Substitutional disorder in a Fibonacci chain: Resonant eigenstates and instability of the spectrum

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The effect of substitutional disorder in a Fibonacci chain is studied. In particular it is shown that the presence of a single impurity affects all the states of the unperturbed system, reducing the fractal dimension of the spectrum. Resonant eigenstates are also observed. The consequences of the instability of the spectrum are discussed in the context of the experimental electronic measurements and also the effect of boundary conditions in theoretical calculations. [S0163-1829(96)07545-5]

I. INTRODUCTION

Over the 12 years after their discovery in 1982, quasicrystals have been the focus of intense experimental and theoretical research devoted to exploring the effects of quasiperiodicity on the properties of these materials. In particular, the self-similarity of the structure was expected to lead to a new type of electronic structure. Many theoretical works, mainly in one- and two-dimensional quasiperiodic systems, confirmed the expectations. In these systems, three kinds of wave functions coexist: extended, localized, and critical.[1] Critical states are neither localized nor extended; they have self-similar wave functions in real space. The band structure of the electronic spectrum of a Fibonacci chain is a Cantor set with a hierarchical distributions of gaps.[2] The spectrum of the Penrose lattice is of a different nature;[3] it does not present self-similarity and shows a δ function of degenerate states at the center of the spectrum, separated from the rest of the states by a sizable gap.[4] The wave functions of the states near the center of the spectrum are localized as opposed to the case of Anderson localization, where localization (due to disorder) is stronger near the band edges.

However, experimental results on transport properties and specific heat measurements had been rather disappointing. Measurements apparently indicated that quasicrystals shared the same transport properties with their crystalline or amorphous counterparts.[5] The origin of this result was considered to be the presence of secondary crystalline phases and of structural defects. The discovery of highly stable quasicrystals with a small defect density was of great advantage in investigating the intrinsic physical properties of quasicrystals. Recent results have shown that in fact quasicrystals are of a different nature than crystals or amorphous concerning their transport properties.[6] For instance, the extremely large resistivities, explainable only by some sort of localization effect, are the most striking physical property of quasicrystals.[7,8] Moreover, in conductor crystals, the electrical resistivity decreases as the perfection of the crystal increases; on the contrary, in quasicrystals resistivity decreases as defects increase, so that they become semiconductors and insulators. Up to now, the effect of disorder in quasiperiodic systems is not completely understood, and there remain some questions such as what is the minimal amount of defects allowed in quasicrystalline samples such that the theoretical predictions of perfect quasiperiodic structres can be measured experimentally?

Studies of the effects of disorder in quasiperiodic structures have shown that a minimal amount of phason disorder dramatically changes the extended states to localized states.[9,10] In a previous paper,[11] we proposed a renormalization approach to study the effect of phason disorder in large Fibonacci chains. The amount of disorder can be easily controlled and it was shown that less than 5% of disorder in a chain of $\sim 10^{20}$ sites was enough to smooth the energy spectrum of the chain.

It is the aim of this paper to explore the effect of substitutional disorder in a Fibonacci chain with a tight-binding Hamiltonian. It shall be shown that all the states of the chain are affected by the presence of a single impurity. The fractal dimension of the spectrum is reduced, and unlike the one-dimensional periodic chain, resonant eigenstates arise. The former result turns out to be relevant in theoretical calculations since the same effect will be observed when considering free boundary conditions.

The paper is organized as follows. In Sec. II we explain the Green's function approach to the treatment of substitutional disorder in a Fibonacci chain. In Sec. III, we evaluate the effect of the impurity on the eigenvalues and the energy spectrum. In Sec. IV the effect of the impurity on eigenstates is described, and finally, conclusions are given in Sec. V.

II. FORMALISM

The Fibonacci sequence is a quasiperiodic alternation of two words, L and S, given by the concatenation rule

$$F(n)=F(n-1)*F(n-2), \quad F(0)=S, \quad F(1)=L,$$

where * denotes string concatenation.

