



Electron pairing in one-dimensional quasicrystals

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ABSTRACT

Electron pairing in one-dimensional binary Hubbard chains is studied for different values of the band-filling using the density matrix renormalization group method. The systems consist of linear arrays of sites with two types of on-site correlations defined by two potentials: U_A being attractive (<0), and U_B repulsive (>0). The atomic levels of the system are modulated with periodic and quasiperiodic ordering, in the latter case following the Fibonacci sequence. We analyze the effect of such modulations and calculate the electron pairing phase diagram as a function of the band-filling. It is observed that there is a critical value of the band-filling where the behavior of the periodic and the Fibonacci binary Hubbard chains is reversed.

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1. Introduction

An impression that low-dimensional systems are an ideal and purely serve as a mathematical example is vanishing from stage. The several nanoscopic low-dimensional devices that have been obtained in the laboratories such as carbon nanotubes, semiconducting quantum wires and quantum dots mean a breakthrough in the engineering of materials with novel physical properties; with desired properties such as superconductivity, and with promising applications, for example, in the area of spintronics. Such systems are inhomogeneous in their structure and intrinsically strongly correlated due to the reduction of the available phase space. Also within the collection of low-dimensional materials are the one-dimensional quasicrystals to be underlined. One of the best known 1D quasicrystals is based on the Fibonacci sequence which started drawing interest after the papers by Kohmoto et al. [1] and Ostlund et al. [2]. The spectral properties of the Fibonacci chain are exotic; the single-particle eigenstates are neither extended nor localized, but critical, and the spectrum corresponds to that of a Cantor set [1–3]. A Fibonacci sequence consists of two elements 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 the letter G_i indicates the i th generation. In a Fibonacci chain, the elements A and B from the Fibonacci sequence may denote two different atoms (diagonal model) or two different bonds separating

identical atoms (off-diagonal model). In this work, we will study the diagonal model, where the site energy takes two values ε_A and ε_B associated to atoms A and B , respectively. In the corresponding diagonal model the number of sites with energy ε_A is $N_A(n)$ and the number of sites with energy ε_B is $N_B(n)$. The total number of sites in a generation n is represented by $N(n)$, $N(0) = N(1) = 1$. These numbers are related by

$$N(n) = N(n-1) + N(n-2),$$

$$N_A(n) = N(n-1),$$

$$N_B(n) = N(n-2).$$

In the quasiperiodic limit ($n \rightarrow \infty$) the ratio $N_A(n)/N_B(n)$ converges towards the golden mean $\sigma = (\sqrt{5} + 1)/2$. Motivated by the work of Alexandrov et al. [4] on the s -wave electron pairing in a one-dimensional binary Hubbard system with two electrons and a total momentum $\mathbf{K} = 0$, we investigate the electron pairing for different values of the band-filling in a Fibonacci lattice. In their paper, Alexandrov et al. considered the possibility of a binary system due to the fact that the CuO chains play a key role in the high-temperature superconductivity. Thus, they considered a Hubbard model with repulsion on copper and attraction on oxygen atoms. For simplicity, the energy of the atomic levels was set the same for all sites. We further want to study the interplay of the binary Hubbard systems under the influence of a modulation of the atomic energy levels, which we model by setting their values along the chain distributed according to the Fibonacci sequence. The results are compared to those of the homogeneous and diatomic chains. The binary Hubbard system proposed by Alexandrov with only two electrons has been solved by means of the Bethe Ansatz method. In our case, we use the density matrix renormalization group method (DMRG) [5–8] which is an efficient method for

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investigating low-energy properties of many-body and strongly correlated systems such as those briefly described above. Although few, recent key studies on quasiperiodic systems including strong interactions have been reported. These include a bosonization approach found in Refs. [9,10], a DMRG study of quasiperiodic Hubbard chains found in Ref. [11], and an exact solution for systems at low-densities using a real-space projection method found in Refs. [12,13].

