Physical nature of critical wave functions in Fibonacci systems

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Abstract

We report on a new class of critical states in the energy spectrum of general Fibonacci systems. By introducing a transfer matrix renormalization technique, we prove that the charge distribution of these states spreads over the whole system, showing transport properties characteristic of electronic extended states. Our analytical method is a first step to find out the link between the spatial structure of these critical wave functions and the quasiperiodic order of the underlying lattice.

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The notion of critical wave function (CWF) has evolved continuously since its introduction in the study of aperiodic systems, leading to a somewhat confusing situation. For instance, references to self-similar, chaotic, quasiperiodic, lattice-like or quasilocalized CWFs can be found in the literature depending on the different criteria adopted to characterize them. Generally speaking, CWFs exhibit a rather involved oscillatory behavior, displaying strong spatial fluctuations which show distinctive self-similar features in some instances. As a consequence, the notion of an envelope function, which has been most fruitful in the study of both extended and localized states, is mathematically ill-defined in the case of CWFs, and other approaches are required to properly describe them and to understand their structure.

Most interestingly, the possible existence of extended critical states in several kinds of aperiodic systems, including both quasiperiodic and non-quasiperiodic ones, has been discussed in the last few years spurring the interest on the precise nature of CWFs and their role in the physics of aperiodic systems. From a rigorous mathematical point of view the nature of a state is uniquely determined by the measure of the spectrum to which it belongs. In this way, since it has been proven that Fibonacci lattices have purely singular continuous energy spectra, we must conclude that the associated electronic states cannot be, strictly speaking, extended in the Bloch’s sense. This result holds for other aperiodic lattices (Thue-Morse, period doubling) as well, and it may be a general property of the spectra of self-similar aperiodic systems. On the other side, from a physical viewpoint, the states can be classified according to their transport properties which, in turn, are determined by the spatial distribution of the wave function amplitudes (charge distribution). Thus, conducting systems are described by periodic Bloch states, whereas insulating systems are described by exponentially decaying wave functions corresponding to localized states. In this sense, since the amplitudes of CWFs in a Fibonacci lattice do not tend to zero at infinity but are bounded below throughout the system, one may expect their physical behavior to be more similar to that corresponding to extended states than to localized ones.

In this letter we are going to show analytically that a subset of the CWFs belonging to general Fibonacci systems are extended from a physical point of view. This result widens the notion of extended wave function to include electronic states which are not Bloch functions, and it is a relevant first step to clarify the precise manner in which the quasiperiodic order of Fibonacci systems influences their transport properties. We shall begin the investigation of this issue by introducing two novel approaches. In the first place, we present a new renormalization approach opening, in a natural way, an algebraic formalism which allows us to give a detailed analytical account of the transport properties of CWFs for certain particular values of the energy. In the second place, we relate the spatial structure of CWFs to the topology of the underlying lattice by means of the study of the Fourier spectrum of the wave function amplitudes and multifractal techniques.

The formalism we are going to introduce is based on the transfer matrix technique where the solution of the Schrödinger equation is obtained by means of a product of $2 \times 2$ matrices. Real-space renormalization group approaches, based on decimation schemes, have proved themselves very successful in order to numerically obtain the energy spectrum of deterministic aperiodic systems. The convenience for such procedures stems from the fact that, by construction, a given transfer matrix relates only three consecutive sites along the lattice, so that by decimating the original chain into successively longer blocks we are
able to describe the electronic state corresponding to sites more and more farther apart. In this context, the key point of our procedure consists of the fact that we renormalize the set of transfer matrices instead of the lattice itself. Since these matrices contain all the relevant information concerning the dynamics of the electrons, our approach becomes specially well suited to describe the characteristic features associated to the long-range order of the underlying Fibonacci system for, as we will see below, it preserves the original quasiperiodic order of the lattice at any stage of the renormalization process.

