

Physical nature of critical modes in Fibonacci quasicrystals

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(Received 24 May 1999)

We report on the possibility of modulating the transport properties of critical normal modes in Fibonacci quasicrystals by using the mass ratio as a tuning parameter. The relationship between the spatial structure and the transport properties of these modes is studied analytically in terms of the transmission and Lyapunov coefficients. Power spectrum analysis of the critical modes indicates a complex modulated structure in agreement with previous experimental results. [S0163-1829(99)11337-7]

The interest in the precise nature of critical states (CS) and their role in the physics of aperiodic systems has witnessed a renewed interest in the last few years, aimed to clarify the relationship between their spatial structure and their related transport properties.¹⁻³ From a mathematical point of view the nature of a state is determined by the measure of the spectrum to which it belongs. Consequently, since it has been proven that Fibonacci lattices have purely singular continuous spectra,⁴ we can properly state that all the states are critical in these systems. However, this fact does not necessarily imply that all these CS behave in exactly the same way from a physical viewpoint.

In fact, physically states can be classified according to their transport properties. Thus, conducting states in crystalline systems are described by periodic Bloch functions, whereas insulating systems exhibit exponentially decaying functions corresponding to localized states. Within this scheme the position of CS is somewhat imprecise because, generally speaking, CS exhibit a rather involved oscillatory behavior, displaying strong spatial fluctuations at different scales.

A first step towards a better understanding of CS was provided by the demonstration that the amplitudes of CS in a Fibonacci lattice do not tend to zero at infinity, but are bounded below through the system.⁵ This result suggests that the physical behavior of CS might be more similar to that corresponding to extended states than to localized ones. Accordingly, the possible existence of *extended* CS in several kinds of aperiodic systems has been extensively discussed,⁶ and arguments supporting the convenience of widening the very notion of extended state to include also states which *are not* Bloch functions have been recently put forward.^{1,7}

The use of multifractal methods to analyze the electronic states in Fibonacci lattices provided conclusive evidence on the *diversity* of different CS, depending on their location in the highly fragmented energy spectra. Thus, while states located at the edges or the band centers of the main subbands exhibit a distinctive self-similar spatial structure, most of the remaining states do not show any specific pattern.⁸ These results were shortly thereafter substantiated by real-space renormalization procedures.⁹

A similar situation can also be expected to occur for the phonon spectrum.¹⁰ In fact, when studying band structure effects in the thermal conductivity of Fibonacci quasicrystals

(FQC) we have found a great variety of *critical normal modes* (CNM),^{11,7} exhibiting quite different physical behaviors, which range from highly conducting extended states to CS whose transmission coefficient oscillates periodically between two extreme values, depending on the system's length.^{7,13}

In this paper we report on the possibility of *modulating* the spatial structure and transport properties of CNM propagating through a FQC by properly selecting the masses' values. The transport properties of the different states are analyzed by means of closed analytical expressions for the Lyapunov and transmission coefficients. The relationship between the spatial structure of CNM and their related transport properties is further explored by means of a power spectrum analysis which allows us to describe the overall structure of CNM as a superposition of two basic contributions involving different scale lengths.

In our study we consider a harmonic chain composed of two kinds of masses, m_A and m_B , which are arranged according to the Fibonacci sequence, and two kinds of springs, K_{AA} and $K_{AB} = K_{BA}$, depending on the type of joined atoms. In this way, the quasiperiodic distribution of masses in the system *induces* an aperiodic (non-Fibonacci) distribution of spring constants in the lattice. This model is physically sound since one expects that the nature of the chemical bonding between the different atoms will depend on the nature of the atoms involved. In this sense, our FQC model is both more *general* and *simpler* than most of the Fibonacci lattices previously discussed in the literature.¹⁴

Making use of the transfer-matrix formalism the stationary equation of motion for the FQC can be cast in the form