A quasiperiodic structure in one dimension can be constructed by arranging two types of bonds following the Fibonacci sequence (bond problem). A simple tight-binding model of electronic states of this quasicrystal is

$$H_0=\sum_i t_{ij}|i\rangle\langle j|, \tag{1}$$

where $|i\rangle$ is the Wannier state associated with the ith site of the chain and t_{ij} is the nearest-neighbor hopping integral,

which in this case is given by the Fibonacci sequence. A different model (site problem) is obtained if the Fibonacci sequence is used to define a self-energy (ϵ) on each site of the chain. The corresponding Hamiltonian of this model is

$$H_0=\sum_i (\epsilon_i|i\rangle\langle i|+t|i\rangle\langle i+1|+t|i\rangle\langle i-1|). \qquad (2)$$

It has been proved that the spectra of previous Hamiltonians are Cantor sets of zero Lebesgue measure,[12,2] with eigenstates which are neither localized nor extended, but critical.[12,2,13–15] This kind of spectra is called singular continuous.

There are powerful ways of solving Eqs. (1) and (2), such as renormalization and techniques which take advantage of the self-similar properties of the Fibonacci chain.[13–15]

We will now consider the case of a Fibonacci chain with a single substitutional impurity at site l. As will be shown, it is enough to understand the consequences of this kind of disorder on the eigenstates and the spectra of H_0.

The easiest way of introducing disorder in a Hamiltonian like Eq. (1) or (2) consists of changing the diagonal element of H_0 at site l, from ϵ_l to $\epsilon_l+\epsilon$. This situation can be thought of as a substitution of the host atom at site l by an impurity with a level lying ϵ times higher than those of the remaining atoms.[16] The new Hamiltonian now reads

$$H=H_0+H_1,$$

where

$$H_1=\epsilon|l\rangle\langle l|$$

is the perturbation due to the substitutional impurity.

The problem is to determine the eigenvalues and eigenfunctions of H. By following a perturbative approach, this task can be divided in parts. Determine first $G_0(E)$, the Green's function of H_0 (one possibility is to use a renormalization procedure as described in Refs. 17–19). Next, express $G(E)$ in terms of $G_0(E)$ and, finally, obtain information about the eigenfunctions and eigenvalues of H from G, defined as

$$G(E)=(E-H)^{-1},$$

where E is the energy.

Using a Dyson expansion, the Green's function of the perturbed system is given by

$$G=G_0+G_0SG_0,$$

where

$$S=H_1+H_1G_0H_1+H_1G_0H_1G_0H_1+\cdots,$$

which in this case is written as

$$S=\epsilon|l\rangle\langle l|+\epsilon^2|l\rangle\langle l|G_0|l\rangle\langle l| +\epsilon^3|l\rangle\langle l|G_0|l\rangle\langle l|G_0|l\rangle\langle l|+\cdots.$$

After a simple summation, a closed expression for S is obtained:

$$S=\frac{\epsilon}{1-\epsilon\langle l|G_0|l\rangle}|l\rangle\langle l|, \qquad (3)$$

with which the final expression for the Green's function reads

$$G=G_0+\frac{\epsilon}{1-\epsilon\langle l|G_0|l\rangle}G_0|l\rangle\langle l|G_0.$$

The discrete eigenvalues of H are the poles of G (or S), that is,

$$\langle l|G_0(E_p)|l\rangle=1/\epsilon, \qquad (4)$$

which is only fulfilled when the imaginary part of G_0 is zero. Since the imaginary part of G_0 is directly related to the local density of states through[16]

$$\rho_{ll}(E)=-\frac{1}{\pi}\mathrm{Im}(\langle l|G_0(E_p)|l\rangle),$$

if there are new states due to the impurity, they must lie inside a gap of the original spectrum.