2. Models and methods

A one-dimensional binary Hubbard chain consists of non-equivalent sites distinguished through two on-site potentials: U_A being attractive (<0), and U_B repulsive (>0) arranged in alternating order. The one-dimensional Hubbard model is one of the few examples of an exactly solvable model using Bethe Ansatz [14], where the N -particle wave function is constructed using plane-wave exponents with coefficients obtained from a two-particle S -matrix. The binary Hubbard system in Ref. [4] was formed by a collection of unit cells consisting of two sites: A and B (see Fig. 1(a)). For the i th unit cell the creation (annihilation) operators with spin σ ($=\uparrow, \downarrow$) are $a_{i,\sigma}^\dagger$ ($a_{i,\sigma}$) and $b_{i,\sigma}^\dagger$ ($b_{i,\sigma}$) at sites A and B , respectively. The following Hamiltonian was then proposed:

$$H = -t \sum_{i,\sigma} \left\{ a_{i,\sigma}^\dagger b_{i-1,\sigma} + b_{i,\sigma}^\dagger a_{i+1,\sigma} + a_{i,\sigma}^\dagger b_{i,\sigma} + b_{i,\sigma}^\dagger a_{i,\sigma} \right\} + \sum_i \left\{ U_A n_{i\uparrow}^a n_{i\downarrow}^a + U_B n_{i\uparrow}^b n_{i\downarrow}^b \right\},$$

with $\varepsilon_A - \varepsilon_B = 0$ and two electrons in the chain. $n_{i,\sigma}^a$ and $n_{i,\sigma}^b$ are the electron number operators on sites A and B , respectively, with U_A the attractive potential on site A and U_B the repulsive potential on site B . From the Bethe Ansatz solution it was then concluded that, given a value U_B for the repulsive interaction, there is a critical value of U_A above which pairing of the electrons was always taking place in the system. The value of the attractive interaction is given by:

$$|U_A| \geq \frac{2U_B}{U_B + 2}. \quad (1)$$

In Ref. [4] it was also left open what would happen for systems with more than two electrons. One possibility mentioned there was that doping the systems would render in less paired-states, which would agree with the fact that for high-temperature superconductors there is a saturation in their critical temperature when doping these materials.

We want now to extend the investigation of electron pairing to binary Hubbard systems with more than two particles and to lattices with different topology like the Fibonacci one. We propose the following Hamiltonian:

$$H = \sum_{i\sigma} \varepsilon_i n_{i,\sigma} - t \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i+1,\sigma} + H.c. + \sum_i U_i n_{i\uparrow} n_{i\downarrow}, \quad (2)$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin σ ($=\uparrow, \downarrow$) at site i and $n_{i\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the electron number operator. ε_i is the atomic energy level and $t = 1$ is the nearest neighbor hopping matrix, which we choose to set the energy scale. U_i is the on-site interaction and will take the value U_A for i odd and U_B for i even. The Hamiltonian in Eq. (2) incorporates the different systems we want to study. We want to compare three different atomic level scenarios: (i) The homogeneous case, which corresponds to the system studied in Ref. [4], and in which $\varepsilon_i = \varepsilon$, i.e., the atomic level is set the same for all sites and we set to zero. (ii) The diatomic case, where there are two different values intercalated, ε_A and ε_B ($\varepsilon_A < \varepsilon_B$). In this case, half of the sites have an atomic level of

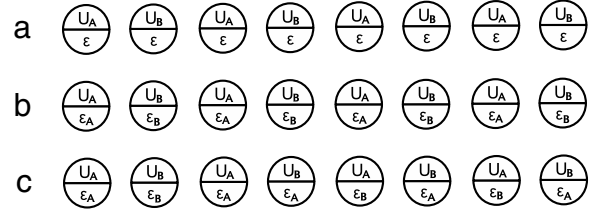


Fig. 1. Structure of one-dimensional binary Hubbard systems. (a) The homogeneous binary Hubbard chain, with $\varepsilon_A = \varepsilon_B = \varepsilon$. (b) The diatomic binary Hubbard chain, with $\varepsilon_A \neq \varepsilon_B$. (c) The Fibonacci binary Hubbard chain, with $\varepsilon_A \neq \varepsilon_B$. Up to the 5th Fibonacci generation is shown in this diagram and $\varepsilon_A < \varepsilon_B$ for (b) and (c).

ε_A and half of them have the value ε_B . (iii) The last system is the Fibonacci case, where we assign each site an atomic energy value following the Fibonacci sequence starting with ε_A and thus we will have more sites with ε_A than with ε_B . The exact number depends on the generation of the Fibonacci set to be used. Fig. 1(a)–(c) show the atomic level structures just described. It is expected that the quantum confinement originated in the diatomic and Fibonacci chains due to the fact that $\varepsilon_A < \varepsilon_B$ will, in general, enhance localization and therefore favor the formation of local electron pairs. On the other hand, the total effect of the different local potentials and confinement might be cumbersome. Furthermore, at half-filling Umklapp scattering plays a key role in the electronic properties of 1D systems. As already mentioned, the interesting materials and systems have an inhomogeneous structure, which on the atomic level induces potentials that modify their properties. In order to investigate such effects we need to consider the strong correlations in many-body quantum systems. Lacking an analytical solution, we make our attempts using the density matrix renormalization group method (DMRG). This method has its origin in the numerical renormalization group formulated by Wilson [15] and allows for accurate calculations of ground state properties in low-dimensional quantum lattice systems for which the basis of the Hilbert space grows exponentially with the number of particles and cannot be handled using exact diagonalization. The DMRG is a variational, real-space method that selects in a systematic way a sector of the Hilbert space that best represents the ground state of a system, which is done by selecting only the m most probable states calculated from the density matrix of the system. The numerical error caused by truncation of the original basis can be calculated directly as the total weight of the states that were discarded. For our systems, with $L = 144$ sites, we kept $m = 256$ density-matrix states, resulting in a maximum truncation error of the order of 10^{-6} . The length of the systems corresponds to the 12th Fibonacci generation, being ε_B the zeroth generation and ε_A the first one.