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} = \begin{pmatrix} \frac{a_n}{K_{n,n+1}} & -\frac{K_{n,n-1}}{K_{n,n+1}} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix} \equiv P_n \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}, \quad (1)$$

where u_n is the displacement of the n th atom from its equilibrium position, $K_{n,n\pm 1}$ denotes the strength of the harmonic coupling between neighbor atoms, $a_n \equiv K_{n,n-1} + K_{n,n+1} - m_n \omega^2$, m_n , with $n = A, B$, is the corresponding mass, and ω is the vibration frequency. Making use of periodic

boundary conditions the allowed regions of the frequency spectrum are determined from the usual condition $|\text{Tr}M(N, \omega)| \equiv |\text{Tr}(\prod_{n=N}^1 P_n)| \leq 2$, where $M(N, \omega)$ is the global transfer matrix, and N is the number of atoms in the

lattice. From the knowledge of the global transfer matrix elements, M_{ij} , we can obtain the transmission, $t(N, \omega)$, and Lyapunov, $\Gamma(N, \omega)$, coefficients through the standard expressions

$$t(N, \omega) = \frac{4 \sin^2 k}{[M_{12} - M_{21} + (M_{11} - M_{22}) \cos k]^2 + (M_{11} + M_{22})^2 \sin^2 k}, \quad (2)$$

and

$$\Gamma(N, \omega) = \frac{1}{N} \ln(M_{11}^2 + M_{12}^2 + M_{21}^2 + M_{22}^2), \quad (3)$$

where $\cos k = m_A/2K_{AA}$ is the dispersion relation for a periodic chain.

Now we will extend the algebraic approach, previously introduced by us to describe the electron dynamics in quasiperiodic^{1,12} and fractal¹³ systems, in order to study the phonon dynamics as well. This approach is based on the transfer matrix technique, where the dynamical equation (1) is determined by the following transfer matrices

$$X \equiv \begin{pmatrix} 2 - \alpha\Omega & -1 \\ 1 & 0 \end{pmatrix}, \quad Y \equiv \begin{pmatrix} 1 + \gamma^{-1}(1 - \Omega) - \gamma^{-1} & \\ & 0 \end{pmatrix},$$

$$Z \equiv \begin{pmatrix} 1 + \gamma - \Omega & -\gamma \\ 1 & 0 \end{pmatrix}, \quad W \equiv \begin{pmatrix} 2 - \Omega - 1 & \\ & 0 \end{pmatrix}, \quad (4)$$

expressed in terms of the model parameters $\alpha \equiv m_B/m_A$, $\gamma \equiv K_{AA}/K_{AB}$, and $\Omega \equiv m_A \omega^2/K_{AB}$. Making use of these matrices, and imposing cyclic boundary conditions, we can *translate* the atomic sequence $ABAAB \dots$ describing the topological order of the FQC to the transfer matrix sequence $XZYXZYXWXZYXW \dots$ describing the phonon dynamics. In spite of its greater apparent complexity, we realize that by renormalizing this transfer matrix sequence according to the blocking scheme $R_A \equiv ZYX$ and $R_B \equiv WX$, we get the considerably simplified sequence $\dots R_B R_A R_A R_B R_A$. The subscripts in the R matrices are introduced to emphasize the fact that the renormalized transfer matrix sequence is also arranged according to the Fibonacci sequence and, consequently, *the topological order present in the original FQC 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 $F_n = F_{n-1} + F_{n-2}$, with $F_1 = 1$ and $F_0 = 1$. It can then be shown by induction that the renormalized sequence contains $n_A \equiv F_{n-3}$ matrices R_A and $n_B \equiv F_{n-4}$ matrices R_B .

Now we realize that the R matrices commute for certain frequency values. In fact, after some algebra we get

$$[R_A, R_B] = \frac{\Omega}{\gamma} \{2\gamma - 1 - \alpha[1 + \Omega(\gamma - 1)]\} \begin{pmatrix} 1 & 0 \\ 2 - \alpha\Omega & -1 \end{pmatrix}. \quad (5)$$

Aside from the trivial, limiting case $\Omega \rightarrow 0$, this commutator vanishes for the frequencies given by the expression

$$\Omega^* = \frac{\alpha - 2\gamma + 1}{\alpha(1 - \gamma)}. \quad (6)$$

A detailed study of the phonon spectrum corresponding to these states has been given elsewhere.^{11,7} In this work we will focus on the particular case given by the condition $K_{AA} = K_{AB}/2$.¹⁵ In this case ($\gamma = 1/2$), expression (6) reduces to $\Omega^* = 2$ for any arbitrary choice of the masses m_A and m_B . In other words, the commutation frequency becomes independent of the values assigned to the mass distribution in the FQC. The renormalized matrices R_A and R_B then adopt the simple form

$$R_A = \begin{pmatrix} 1 & 0 \\ 2(\alpha - 2) & 1 \end{pmatrix}, \quad R_B = \begin{pmatrix} -1 & 0 \\ 2(1 - \alpha) & -1 \end{pmatrix}, \quad (7)$$

and the corresponding power matrices can be easily evaluated by induction, so that the transfer matrix becomes

$$M(N, \Omega^*) \equiv R_A^{n_A} R_B^{n_B} = (-1)^{n_B} \begin{pmatrix} 1 & 0 \\ 2(\alpha F_{n-2} - F_{n-1}) & 1 \end{pmatrix}. \quad (8)$$