In a periodic chain, the poles E_p are outside the band of H_0, because inside the band, the spectrum is continuous (there are no gaps) and Eq. (4) cannot be satisfied. On the contrary, the singular continuous spectrum of a Fibonacci chain contains an infinite number of gaps, and so relation (4) can in principle be satisfied between any two eigenvalues of H_0. Consequently, substitutional disorder affects all the states of a singular continuous spectrum and not only those at the top of the band as in the case of a periodic chain. As will be shown in Sec. III, this effect consists of a shifting of all the original eigenstates.

One may visualize this effect of the impurity in a Fibonacci chain using the following arguments. Let us first consider a perfect periodic chain with lattice parameter a. When a defect is introduced, the most scattered modes are those at the top of the band and a localized impurity mode appears outside the original band, that is, near $k=\pi/a$, where k is the usual wave vector of a periodic system. Now suppose that the chain is transformed onto a diatomic linear chain. Since the cell parameter is doubled, the new spectrum is obtained by folding the original spectrum around $k=\pi/2a$ and a gap of size V_k arises at the limit of the new Brillouin zone. In this diatomic chain there are two impurity modes which now appear due to disorder, the one at $k=\pi/2a$ and the other at $k=0$. Since the Fibonacci chain is obtained by folding the Brillouin zone an infinite number of times[20] (each folding corresponding to a rational approximant), an infinite number of gaps are opened and also an infinite number of impurity modes are created.

III. EIGENVALUES AND SPECTRUM

In general, the introduction of disorder in a finite lattice with $\epsilon>0$ leads to a shift of the states to higher energies.[21] An estimation of these shifts, arising from one single impurity, can be given as follows. In a discrete or a singular continuous spectrum, the imaginary part of the Green's function is written as a sum of δ functions at the poles E_n of H_0 with a weight given by the amplitude $|\phi_n(l)|^2$ of the

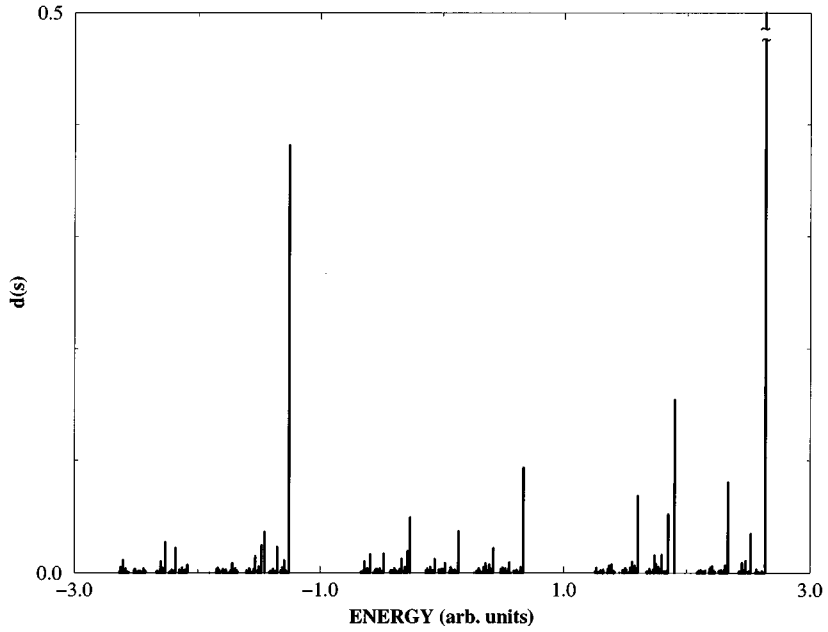

FIG. 1. Displacement $d(s)$ of the eigenvalues of the Fibonacci chain with a single impurity from the eigenvalues of the perfect chain. Calculations were made for a chain with 987 sites.

wave function at site l, that is,

$$\mathrm{Im}\langle l|G(E)|l\rangle = -\pi \sum_n |\phi_n(l)|^2 \delta(E-E_n).$$