Let us start by considering a general Fibonacci system in which both diagonal and off-diagonal terms are present in the Hamiltonian

\[ H = \sum_n \{ V_n |n\rangle\langle n| + t_{n,n+1} |n\rangle\langle n+1| + t_{n,n-1} |n\rangle\langle n-1| \}, \]

where \( V_n \) is the on-site energy and \( t_{n,n\pm 1} \) are the nearest-neighbor hopping integrals. This Hamiltonian can be rewritten in terms of the following matrices

\[
X \equiv \begin{pmatrix}
\frac{E - \beta}{t_{AB}} & -1 \\
1 & 0 
\end{pmatrix},
Y \equiv \begin{pmatrix}
\gamma^{-1} \frac{E - \alpha}{t_{AB}} & -\gamma^{-1} \\
1 & 0 
\end{pmatrix},
Z \equiv \begin{pmatrix}
\frac{E - \alpha}{t_{AB}} & -\gamma \\
1 & 0 
\end{pmatrix},
W \equiv \begin{pmatrix}
\frac{E - \alpha}{t_{AB}} & -1 \\
1 & 0 
\end{pmatrix},
\]

where \( E \) is the electron energy, \( \alpha (\beta) \) denote the on-site energies of sites A (B), \( t_{AB} = t_{BA} \) and \( t_{AA} \) are the corresponding hopping integrals and \( \gamma \equiv t_{AA}/t_{AB} > 0 \). Making use of these matrices we can translate the atomic sequence ABAAB . . . describing the topological order of the Fibonacci lattice to the transfer matrix sequence XYZXWXYZXW . . . describing the behavior of electrons moving through it. In spite of its greater apparent complexity, we realize that by renormalizing this TMS according to the blocking scheme \( R_A \equiv XYZ \) and \( R_B \equiv XW \), we get the considerably simplified sequence \( R_AR_BR_AR_AR_B \ldots \) The subscripts in the Rs matrices are introduced to emphasize the fact that the renormalized TMS is also arranged according to the Fibonacci sequence and, consequently, the topological order present in the original lattice is preserved by the renormalization process. Let \( N = F_n \) be the number of lattice sites, where \( F_n \) is a Fibonacci number obtained from the recursive law \( F_k = F_{k-1} + F_{k-2} \), with \( F_1 = 1 \) and \( F_0 = 1 \). It can then be readily shown that the renormalized TMS contains \( n_A \equiv F_{n-3} \) matrices \( R_A \) and \( n_B \equiv F_{n-4} \) matrices \( R_B \).

We will now use several properties of the Rs matrices to develop our procedure. Firstly, they are unimodular (i.e. their determinant is one) for any choice of the system parameters and for any value of the electron energy. Secondly, they commute for certain values of the energy. In fact, after some algebra we get

\[
[R_A, R_B] = \frac{P(E)}{\omega^2 \gamma} \begin{pmatrix}
-1 & E + \alpha \\
0 & 1 
\end{pmatrix},
\]

where we have defined the origin of energies in such a way that \( \beta = -\alpha \) and \( t_{AB} \equiv 1 \), and

\[
P(E) = (\gamma^2 - 1)(E + \alpha)((E - \alpha)^2 - \omega^2) + 2\alpha \omega^2 \gamma^2,
\]

