Energy spectra and level statistics of Fibonacci and Thue-Morse chains

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(Received 31 October 1994)

We study the density of states, the distribution of energy spacings, and the transmission coefficient of one-dimensional quasiperiodic Fibonacci and Thue-Morse systems. We consider arrays of δ potentials with constant separation and two potential strengths, and tight-binding systems with constant nearest-neighbor couplings and two different on-site energies. The quasiperiodicity lies in the arrangement of the two possible values of either the potential strengths or the on-site energies. We analyze the fractal character of the energy spectra of these systems through their integrated density of states and fractal dimensionality. We study the average with respect to energy of the transmission coefficient, which turns out to be a good way to measure the regularity of the system.

I. INTRODUCTION

During the last few years great attention has been devoted to the study of physical properties of quasiperiodic one-dimensional systems.[1] The Fibonacci lattice, which is made by juxtaposing two different building blocks A and B arranged in a Fibonacci sequence, has become a standard model for the study of these systems.

The Fibonacci sequence S_∞ is obtained by the recursion relation $S_{l+1} = \{S_l S_{l-1}\}$ for $l \geq 1$ with $S_0 = \{B\}$ and $S_1 = \{A\}$. The Fibonacci number F_l is the total number of building blocks A and B in S_l, and obeys the recursion relation $F_{l+1} = F_{l-1} + F_l$ for $l \geq 1$ with $F_0 = F_1 = 1$. It is easy to obtain that in the limit $l \to \infty$, the ratio F_l/F_{l-1} tends to the golden mean $\tau = (1+\sqrt{5})/2$.

A Thue-Morse sequence is a different type of aperiodic system, with a very different kind of aperiodicity from that of Fibonacci sequences.[2–5] The Thue-Morse sequence is obtained by the recursion relation $M_{l+1} = \{M_l M_l^*\}$ for $l \geq 0$ with $M_0 = \{AB\}$ and where M_l^* is the complement of M_l, obtained by interchanging A and B.

The electronic spectra of quasiperiodic Fibonacci lattices have been analyzed by a renormalization group type theory.[6,7] The spectra are Cantor set with a self-similar structure.[8] The transmission coefficient also shows self-similarity, which has been interpreted as a sign of quasilocalization.[9]

In this paper, we want to study numerically the fractal properties of the density of states and of the transmission coefficient. We also analyze the self-similarity of the energy spectra, which is best shown by the integrated densities of states. We will see that a recent experiment by Hattori *et al.*,[10] about the phase change of the light transmitted through a one-dimensional quasicrystal arranged in a Fibonacci sequence, shows a similar behavior between electromagnetic waves and our results for electrons in quasiperiodic structures.

Level statistics reflect very clearly the properties of disordered systems.[11] When the states are localized the nearest neighbor distribution of quantum levels is Poisson-like, while for systems with extended states it is of Wigner type. On the other hand, the (normalized) nearest-neighbor separation of levels in periodic systems is constant. Quasiperiodic chains could be considered as intermediate systems between periodic and random systems and we would like to study how this fact reflects itself in the level statistics.

II. METHOD OF CALCULATION

We consider two different models: a set of δ functions with two possible strengths arranged in Fibonacci or Thue-Morse sequences, and a tight-binding Hamiltonian with two types of atoms also arranged in Fibonnacci or Thue-Morse sequences. The separation between the δ functions is constant and, in the tight-binding model, we assume constant nondiagonal elements between nearest neighbors only. So, the quasiperiodicity only induces diagonal "disorder."

To calculate the energy spectrum we enclose our system between two infinite potentials to make it a close system and calculate the zeros of the characteristic determinant D, introduced by Aronov *et al.*[12] This determinant can be computed recursively for the two cases considered, and give us most magnitudes of interest, since it is directly related to the Green function of the system. For the tight-binding model we check that the energies obtained coincide with the eigenvalues of the tridiagonal Hamiltonian matrix. Our procedure is computationally more efficient than the direct evaluation of the levels.