The real part of G is obtained with the help of the Kramers-Kronig relations

$$\mathrm{Re}\langle l|G(E)|l\rangle = \frac{1}{\pi} P\left[\frac{\pi \Sigma_n |\phi_n(l)|^2 \delta(E'-E_n)}{(E-E')}\right] = \sum_n \frac{|\phi_n(l)|^2}{(E-E_n)}, \tag{5}$$

where P stands for the principal part. In the region between two states, say, E_s and E_{s+1}, the main contribution to the sum comes from the terms with $n=s$ and $n=s+1$, so that the right-hand side of Eq. (5) can be approximated by

$$\frac{|\phi_s(l)|^2}{(E-E_s)} + \frac{|\phi_{s+1}(l)|^2}{(E-E_{s+1})} = \frac{1}{\epsilon}. \tag{6}$$

Now if $d(s)$ denotes the shift of the state s, then we have $d(s)=(E-E_s)$ and $(E-E_{s+1})=d(s)-\Delta_s$, where Δ_s is the separation between levels E_s and E_{s+1}.

With these definitions, Eq. (6) is reduced to a second-order equation with the solution

$$d(s) = \frac{\Delta_s}{2} + \epsilon \overline{|\phi_s(l)|^2} - \sqrt{\left(\frac{\Delta_s}{2} + \epsilon \overline{|\phi_s(l)|^2}\right)^2 - \epsilon \Delta_s |\phi_s(l)|^2}, \tag{7}$$

where $\overline{|\phi_s(l)|^2} = [|\phi_s(l)|^2 + |\phi_{s+1}(l)|^2]/2$, and the minus sign was chosen to assure that $d(s)$ is zero for $\varepsilon = 0$.

In a periodic but finite lattice $|\phi_s(l)|^2$ and the spacing between levels scale as the inverse of the number of sites N, then $d(s)$ is also scaled by $1/N$. Consequently, in the limit $N \to \infty$, new solutions arise only at an energy higher than the top of the band, since the other solutions are undistinguishable from the original ones.

In a Fibonacci chain the space between levels follows an anomalous $1/N^{\beta(E)}$ law.[22] This is also true for the size dependence of wave functions which follows the law $|\phi_s(l)|^2 \sim 1/N^{\gamma(E_s)}$.[22] As a consequence of the singularity of the spectra, both γ and β are smaller than one in the regions of the largest gaps and larger than one in the remaining regions. From Eq. (7) it can be seen that, in an infinite lattice, the tendency of the spectrum is to be smoothed, since d is larger (smaller) in regions where β and γ are smaller (larger) than 1. The smoothening effect is enhanced at the edges of the spectra where β and γ take their minimum values.[22] The self-similarity of the spectra also means that states are shifted at all scales.

Numerical direct diagonalization of H was carried out in order to confirm the above considerations. Figure 1 shows a plot of $d(s)$ against the eigenvalues for the bond problem ($t_L=-1.5$ and $t_S=-1.0$) of a Fibonacci chain with $N=987$ and with a single defect ($\epsilon=10$) at the middle of the lattice. The largest value of $d(s)$ is at the top of the band and corresponds to the localized state that appears outside the band near $E \sim \epsilon$. In general, $d(s)$ is larger for states near to the largest gaps, as is expected from Eq. (7). Observe that $d(s)$ is self-similar as a consequence of the self-similarity of $|\phi_s(l)|^2$ and Δ_s.

The integrated density of states (IDOS) of a perfect Fibonacci chain has a devil's staircase structure which is typical of a Cantor-like set. When the defect is introduced, and since $d(s)$ is self-similar, all the steps of this devil's staircase are reduced and the IDOS is transformed into a Besicovitch staircase which is a multifractal curve with a larger fractal dimension.[23] Albeit this tendency should be observed with a single defect, the transition to a Besicovitch staircase is even more evident in a Fibonacci lattice with two defects of the same type. In Fig. 2 an enlarged view of a section of the