with \( \omega^2 \equiv (1 + \gamma) t_{AB}^2 \). This commutator considerably simplifies for the two cases mostly discussed in the literature, namely the on-site (\( \gamma \equiv 1 \)) and transfer (\( \alpha \equiv 0 \)) models. The
expression (2) shows that the on-site model is *intrinsically* non-commutative, for the commutator vanishes only in the trivial periodic case. On the contrary, there exist three energy values for which the R matrices commute in the transfer model, corresponding to $E = 0$ and $E = \pm \omega$. Most interestingly, since $P(E)$ is a real cubic polynomial in $E$, there exists at least one energy satisfying the relation $P(E) = 0$ for any realization of the mixed model (i.e. for any $\gamma$ value). For these energies the condition $[R_A, R_B] = 0$ is fulfilled and, making use of the Cayley-Hamilton theorem for unimodular matrices, the global transfer matrix of the system, $M(N) \equiv R_A^N R_B^N$, can be explicitly evaluated in terms of Chebyshev polynomials of the second kind, $U_m(x)$, where $x$ is $\text{Tr}(R)/2$. Alternatively, the required power matrices can be evaluated by diagonalizing them to a common basis. From the knowledge of $M(N)$ the condition for the considered energy value to be in the spectrum, $|\text{Tr}[M(N)]| \leq 2$, can be readily checked and, afterwards, relevant parameters describing their transport properties can be determined explicitly. In this way, given any arbitrary Fibonacci lattice, we are able to obtain a subset of its energy spectrum whose eigenstates can be studied analytically.

Although our approach is completely general, the solutions of the algebraic equation $P(E) = 0$ are rather involved in most cases. For convenience, model parameters for which the algebra considerably simplifies will be discussed henceforth. In Fig. 4 we show the charge distribution of two electronic states, for which the R matrices commute, corresponding to Fibonacci lattices with $N = F_{16} = 1597$. Figure 4(a) corresponds to the energy $E = 2$ and lattice parameters $\gamma = 3$ and $\alpha = 1$. Figure 4(b) shows the result for the energy $E = \sqrt{1 + \gamma}$ for a transfer model ($\alpha = 0$) with $\gamma = 1 + \sqrt{2}$, the so-called silver mean. The overall periodic-like behavior of the wave function amplitudes, which we have calculated exactly with the aid of our matrix formalism, clearly indicates their extended character.

In order to discuss this point from a more rigorous physical perspective we will focus our attention on the transmission coefficient, $\tau(E)$. For the transfer model the global transfer matrices corresponding to the energies $E = \pm \omega$ in the interval $0 \leq \gamma \leq 3$ can be expressed, after lengthy algebra, in the closed form

$$M(N, \pm \omega) = R_A^{-p} = \begin{pmatrix} U_p(\theta^\pm) & U_{p-1}(\theta^\pm) \\ -U_{p-1}(\theta^\pm) & -U_{p-2}(\theta^\pm) \end{pmatrix},$$

(4)

where $p \equiv 2n_B - n_A = F_{n-1}$. From expression (4) we get $\text{Tr}[M(N)] = 2 \cos \theta^\pm$ and, consequently, we can ensure that the energies $E = \pm \omega$ belong to the spectrum in the quasiperiodic limit ($N \to \infty$). Now, we proceed to the calculation of the transmission coefficient by embedding the Fibonacci lattice in an infinite periodic arrangement of identical atoms connected by hopping integrals $t$. In this way we obtain

$$\tau(\pm \omega) = \frac{1}{1 + \frac{4\omega^2(t+1)^2}{(4\omega^2)\sin^2 p\theta^\pm}}.$$ 

(5)

Two important conclusions can be drawn from this expression. In the first place, the transmission coefficient is always bounded below for *any* lattice length, which proves the true extended character of the related eigenstates. In the second place, we observe that the transparency condition $\tau = 1$ is obtained, for any value of $t$, for certain chain sizes satisfying $p\theta^\pm = k\pi$, $k = 1, 2, \ldots$, which in turn implies $\pm \omega = \mp 2 \cos(k\pi/p)$. In this way the transparent states $\tau = 1$ can be classified according to a well defined scheme determined by the
integers $k$ and $p$. Thus the state shown in Fig. 1(b) corresponds to the choice $k = 1$ and $p = 8$.