D is the determinant of a tridiagonal matrix and satisfies the following recurrence relationship:

$$D_n = A_n D_{n-1} - B_n D_{n-2} \,, \tag{1}$$

where the index n goes from 1 to the number of δ functions (or sites in the tight-binding case). The initial conditions are

$$A_1 = 1, \qquad D_0 = 1, \qquad D_1 = 0 \,, \tag{2}$$

and we have for $n > 1$,

$$A_n = 1 + \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1} - r_{n-1,n-2}) \tag{3}$$

and

$$B_n = \lambda_{n-1,n}\frac{r_{n-1,n}}{r_{n-2,n-1}}(1 - r_{n-2,n-1})(1 - r_{n-1,n-2}). \quad (4)$$

The values of $r_{n,n-1}$ are model dependent, and for both, a tight-binding model and a set of δ functions, we obtain

$$r_{n,n-1} = \frac{V_n G_n^{(0)}}{1 + V_n G_n^{(0)}} \quad (5)$$

and $r_{n-1,n} = r_{n,n-1}$, where V_n is the nth diagonal energy in the tight-binding case, and the strength of the nth δ function in the other case. $G_n^{(0)}(x,x)$ is the unperturbed GF, for each case.

The density of states $\nu(E)$ can be obtained by counting the number of states in any given small energy interval or, alternatively, with the help of the characteristic determinant through the expression[13]

$$\nu(E) = \nu_0 - \frac{1}{\pi L}\,\mathrm{Im}\frac{\partial \ln D}{\partial E}, \quad (6)$$

where $\nu_0 = 1/2\pi k$ is the density of states of free electrons. For a closed system, $\nu(E)$ is a set of δ functions. It is easier to study $\nu(E)$ for the corresponding open system (where we suppress the two infinite potentials surrounding the system) for which the δ functions are smeared out.

The transmission coefficient and the resistance of the system can also be calculated from the characteristic determinant of the open system. The transmission amplitude t is the inverse of the characteristic determinant, $t = 1/D$, and so the transmission coefficient T is equal to[12]

$$T = |D|^{-2}. \quad (7)$$

Our method is very suitable to study if a very small value of the transmission coefficient is due to localization or to a gap, because all the quantities are obtained from the same basic entity, the characteristic determinant.

III. DENSITIES OF STATES

It is well known that the energy spectrum of a Fibonacci chain is a Cantor set. This property is more clearly seen by representing the integrated density of states as a function of energy. This is done in Fig. 1 for a tight-binding Fibonacci chain with 6765 sites; the atomic energies of the two types of atoms are $V_A = 1$ and $V_B = 0$, and the nearest neighbor transfer energy is equal to 1 (we choose this as our unit of energy throughout the paper). The self-similarity of the figure is evident. The flat regions are the energy gaps and the number of states between any two gaps is a Fibonacci number. For example, the number of states up to the first big gap is equal to 2584, which is the Fibonacci number two positions before than the total number of states (6765). The number of states between the two big gaps is 1597, which is the Fibonacci number previous to 2584. Thus the proportion of states in any of the two lateral pseudobands is equal to the square of the golden mean, and in the central pseudoband is equal to the golden mean to the third power. Changing the values of the atomic energies only varies the width of the gaps, keeping constant the number of states between the gaps.