3. Results and discussion

The systems described above were investigated for different values of the band-filling under open boundary conditions, which favors convergence in the DMRG method. Finite-size effects such as particle density oscillations and charge accumulation close to the edges of the systems are present specially in the homogeneous system away from half-filling. The diatomic and Fibonacci chains behave according to the energy considerations of their arrangements even at the edges of the systems.

To obtain the pairing phase diagram we calculate the binding energy Δ as the difference in the ground state energy E_{GS} when the on-site potentials are all off and after they were switched on:

$$\Delta(f(\varepsilon)) = E_{GS}(U_A = U_B = 0; f(\varepsilon)) - E_{GS}(U_A \neq U_B \neq 0; f(\varepsilon)), \quad (3)$$

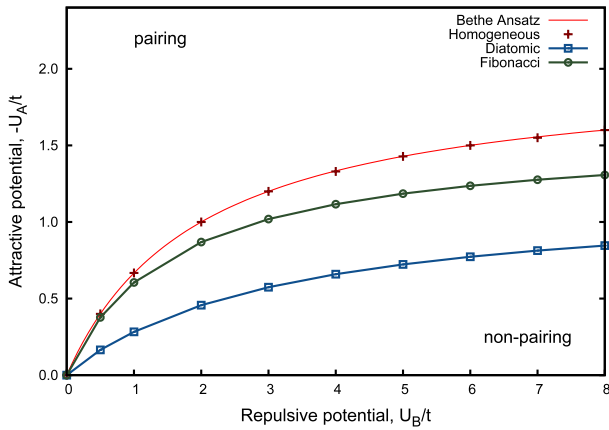


Fig. 2. Ground state pairing phase diagram for binary Hubbard systems with 2 electrons.

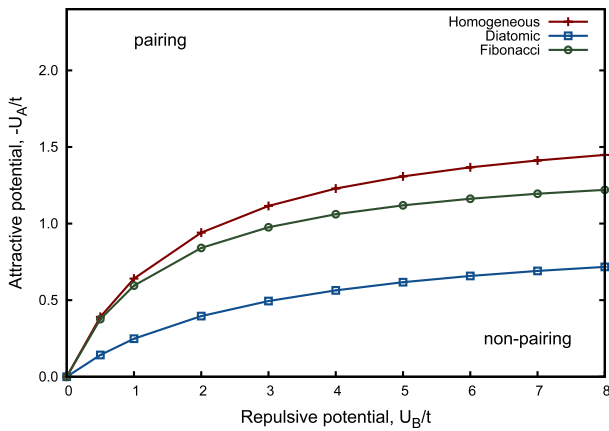


Fig. 3. Ground state pairing phase diagram for binary Hubbard systems at quarter-filling.

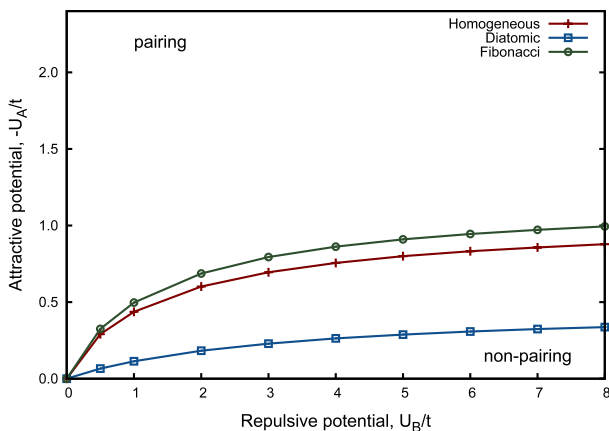


Fig. 4. Ground state pairing phase diagram for binary Hubbard systems at half-filling.

where $f(\varepsilon)$ refers to the homogeneous, diatomic or Fibonacci arrangement of the atomic levels ε . A positive Δ means there is local pair formation in the system. In Figs. 2–4 we show the ground state phase diagram for binary Hubbard chains with homogeneous, diatomic and Fibonacci ordering of the site energies ε . In all cases, the area above (and including) each line corresponds to paired states. The area below the line corresponds to non-paired states.