After having discussed the transport properties of this class of critical wave functions, we turn our attention to their spatial structure. To this end we shall consider the example shown in Fig. 2 which corresponds to the energy $E = \sqrt{2}\sigma$, where $\sigma \equiv (\sqrt{5} + 1)/2$ is the so-called golden mean, and model parameters $\gamma = \sqrt{5}$ and $\alpha = 0$. In Fig. 2(a) we show the overall charge distribution through a lattice with $N = F_{21} = 17711$ sites. From this plot we notice the existence of two different superimposed structures. In fact, a periodic-like long-range oscillation with a typical wavelength of about 18000 sites is observed to modulate a quasiperiodic series of short-range minor fluctuations of the wave function amplitude, typically spreading over 122 lattice sites. This qualitative description receives a quantitative support from the study of its Fourier transform, as it is shown in Fig. 2(b). In fact, we observe two major components in the Fourier spectrum corresponding to the low and high frequency regions, respectively. In the low frequency region two relevant features at frequencies $\nu_1 \simeq 1.11 \times 10^{-4}$ and $\nu_2 \simeq 8.18 \times 10^{-3}$ are present, in agreement with the short- and long-range structures of the charge distribution observed in Fig. 2(a). On the other side, in the high frequency region we observe a series of features grouped around frequency positions given by successive powers of the inverse golden mean $\sigma^{-1} \equiv (\sqrt{5} - 1)/2$. These features are labelled correspondingly in Fig. 2(b) and are characteristic of the quasiperiodic nature of the charge distribution of the considered states. By this we mean that we have observed that their weights in the Fourier spectrum increase and their positions approach the reported powers of $\sigma^{-1}$ as the system size increases.

Finally, to gain further insight into the behavior of the wave function at all length scales we have performed a multifractal analysis of the states belonging to the subset $E = \pm \omega$. The amplitude distribution of the electronic states has been characterized by the scaling of moments $\mu_q(N)$ of order $q$, associated to their charge distribution, with the system size (for a definition of those moments see, e.g, Ref. 21). The multifractal dimension $D_q$ is determined via the scaling $\mu_q(N) \sim N^{(1-q)D_q}$ for $q \neq 0$. In all cases studied we have found that $D_q = 1$, for all $q$, and for system sizes as large as $N = F_{30} = 1346269$. Thus the lack of multifractality along with the fact that $D_q$ equals the spatial dimension proves our claim that these states uniformly spread over the whole system.

In summary, in this letter we prove the existence of a subset of the singular continuous spectrum characteristic of Fibonacci systems whose eigenstates are extended in the physical sense previously discussed. This we have shown by means of a transfer matrix renormalization technique which allows us to unveil the effects of short-range correlations by grouping ABA sites and AB sites into the matrices $R_A$ and $R_B$, respectively. In this sense we can properly state that these states are characteristic of the quasiperiodic order of the underlying lattice. Interestingly we note that similar results concerning extended states in Thue-Morse chains have been recently reported in the literature. We wish to stress that the algebraic approach presented in this work can be extended in a straightforward manner to other kinds of aperiodic systems based on substitution sequences, and therefore it can be relevant in order to attain a unified treatment of physical properties of aperiodic systems. In closing, we note that the transparency condition $\tau = 1$ obtained for extended Fibonacci states is similar to that appearing in random dimer models and this fact suggests that sets of extended states may arise in general aperiodic systems.
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FIGURES

FIG. 1. Electronic charge distribution in Fibonacci lattices with $N = F_{16}$ and (a) $\gamma = 3$, $\alpha = 1$, $E = \omega = 2$ and (b) $\gamma = 1 + \sqrt{2}$, $\alpha = 0$, $E = \omega = \sqrt{2 + \sqrt{2}}$. Insets show finer details of the squared wave functions.

FIG. 2. (a) Electronic charge distribution in a Fibonacci lattice with $N = F_{21}$, $\gamma = \sqrt{5}$, $\alpha = 0$, and $E = \omega = \sqrt{1 + \sqrt{5}}$. Inset shows finer details of the squared wave function. (b) The corresponding Fourier spectrum. Inset shows the lower frequency region.