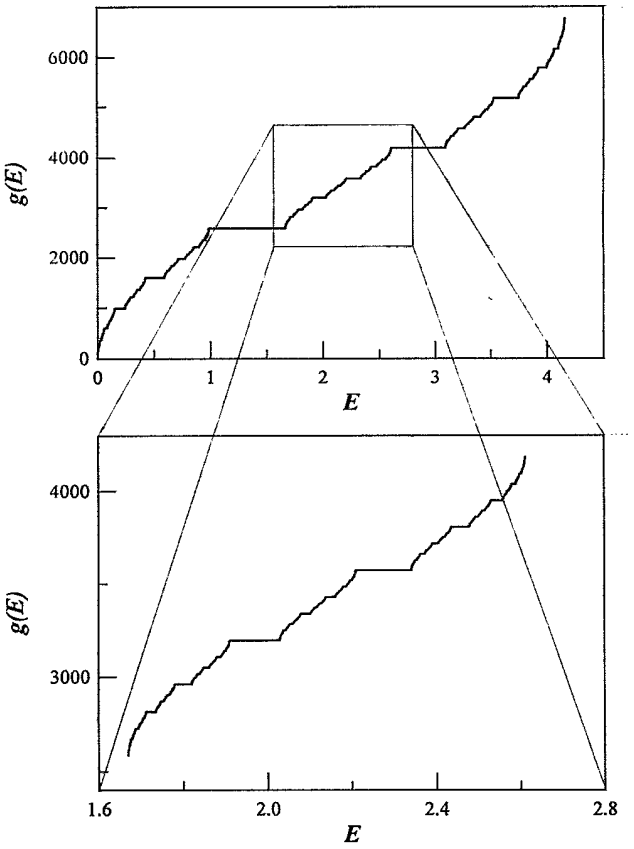

FIG. 1. Integrated density of states as a function of energy for a tight-binding Fibonacci chain with $V_A = 1$ and $V_B = 0$.

The results for a Fibonacci chain of δ functions are similar to those for the tight-binding model, although the relative width of the gaps changes noticeably, and an infinite number of pseudobands appears at higher energies.

The integrated density of states as a function of energy resembles the devil's staircase found by Bak and Bruinsma[16] for the chemical potential as a function of the relative occupancy of a periodic interacting one-dimensional system.

Integrating Eq. (6) with respect to energy and taking into account that $D = 1/t$, we find that the integrated density of states is proportional to the phase of the transmission amplitude. Hattori *et al.*[10] have recently measured this phase for photonic Fibonacci lattices and have found experimental curves very similar to Fig. 1.

The integrated densities of states as a function of energy for Thue-Morse chains are similar to those for Fibonacci chains, showing a whole sequence of gaps. The only major difference between these densities of states is the position of the gaps, which reflects the structure of the corresponding lattice.

In order to have a more quantitative idea of the importance of the gap structure we have obtained the fractal dimensionality of the energy spectra of Fibonacci and Thue-Morse sequences. We have done this by a direct computation of the definition of fractal dimensionality.[17]

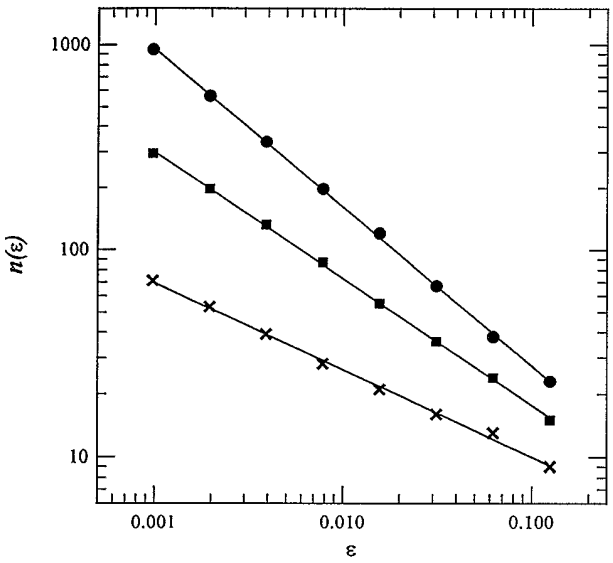

FIG. 2. Number of segments needed to cover the spectrum of a tight-binding Fibonacci chain versus the size of each segment for three values of $V_B - V_A$, 1 (solid dots), 2 (solid squares), and 5 (crosses). The corresponding fractal dimensionalities are 0.77, 0.61, and 0.42, respectively.

We considered line segments of different sizes and calculated how many of them are needed to cover all the eigenenergies of a closed system. The number of segments n is of the form

$$n(\epsilon) \propto \epsilon^{-d} , \tag{8}$$

where ϵ is the size of the line segment considered and d is the fractal dimensionality.[17] We checked that our method produces a dimension equal to unity for both an ordered and a random tight-binding system.