Two interesting consequences can be extracted from Eq. (8). In the first place, we realize that the frequency $\Omega^* = 2$ belongs to the spectrum regardless of the system length, since $|\text{Tr}[M(N, \Omega^*)]| = 2$ in this particular case. In the second place, if we choose the values for the masses in such a way that their ratio satisfies the relationship $\alpha = F_{n-1}/F_{n-2}$, we get $M(N, \Omega^*) = \pm I$, where I is the identity matrix. Consequently, when the parameter α is a rational approximant of the golden mean $\tau = \lim_{n \rightarrow \infty} (F_{n-1}/F_{n-2}) = (\sqrt{5} + 1)/2$, the state corresponding to the resonance frequency Ω^* is a *transparent* state with $t = 1$. An illustrative example of this kind of state is shown in the inset of Fig. 1 for a lattice with $N = 2584$ and $\alpha = 1597/987$. The normal mode amplitudes have been obtained by iterating the dynamical equation (1) with the initial conditions $u_0 = 0$ and $u_1 = 1$. The extended nature of the state is clearly appreciated. At this point, however, we must stress that the spatial structure of this CNM is determined by two different contributions, which correspond to two separate scale lengths. Thus, although at long scales (greater than, say, 100 sites) the state shows a distinct periodiclike¹⁶ pattern, such an alternating pattern resolves into a series of quasiperiodic oscillations at shorter length scales. The existence of both contributions is conveniently illustrated in the main frame of Fig. 1, where we plot the power spectrum of the CNM shown in

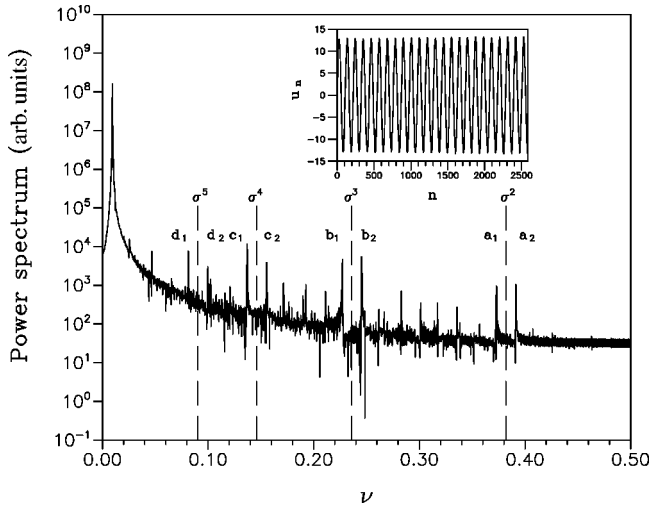


FIG. 1. Power spectrum of the extended CNM shown in the inset and atomic displacements in a FQC with $N=2584$ and $\alpha_1 = 1597/987$ at the resonance frequency $\Omega^*=2$ (inset).

the inset. In fact, we observe two main contributions in the power spectrum. In the low frequency region, a major peak located at $\nu=0.00921$ ($\lambda \approx 108.5$ sites), describes the overall periodiclike pattern. On the other hand, starting at about $\nu=0.09$, we observe a series of nested, subsidiary features, characterized by the *twin peaks* labeled by the letters a_i , b_i , c_i , and d_i ($i=1,2$). Each couple of peaks groups around a frequency value given by some of the successive powers of the inverse golden mean $\sigma = 1/\tau$. These features arrange according to a self-similar pattern, which extends through the entire high frequency region of the power spectrum up to $\nu \approx 0.4$. This self-similar component of the power spectrum reveals the quasiperiodic nature of the corresponding CNM when it is observed at shorter scales. The relative importance of the periodiclike versus the quasiperiodiclike contribution can be roughly measured by the height ratio of their related peaks in the power spectrum, i.e., $I_{QP}/I_P \approx 10^{-4}$. Therefore, we are considering a CNM which behaves as an extended, transparent state, but *still preserves a significant degree of quasiperiodic order* in its inner structure.

