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Wave function behavior in a Fibonacci lattice with electronic correlation

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Abstract

The electronic correlation and the spatial symmetry in quasicrystals are by themselves two very complicated research topics since we cannot use the reciprocal space to study quasicrystals and the electronic correlation in many-body system has been solved exactly only for one and for infinite dimension. We should note that 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 case of two interacting particles in a Fibonacci lattice using a real-space method and the Hubbard model. The real-space 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. Within the Hubbard Hamiltonian we obtained the behavior of the wave function and the analysis of these eigen-functions in the Fibonacci lattice when correlation is off shows a critical behavior.

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Keywords: Quasicrystals; Electrical and electronic properties

1. Introduction

Two of the most important discoveries in the last two decades within the condensed matter physics, were the discovery of quasicrystals in 1984 by Shechtman et al. [1] and the high-T_c superconductivity in ceramic materials by Bednorz and Muller in 1987 [2]. These topics have generated a large number of studies both experimental and theoretical in the physics of low dimension. Also, these two discoveries have modified some of the concepts in the solid state physics, for instance, it was believed that the fivefold symmetry was incompatible with a long-range order and it was not expected superconductivity in ceramics materials with a high-T_c and a short coherence length. So, it has been very important to revise both the spatial symmetry and the electronic correlation to see how it affects the physical properties in materials. In one-dimensional quasiperiodic structures, the interactions between electrons have often been neglected and only few results have been obtained [3,4].

The most widely studied model in one-dimensional quasicrystals is based on the Fibonacci sequence which started drawing interest after the two interesting papers by Kohmoto et al. [5] and Ostlund et al. [6]. The spectral properties of Fibonacci chain are exotic, the single-particle eigenstates are neither extended nor localized but critical and the spectrum is a Cantor set [5–8]. 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 $G_0 = \mathrm{B}$, $G_1 = \mathrm{A}$, $G_2 = \mathrm{AB}$, $G_3 = \mathrm{ABA}$, $G_4 = \mathrm{ABAAB}, \ldots, G_i = G_{i-1}G_{i-2}$ for $i \geqslant 2$, where the letter G_i indicates the generation i. In a Fibonacci chain, the letters A and B of the Fibonacci sequence may denote two different atoms (site model) or two different bonds separating identical atoms (transfer model). In this work, we will study the transfer model, where the hopping integrals take two values t_A and t_B corresponding to a short bond and a large bond, respectively. In the transfer model the number of short bonds is $N_A(n)$

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and the number 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 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 ($n \to \infty$), the ratio $N_A(n)/N_B(n)$ converges toward the golden mean $\sigma = (\sqrt{5}+1)/2$. The Hubbard model [9] is the simplest one used to describe correlations in narrow-band systems and has been studied extensively [10,11]. However, even when the Hubbard model is conceptually very simple, this model is very difficult to solve in general. The Hubbard Hamiltonian may be written in real space as [12]

$$H = \sum_{\langle i,j\rangle,\sigma} t_{i,j} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

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 $n_{i,\sigma} = c^{+}_{i,\sigma} c_{i,\sigma}$. The parameters of the Hamiltonian are $t_{i,j}$ the hopping integral and U the on-site Coulomb interaction. It is worth mentioning that in principle, the parameter U is positive because it is a direct Coulomb integral. However, U 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 will study the behavior of the wave function in a Fibonacci lattice with two interacting electrons of opposite spin.

2. Results and discussion

The Hamiltonian in Eq. (1) is analyzed by using the mapping method previously reported [12]. This method maps the original many-body problem onto a one-body problem with some ordered site-impurities in a *nd*-dimensional lattice, n being the number of particles and d the dimensionality of the original system. In our case $n = 2$ and $d = 1$, so the mapped one-body problem is in two-dimensional lattice, see Fig. 1.

In our calculations we use a Fibonacci lattice with 90 sites (10th generation) and hopping parameter given by $t_A = -1.0$ and $t_B = -2.0$. In Fig. 2, we show the results when the on-site electronic interaction is $U = 0$, for the periodic linear chain (Fig. 2(a)), which was calculated only to compare with the Fibonacci lattice, and for the Fibonacci lattice (Fig. 2(b)). The wave functions correspond to the band edge eigenvalues ($E_L = -3.997616562204283$ and $E_F = -5.661148600328795$ for the periodic chain and

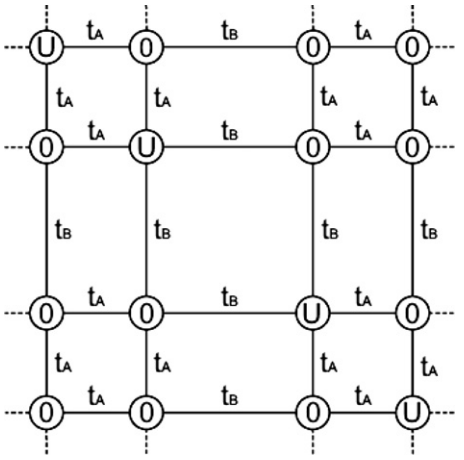

Fig. 1. Geometric representation (lattice of states) of the states of two electrons with opposite spin in a Fibonacci lattice, the states are represented by circles and the self-energy is indicated inside.