In Fig. 2 we plot n versus ϵ on a double logarithmic scale for a Fibonacci tight-binding system with 6765 states and $V_B - V_A$ equal to 1 (solid dots), 2 (solid squares), and 5 (crosses). The data for each case fit a fairly good straight line, whose slope is equal to minus the fractal dimensionality. This is equal to 0.77, 0.61, and 0.42, respectively, for the three cases considered. There is a systematic decrease of the effective dimensionality with increasing values of $V_B - V_A$.

Thue-Morse systems show a more similar dependence of the fractal dimensionality with $V_B - V_A$ than Fibonacci chains. For example, for a Thue-Morse chain with 4096 sites, the fractal dimensionality is 0.68 for $V_B - V_A = 1$, and 0.58 when $V_B - V_A = 2$. For the same value of the difference $V_B - V_A$, the dimensionality of the Fibonacci chain is bigger than that of the Thue-Morse chain.

IV. LEVEL STATISTICS

It is clear from the results of the integrated density of states for a Fibonacci chain that from a strict point of view we cannot talk about a normalized level distribution of nearest neighbor energies, since the infinite structure of gaps does not allow us to define an average separation.

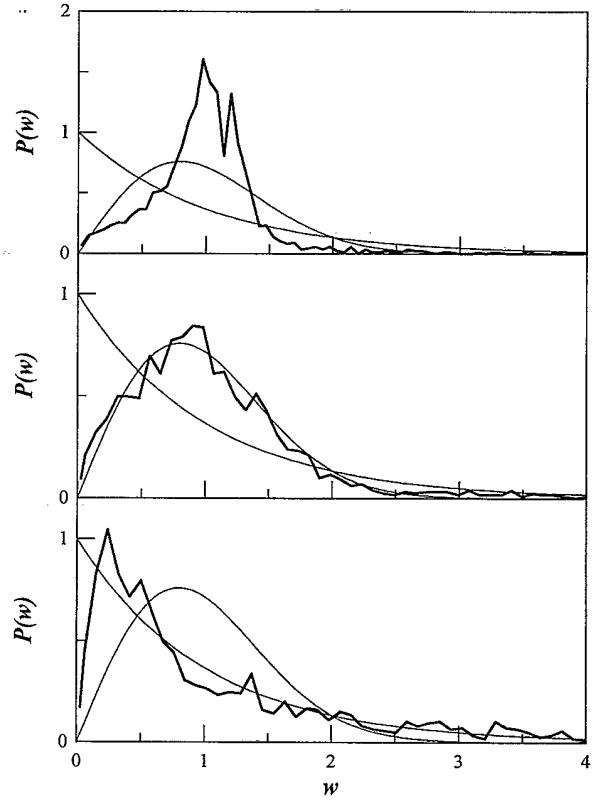

FIG. 3. Energy spacing distributions for the central band of a tight-binding Fibonacci chain. The upper curve corresponds to $V_B - V_A = 1$, the middle curve to $V_B - V_A = 5$, and the lower curve to $V_B - V_A = 10$.

We can only obtain an absolute distribution of energy spacings, in a small enough energy window.

In Fig. 3 we show the distribution of energy spacings for the central pseudoband of a tight-binding Fibonacci chain with 6765 sites. The upper curve corresponds to $V_B - V_A = 1$, the middle curve to $V_B - V_A = 5$, and the lower curve to $V_B - V_A = 10$. For comparison, we also plot Poisson and Wigner distributions. We can note that when $V_B - V_A$ is small, the distribution resembles that of the ordered case, which corresponds to a δ function. For intermediate values of the difference $V_B - V_A$, the distribution is close to Wigner, and when this difference increases the distribution approaches Poisson.

The results are similar for other pseudobands and for Thue-Morse chains, although the typical values of the potentials which one can associate with changes in the distribution of energy spacings vary from one case to another (for the same length of the system).