Now we shall consider the following question. According Eq. (8) the transparency condition $t=1$ is achieved when $\alpha = F_{n-1}/F_{n-2}$, which corresponds to the *best* rational approximant to τ for a given FQC of length N . Let us consider the case where we assign to the parameter α the successive values of the series $\alpha_m \equiv \{F_{n-m}/F_{n-(m+1)}\}$, with $m = 1, 2, \dots$ giving progressively *worse* rational approximants of τ . What will the spatial structure and related transport properties of the corresponding critical states be? To this end, we shall perform an analytical study of the transmission and Lyapunov coefficients. By plugging Eq. (8) into Eq. (2) and Eq. (3), respectively, we obtain

$$t(N, \Omega^*) = \frac{1}{1 + \frac{4}{3}(\alpha F_{n-2} - F_{n-1})^2}, \quad (9)$$

and

TABLE I. Systematic variation of the transmission and Lyapunov coefficients with the mass ratio parameter α_m for the resonant CNM $\Omega^*=2$ corresponding to a FQC with $N=2584$.

m	α_m	$t(2584, \Omega^*)$	$L/2584$
1	1597/987	1.000000	1.44269
2	987/610	0.999996	1.44268
3	610/377	0.999990	1.44266
4	377/233	0.999902	1.44239
5	233/144	0.999421	1.44089
6	144/89	0.995809	1.42971
7	89/55	0.972565	1.36131
8	55/34	0.836873	1.05302
9	34/21	0.428571	0.55811
10	21/13	0.098811	0.29588
11	13/8	0.015619	0.19038

$$\Gamma(N, \Omega^*) = \frac{1}{N} \ln[2 + 4(\alpha F_{n-2} - F_{n-1})^2], \quad (10)$$

where, without any loss of generality, we have adopted the reference values $m_A = K_{AA} = 1$. Then assigning different α_m values into Eq. (9) and Eq. (10) we can study the mass ratio dependence of t and Γ coefficients for different system lengths. In Table I we summarize the results for a FQC with $N=2584$, where $L = \Gamma^{-1}$ estimates the localization length of the corresponding states.

From the results listed in Table I several conclusions can be drawn. In the first place, as α_m progressively worsens as a τ approximant, we observe a systematic *degradation* of the transport properties of the resonant state, which evolves from an extended character ($t \approx 1$, $L/N > 1$) to a clearly localized one ($t \approx 0.1$, $L/N < 1$). In the second place, we observe that the extended-localized transition is a relatively sudden episode, taking place in a narrow window of mass ratio values around the critical value $\alpha^* = \alpha_8$. We have checked that this transition also occurs for other system lengths, although the precise value of α^* depends on N . In Fig. 2 we show the power spectrum and the amplitude dis-

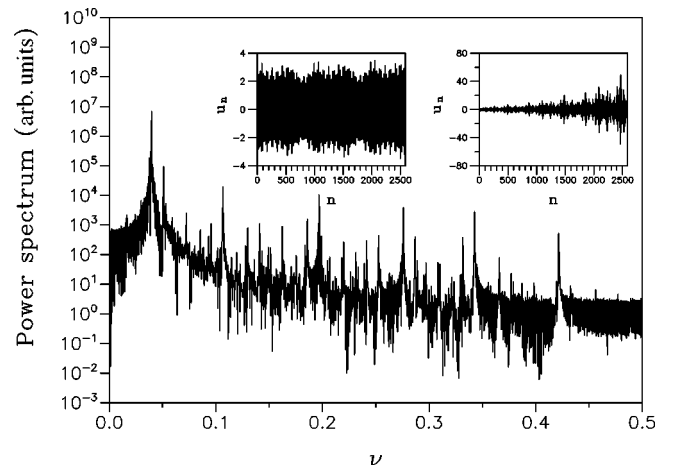


FIG. 2. Power spectrum of the CNM shown in the left-hand inset and atomic displacements in a FQC with $N=2584$ at the resonance frequency $\Omega^*=2$ for $\alpha_7=89/55$ (left-hand inset) and $\alpha_8=55/34$ (right-hand inset).