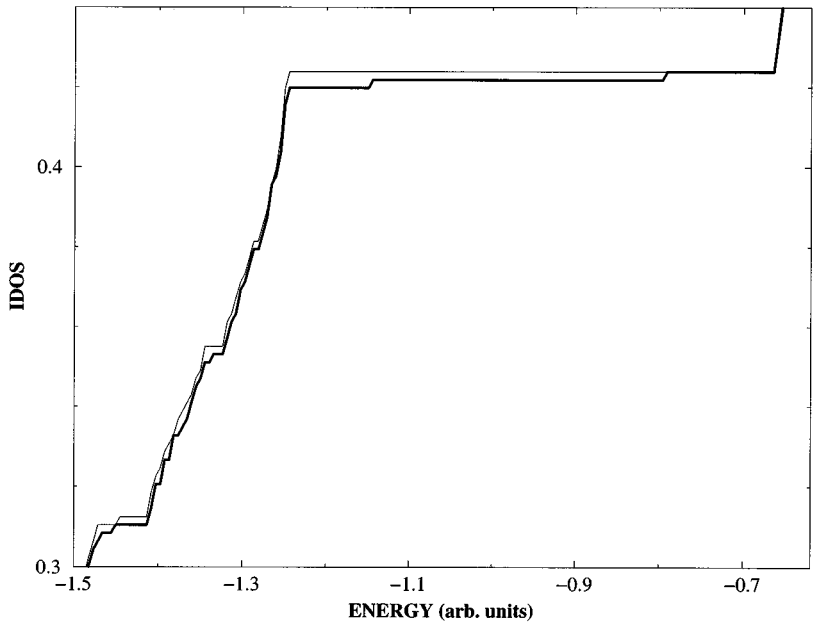

FIG. 2. Enlarged view of a section of the integrated density of states of the perfect Fibonacci chain (thin line) compared with the chain with two defects (bold line).

IDOS of the Fibonacci chain with two defects is shown (bold line) and compared with that of the perfect chain (thin line).

The scaling properties of the DOS can be obtained by means of a multifractal analysis.[25] First, observe that the level spacing for a finite system is given by $\Delta E = 1/N\rho(E)$ where ΔE is the separation between two eigenvalues. Then, the system size dependence of the level spacing (δE) is given by $\delta E = \rho(E)\Delta E$. In a periodic system δE is always $1/N$.

Now, let us define a scaling exponent (α) through[24]

$$\alpha = -\frac{\ln(\delta E)}{\ln N}. \tag{8}$$

The fractal dimension for each exponent is given by[25]

$$f(\alpha) = -\frac{\ln\Gamma(\alpha)}{\ln(\overline{\delta E})}, \tag{9}$$

where $\overline{\delta E}$ is the average of δE, and $\Gamma(\alpha)$ is the number of level spacings with a scaling exponent between α and $\alpha + \delta\alpha$.

The spectrum is the union of fractal sets, each of them with a fractal dimension given by $f(\alpha)$. The fractal dimension of the whole set, which is the Hausdorff-Besicovitch dimension of the DOS, is the maximum of $f(\alpha)$. If this maximum is smaller than 1, the spectrum is singular continuous.[25]

In Fig. 3 we show $f(\alpha)$ for the lattice with a single defect. The maximum of $f(\alpha)$ is ~ 0.45. This value is smaller than the maximum of the same curve obtained from the Fibonacci