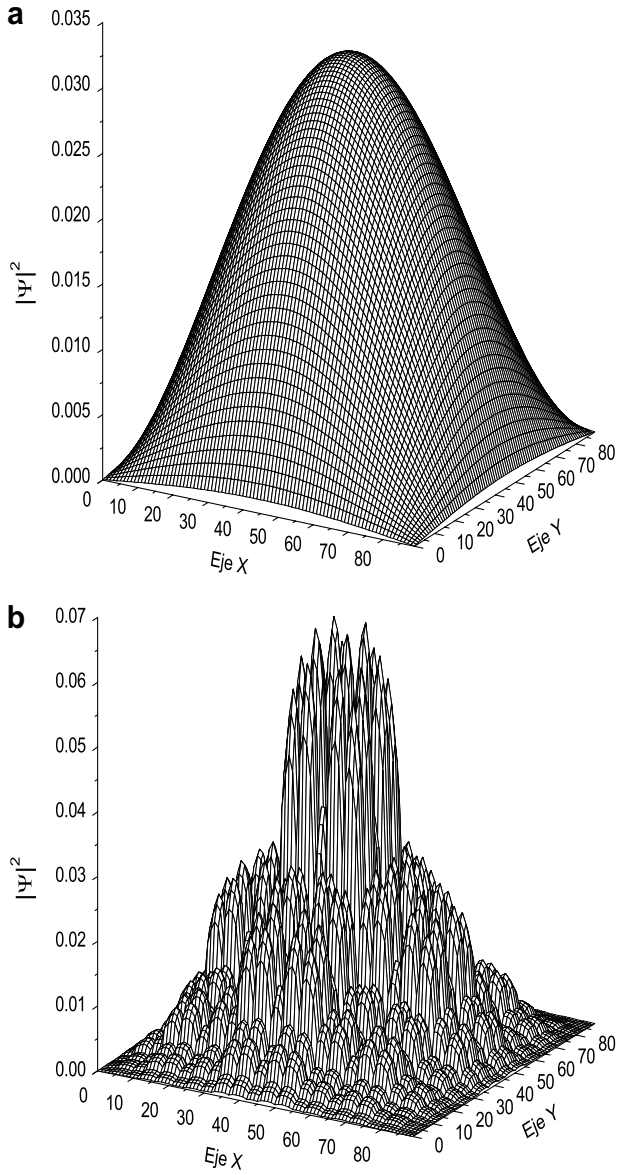

Fig. 2. Wave function in a linear chain (a) and in a Fibonacci lattice (b) with two non-interacting electrons with opposite spin, the wave function is associated to the band edge eigenvalues.

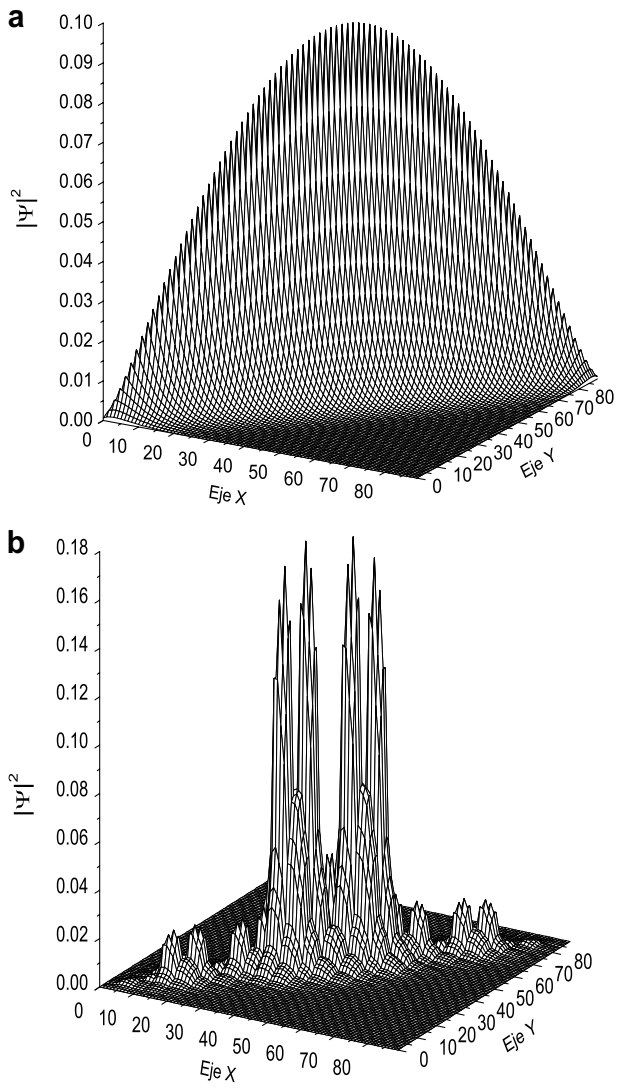

Fig. 3. Wave function in a linear chain (a) and in a Fibonacci lattice (b), with two attractive interacting electrons. The results are associated to the band edge eigenvalues.

Fibonacci lattice, respectively). The results in the Fibonacci lattice show us qualitatively the critical behavior of the wave function. It is worth to mention that we obtained the same results for the positive side of the band edge since the Fibonacci lattice is also bipartite.

In Fig. 3, the results including a small on-site attractive electronic interaction $U = -1.0$ are presented for the same hopping parameters mentioned above. The attractive electronic interaction is similar to that used for the Cooper pair formation in high temperature superconductors. The wave functions presented here were also calculated for that associated to the band edge eigenvalues ($E_L = -3.994528104688936$ and $E_F = -5.661648478876018$ for the periodic chain and Fibonacci lattice, respectively). We can observe that the wave functions are localized along the principal diagonal of the two-dimensional lattice of states, since in this diagonal are localized the parameters of the attractive on-site interaction. The critical behavior of the wave function is still there.

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