tributions of a CNM undergoing this transition. The CNM shown at the left-hand inset (α_7) has a high value of the transmission coefficient ($t \approx 0.97$), and uniformly spreads through the FQC ($L/N \approx 1.36$). Conversely, the transmission coefficient of the CNM shown at the right-hand inset (α_8) has significantly decreased ($t \approx 0.84$) and $L/N \approx 1$, indicating a sudden stretching of its spatial extent. The overall structure of the power spectrum is analogous to that shown in Fig. 1, but a closer inspection reveals some interesting differences. Thus we observe a shift of the periodiclike peak position towards higher frequencies describing the presence of the long-range modulation amplitude. Conversely, the nested twin peak features broaden, undergoing a substantial shift towards the lower frequency region of the spectrum. Finally, the ratio $I_{QP}/I_P \approx 10^{-3}$ increases by an order of magnitude, indicating the progressive relevance of the role played by the quasiperiodic contribution.

It is worth noting that the spatial structure of the CNM shown in the left-hand inset exhibits a long-range (about 900 sites) amplitude modulation containing a series of higher frequency quasiperiodic oscillations of minor amplitude. This complex spatial modulation has been previously reported as a characteristic signature of wave propagation on quasilattices in a few experimental studies dealing with Rayleigh surface acoustic waves propagating on the quasiperiodically corrugated surface of a piezoelectric substrate (LiNbO_3),¹⁷ and coherent acoustic phonons in GaAs/AlAs Fibonacci superlattices.¹⁸

Finally, we will briefly comment on the interesting behavior of the CNM when the FQC satisfies the condition $\alpha F_{n-2} - F_{n-1} = 1$. In this case the amplitude distribution exhibits a peculiar signature, where a complex arrangement of self-similar fluctuations of the normal mode amplitudes seems to be *modulated* by a broad, smooth envelope covering the entire system's length, as shown in the inset of Fig. 3. The overall structure of the corresponding power spectrum exhibits an intricate pattern, where a significant overlapping of different nested peaks occurs as a consequence of their progressive broadening. Notwithstanding, we can clearly appreciate the significant influence of the quasiperiodic contribution over the periodiclike one, as indicated by the relatively high value of the ratio $I_{QP}/I_P \approx 0.01$.

In summary, this work conveniently illustrates the *rich*

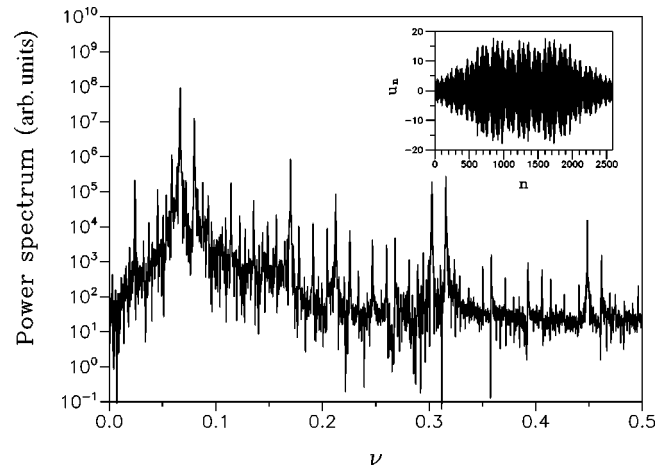


FIG. 3. Power spectrum of the CNM shown in the inset and atomic displacements in a FQC with $N=2584$ and $\alpha_9=34/21$ at the resonance frequency $\Omega^*=2$ (inset).

physical behavior of CS and the way the different spatial structures they display can affect their related transport properties, as measured in terms of the Lyapunov and transmission coefficients. 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, it is quite reasonable to assume that the transport properties of these critical normal modes are substantially affected by the quasiperiodic order of the underlying lattice. It is also worth noting that similar results concerning the existence of extended states in other kinds of self-similar structures, such as Thue-Morse chains and hierarchical lattices, have been recently reported in the literature.^{19,20} Consequently, we deem that the algebraic approach presented in this work may be extended in a straightforward manner to other kinds of aperiodic systems based on substitution sequences, and therefore it can be a promising starting point in order to attain a unified treatment of certain physical properties of aperiodic systems.²¹

I acknowledge M. Victoria Hernández for a critical reading of the manuscript. This work was supported by UCM under Project No. PR64/99-8510.

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