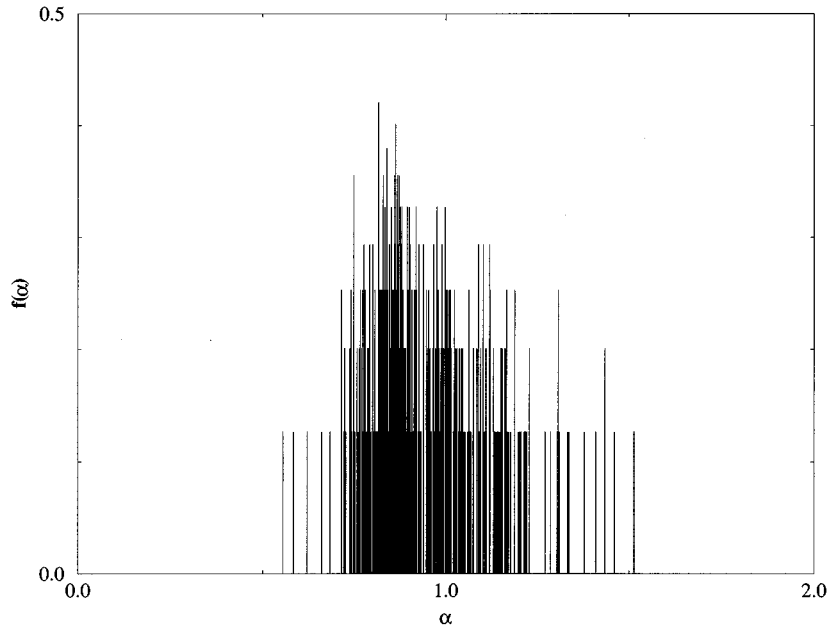

FIG. 3. The multifractal distribution of scaling exponents for the energy spectrum of the Fibonacci chain with a single defect.

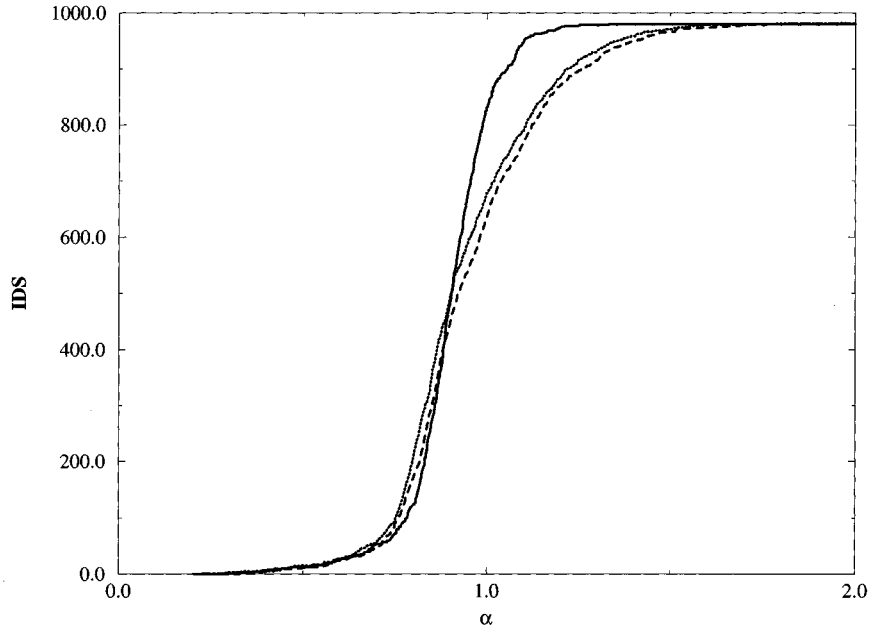

FIG. 4. Integrated distribution of scaling exponents for the perfect Fibonacci chain (solid line), chains with one (dotted line), and two (dashed line) defects.

chain where $f_{\max}\sim 0.56$ for a lattice of size $N=987$. If $N\to\infty$, the fractal dimension lies between 0.6 and 0.7.[22]

