing is:

$$\sqrt{(1+u)(1+w)} - 1 < 0 \,, \tag{4}$$

with $u = U/B$, $w = 2V/B$ and $B = 2\beta$. The above equation gives the phase diagram between the pairing and non-pairing regions for all the parameters involved in the extended Hubbard Hamiltonian. The effects of the quasiperiodicity in the analytical expression for the pairing condition (Eq. (4)) are introduced

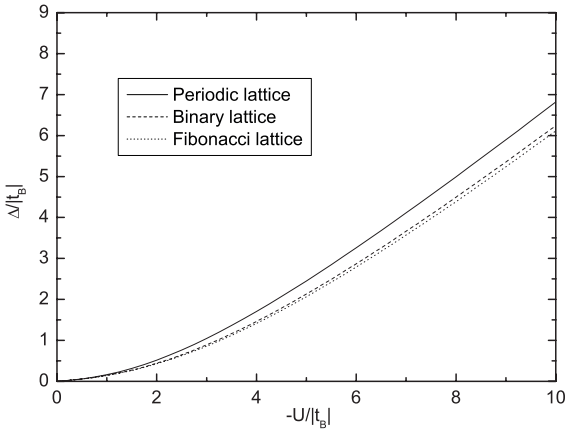

Fig. 1 Binding energy as a function of the on-site attractive interaction ($U<0$) with the nearest-neighbor interaction $V=0$, for the one-dimensional periodic, binary and quasiperiodic lattices.

through the effective hopping parameter β. The solution is exact for $f=1$ (periodic case) and is an approximation for $f\neq 1$. The approximation is valid for values not far from $f=1$.

For the three-particles with non-parallel spins in a Fibonacci chain, we found that the state configuration has a geometric representation in a three dimensional lattice with bond-quasiperiodic symmetry in different directions, which is also described by a tight-binding Hamiltonian.

The three dimensional network of states is solved using a projection technique [7]. For the ground state ($K=0$) it is possible to approximate the network of states onto a two-dimensional effective lattice of states. The effective hopping between effective states is given by

$$\beta = t_B\left(\frac{\sigma f+1}{\sigma+1}\right). \tag{5}$$

It is important to emphasize that the numerical solution presented here is for the case of three non-parallel ($\uparrow\downarrow\uparrow$) electrons in an infinite one-dimensional quasiperiodic lattice, within the extended Hubbard Hamiltonian. In order to analyze the pairing state, the binding energy was considered, which has been calculated from the energy difference between the lowest correlated state and the lowest non-correlated state localized at the lower non-interacting ($U=V=0$) three-particles band edge. The final numerical diagonalization was carried out for a truncated two-dimensional triangular lattice of 1751 effective states. The matrix sizes for numerical diagonalizations were chosen as small as possible so that the physical quantities will not vary significantly with the matrix size.

Figure 1 shows the binding energy as a function of the on-site interaction parameter (U) for the three particles in a Fibonacci lattice. It is important to remember that the interaction is always a two-body interaction as given by the Hamiltonian in (2). The results are compared with those of a periodic linear chain and the binary linear lattice. For the Fibonacci and the binary lattices the calculations were done for $t_A=2t_B$, $t_B=t$ and the nearest-neighbor interaction (V) equal cero. The parameter t is the hopping amplitude for a periodic lattice when correlations are not included and we will use it as our unit of energy, usually it is taking as $t=-1$ for electrons. As shown in Fig. 1 the pairing on-site electrons in a Fibonacci lattice require much more energy than the same pairing in a periodic linear chain.

Figure 2 shows the three particles binding energy as a function of the V parameter, with $U=0$ for the same cases mentioned above. As shown in Fig. 2 pairing electrons with nearest-neighbor interactions are easier to occur than electrons with on-site interaction in the three lattices already mentioned. Preliminary results for four and five number of electrons shows that the pairing difference with the two interacting parameters increases when the number of particles is odd. They also showed that the general behavior of the pairing between the three lattices remains similar to that already described above.

In conclusion, it has been studied the correlation in a one-dimensional quasiperiodic lattice within the dilute limit, using the Hubbard model and the mapping method. This was achieved by approaching the projection of the nd-dimensional lattice of states onto a $(n-1)d$-dimensional one with effective states.

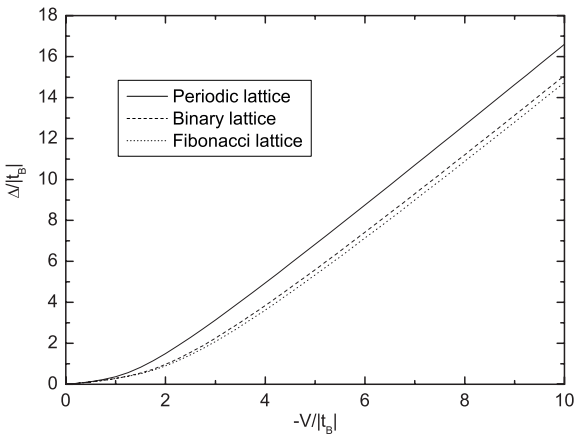

Fig. 2 Binding energy calculated for the same cases as in Fig. 1 except that here we have $V<0$ and $U=0$.

This allow us to find the pairing conditions, in particular, we solve the two- and three-interacting particles cases. In general, it was found that pairing electrons in a quasiperiodic lattice it is more difficult than in periodic or binary lattice.

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