When browsing from Fig. 2 to Fig. 4, one observes that the electron pairing is indeed enhanced due to quantum confinement and it also increases with the number of electrons in the system.

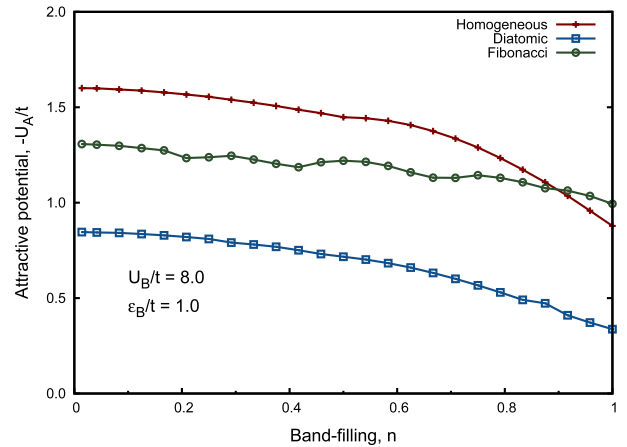


Fig. 5. Minimum value of the attractive potential U_A for the systems to have electron pairing with a fixed repulsive potential $U_B/t = 8.0$ as a function of the band-filling, n .

In Fig. 2 we compare our results directly to those obtained using Bethe Ansatz (Eq. (1)), for the case of a binary Hubbard system with $\varepsilon_A - \varepsilon_B = 0$ and two electrons. In Fig. 2, it is also shown how a completely periodic modulation of ε , as in the case of the diatomic chain, enhances the most the electron pairing, whereas an aperiodic modulation, such as that of the Fibonacci chain, enhances the electron pairing as well but this is only significant when compared to the homogeneous case. These results are comprehensible if we consider what was explained about the Fibonacci chains: There are more sites with energy values $\varepsilon_A = 0$ (a total of 89) than sites with energy values $\varepsilon_B = 1$ (a total of 55). This fact makes it plausible to observe the results of the Fibonacci chain rather closer to those of the homogeneous system than to those of the diatomic case. The same behavior of the phase diagram was found in the systems at quarter-filling (see Fig. 3) where it is even observed that the distance between the curves for both homogeneous and Fibonacci chains decreases. This result indicates a sort of competition between these two systems as a function of the band-filling. An effect which close to half-filling renders interesting results. In Fig. 4 we show the results for the binary Hubbard chains at half-filling. While the diatomic chain remains well below the other two cases, the homogeneous and Fibonacci chains seem, at first glance, to behave the other way around, i.e., there are now more electrons paired for the homogeneous than for the Fibonacci system. We investigated this behavior further in the next way: After fixing a value of the repulsive on-site potential U_B , we obtained the minimum value of attractive on-site potential U_A for which the systems have electron pairing. The results (see Fig. 5) show for the Fibonacci chain a uniform, though oscillating behavior in U_A . On the contrary, for the homogeneous case, and for values of the band-filling close to $n = 1$, the minimum U_A values decrease faster than the Fibonacci case. This situation results in a critical value of the band-filling of $n = 0.895$ after which the behavior of the homogeneous and Fibonacci binary Hubbard chains is inverted. In general, quantum confinement enhances electron pairing in binary Hubbard chains. However, the topology of the confinement determines strongly the electronic properties. The behavior of the homogeneous and Fibonacci chains close to half filling indicate that the quantum confinement effect is overridden by the effect of the aperiodic structure, as this is not happening in the diatomic chain.

4. Conclusions

In conclusion, we considered a system of spin- $\frac{1}{2}$ fermions in a one-dimensional lattice with position dependent atomic level

ε_i , embedded in a binary on-site potential. Our results illustrate how the modulation of the atomic energy levels in a periodic and non periodic way affects the formation of local electron pairs in binary Hubbard chains with attractive and repulsive on-site potentials. We found a combined effect on the electron pairing due to the atomic level ordering and the increasing band-filling. The number of paired-states increases with the band-filling for the homogeneous, diatomic and Fibonacci chains. Moreover, there is a critical value of the band-filling for which the effect of aperiodicity compared to the homogeneous case is reversed.

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