The reduction of the fractal dimension has its origin in the widening of the function $\Gamma(\alpha)$. Since $\Sigma_\alpha \Gamma(\alpha)=N$, a dispersion in the scaling leads to a reduction of the maximum value of $\Gamma(\alpha)$ which in fact determines the fractal dimension since the factor $\ln(\overline{\delta E})$ is almost the same for both lattices. For the sake of comparison, we calculate the integrated distribution of scaling exponents (IDS), defined as $\int_0^\alpha \Gamma(\alpha)d\alpha$, for the perfect Fibonacci chain, and chains with one and two defects. In all the cases it was found that $\overline{s}$ approaches $1/N$. The dispersion of $\Gamma(\alpha)$ is evident in Fig. 4 where the IDS is shown. In a periodic chain, the IDS jumps from 0 to N when $\alpha=1$, but for the Fibonacci chain it shows dispersion near $\alpha=1$. As can be seen, the IDS of the chain with a single defect shows a larger dispersion than the perfect one and the IDS of a chain with two defects shows even more dispersion. From here it is clear that the reduction of the fractal dimension is a consequence of a change in the level statistics.

It is interesting to comment that a similar reduction of the Hausdorff-Besicovitch dimension was found in the transition from a singular continuous to a pure point spectrum in the Harper potential.[26] In that case, the Hausdorff-Besicovitch dimension of the pure point spectrum (which corresponds to localized eigenstates) is zero while in the singular continuous regimen is given by the fractal dimension of a Cantor set.[26]

IV. EIGENSTATES

We consider here the eigenstates of H which are given by[16]

$$|\psi(E)\rangle=|\phi(E)\rangle+G_0^+(E)S^+(E)|\phi(E)\rangle, \tag{10}$$

where $|\phi(E)\rangle$ are the eigenfunctions of the unperturbed Hamiltonian. The plus sign in G and S denotes the use of the retarded Green's function, in such a way that only physically outgoing solutions are admitted.

Substituting Eq. (3) into Eq. (10), the wave function at site n results:

$$\langle n|\psi(E)\rangle=\langle n|\phi(E)\rangle+\epsilon\frac{\langle n|G_0^+(E)|l\rangle\langle l|\phi(E)\rangle}{1-\epsilon\langle l|G_0^+(E)|l\rangle}.$$

At the site l of the impurity, the above expression is reduced to

$$\langle l|\psi(E)\rangle=\frac{\langle l|\phi(E)\rangle}{1-\epsilon\langle l|G_0^+(E)|l\rangle}, \tag{11}$$

from where the amplitude at site l is easily obtained:

$$\langle l|\psi(E)\rangle^2=T\langle l|\phi(E)\rangle^2, \tag{12}$$

where T is defined as

$$T=\frac{1}{|1-\epsilon\langle l|G_0^+(E)|l\rangle|^2}. \tag{13}$$

Some words about the quantity T can be said here. In one-dimensional lattices T usually stands for the transmission coefficient. In a quasiperiodic lattice, it turns out that k is not a good quantum number, and so Eq. (13) does not represent the transmitted amplitude across the chain since also the system without defects shows scattering. Then, in this case T is a measure of the scattering of critical states due to the presence of defects.