V. TRANSMISSION COEFFICIENT

In order to study transport properties of one-dimensional quasiperiodic sequences or of commensurate-incommensurate systems, it is convenient to solve first the problem of the scattering of a plane wave from these systems. In Refs. 14 and 15 the transmission and reflection amplitudes of electrons in one-dimensional arrays

of δ-function potentials, with the same strength and on locations whose separations follow a Fibonacci or a Thue-Morse sequence, were obtained.

In this section we study the scattering of a plane wave from a one-dimensional sequence of δ potentials located on a regular lattice and with two possible strengths distributed according to a Fibonacci or a Thue-Morse sequence. We calculate the transmission coefficient as a function of energy from Eq. (7). This coefficient shows marked oscillations between values close to unity and others very small, corresponding to gaps in the density of states.

The gap structure is reflected in the length dependence of the average with respect to energy of the transmission coefficient. When we increase the size of the system, more gaps open up and the average transmission coefficient decreases, since it is very small in the gaps. In Fig. 4 we plot, on a double logarithmic scale, the average transmission coefficient as a function of the length of the system for regular (triangles), Fibonacci (squares) and Thue-Morse (diamonds) sequences of delta functions. For each quasiperiodic lattice, we consider two set of parameters $V_A = 2$ and $V_B = 1$ (open figures), $V_A = 3$ and $V_B = 0.1$ (solid figures). The slopes of the straight line fits to these data are -7.1×10^{-5} for the regular system, -0.098 for the open squares, -0.15 for the open diamonds, -0.16 for the solid squares and -0.21 for the solid diamonds. The lines corresponding to Thue-Morse systems are systematically steeper than those for Fibonacci chains. This indicates that, as far as the transmission coefficient is concerned, Thue-Morse systems are more irregular than Fibonacci systems.

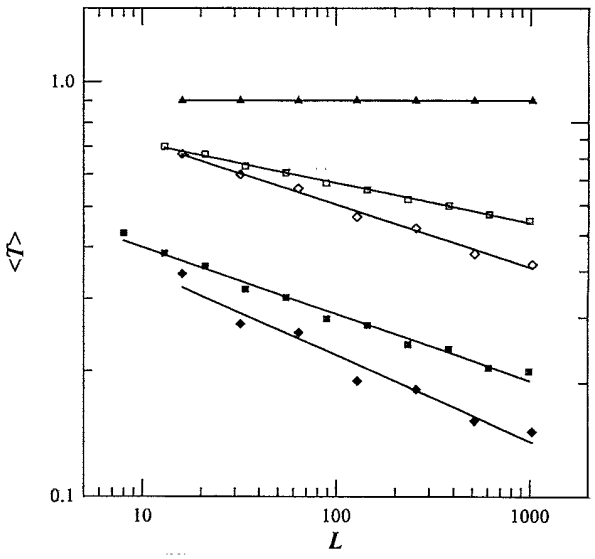

FIG. 4. Average transmission coefficient as a function of the length of the system, on a double logarithmic scale, for regular (triangles), Fibonacci (squares), and Thue-Morse (diamonds) sequences of δ functions. $V_A = 2$ and $V_B = 1$ for the open figures, and $V_A = 3$ and $V_B = 0.1$ for the solid figures.

VI. DISCUSSION

We have calculated the density of states, the energy-level distribution, and the transmission coefficient of Fibonacci and Thue-Morse sequences from the characteristic determinant of the system, which ensures a complete self-consistency of the data. The method is computationally very effective, and can be extended to many situations.

The distribution of the nearest neighbor energy level spacings resembles that of a regular system when the tight-binding parameters or the δ potential strengths are similar, and becomes successively Wigner-Dyson and Poisson type when the difference between these parameters increases.

Our results indicate that Fibonacci systems behave more regularly than Thue-Morse systems as far as the average value of the transmission coefficient is concerned, in disagreement with some recent claim.[2]

ACKNOWLEDGMENTS

We would like to acknowledge the Dirección General de Investigación Científica y Técnica, project number PB 93/1125, sabbatical support for V.G. and a grant for P.C., and the European Economic Community, Contract No. SSC*-CT90-0020, for financial support.

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