Equation (13) can be written as

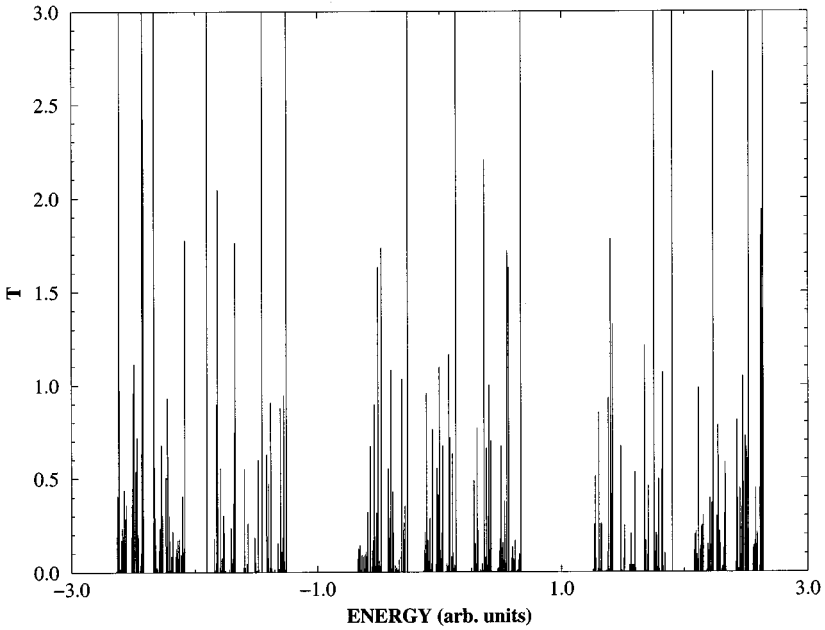

FIG. 5. T is plotted as a function of the energy. States with $T>1$, $T\approx 1$, and $T\approx 0$ are, respectively, localized, resonant, and scattering eigenstates.

$$T=\frac{1}{[1-\epsilon \mathrm{Re}\langle l|G_0^+(E)|l\rangle]^2+[\pi\rho(E,l)]^2}. \qquad (14)$$

T has its maximum value whenever $\rho(E,l)$ is small and $1-\epsilon \mathrm{Re}\langle l|G_0^+(E)|l\rangle$ approaches zero, which is indicative of a resonant eigenstate. Observe that for the original states inside the band, $\langle l|G_0^+(E)|l\rangle$ is always a complex number so that $T\leqslant 1$. Therefore, a resonant eigenstate of H_0 leads to a peak of size 1 in the curve of T plotted against E.

For instance, in a perfect periodic chain $\rho(E,l)$ is small at the center of the band and tends to infinity at the band edges, and so states at the band edges (the most coherent ones) are more strongly scattered than those at the middle. In this kind of chain, T does not exhibit any resonance since there are no possibilities for interference effects.[16]

T can also be calculated considering Eq. (12) as a definition for all the states, i.e., for states inside the band and for the new states that appear with the defects. In that case T can be larger than 1 for the defect states, meaning that defect states are localized.

Figure 5 shows T as a function of the eigenvalues of the perfect Fibonacci chain calculated using Eq. (12) as the definition of T. Observe that states at the edge of the largest gaps fulfill $T>1$ since they become defect states and are localized. Eigenstates with T approaching zero are strongly scattered by the defect. Resonant states are those with T approaching 1 and are less scattered by the disorder.

The existence of scattering and resonant eigenstates is preferable due to the infinity folding of the Brillouin zone. In a periodic chain, states with larger T are at the middle of the band. Each time that a new folding takes place, a new region appears in the middle of each subband that can support resonant eigenstates.

V. CONCLUSIONS

In this article we studied the consequence of introducing a single defect on a Fibonacci chain. Our results can be summarized as follows. As a consequence of the self-similarity of the spectra, the disorder affects all the states of the unperturbed system and consequently the fractal dimension of the IDOS increases. On the contrary, the fractal dimension of the DOS with a defect is reduced since the multifractal distribution of the scaling exponents shows a larger dispersion respect to the perfect Fibonacci chain. This change in the multifractal distribution is a consequence of the change in the level statistics. This last is expected since a singular continuous spectrum shows a tendency toward clustering of levels, producing a new class of level statistics,[27] while a disordered system follows a Poisson distribution with a width proportional to $1/N$.[28] Finally, unlike the case of periodic one-dimensional chains, resonant eigenstates appear.

The present study, in spite of the simplicity of introducing a single defect, is capable of showing the essential consequences of the presence of substitutional disorder in one-dimensional quasiperiodic structures. Two conclusions can be drawn. First, since free boundary conditions can be viewed as impurities, the use of periodic boundary condition is preferable in numerical calculations. As was shown, free boundaries lead to surface states appearing at all energies. Second, singular continuous spectra and critical states may be very difficult to observe in a real quasicrystal since even a small amount of disorder can destroy these features.

All the ideas portrayed here can be extended to the vertex problem for the Penrose lattice where an infinite series of gaps appears near the center of the spectrum,[29] and therefore this region is expected to be strongly affected by disorder.

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