Use of the trace map for evaluating localization properties

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The use of Lyapunov exponents for evaluating localization lengths of wave functions in one-dimensional lattices is discussed. As a result, it is shown that it is more practical to calculate this length by using the scaling properties of the trace map of the transfer matrix. This leads to a relationship between localization and the fixed points of the map, which is considered as a dynamical system. The localization length is then defined by a Lyapunov exponent, used in the sense of chaos theory. All these results are discussed for periodic, disordered, and quasiperiodic chains. In particular, the Fibonacci quasiperiodic chain is studied in detail. [S0163-1829(99)05217-0]

I. INTRODUCTION

Much work has been devoted to study the localization of waves, following the seminal work by Anderson,[1] and the subsequent intensive research in the field of disordered materials.[2] At present, there exist several different criteria to evaluate when localization occurs, and how to measure it, although many of these criteria are not rigorously proven.[3] Furthermore, with the advent of the intensive use of computer calculations, it is clear that these criteria must be adapted to extrapolate conclusions from finite to infinite systems. One of the most dramatic pieces of evidence of this fact was found after the discovery of quasicrystals in 1984.[4] Quasicrystals present a peculiar kind of order: despite lacking translational order, the positions of the atoms are not arbitrary, as in an amorphous solid, but precisely determined. Thus, neither of the methods developed to deal with crystals or amorphous apply to this case. One could approximate a quasicrystal by a crystal, with a large unit cell. However, still there is no consensus about the nature of the spectrum and wave functions, since quasiperiodic systems present anomalous dependences on the system size.[5]

In one-dimensional systems (1D), the transfer matrix formalism has been very useful to determine the spectrum and to describe the propagation of waves as they travel across periodic, disordered, and quasiperiodic lattices. Within this method for a tight-binding Hamiltonian, the spectrum is found by using the trace of the transfer matrix. This is extremely successful in the field of 1D quasicrystals, since Kohmoto, Kadanoff, and Tao[6] found a recurrence relation for the trace of a Fibonacci chain.[6] This relation defines a trace map, from which the spectrum can be found by successive iterations. After its introduction, this technique has produced many interesting results concerning the nature of the spectrum for diverse quasiperiodic systems, such as the period-doubling[7] and Thue-Morse[8] chains. More recently, this formalism has been extended to aperiodic systems where the complexity of the transfer matrix makes such a formalism particularly involved.[9]

Since the trace is a powerful tool for determining the spectrum, one is lead to ask if it is possible to use it in order to investigate localization. In this paper, this question is answered by finding expressions that relate the localization of waves with the properties of the trace map, considered in the sense of a dynamical system. Furthermore, this way to investigate localization is much more efficient than the use of the Lyapunov exponents of the wave functions,[10] since this method presents some problems in practice, as we shall see in Secs. II and IV. The results presented in this paper also show that the stability properties of the trace map and their related Lyapunov exponents (used in the sense of chaos theory) are suitable tools to classify the nature of eigenstates in extended, critical, and localized, and thus must be referred as a diagnostic tool for localization.[11]

The structure of the paper is as follows. In Sec. II the formalism of the transfer matrix is introduced, and the problems of the Lyapunov exponents are discussed. In Sec. III, the relation between the localization length, scaling of bands, and the stability of trace map is discussed. Section IV is devoted to show two applications of the concepts developed in Sec. III: a periodic chain with an impurity and a Fibonacci chain. Finally, in Sec. V the conclusions are given.

II. TRACE MAPS AND THE LYAPUNOV EXPONENTS

In one-dimensional systems, the tight-binding Hamiltonian is very appropriate to describe electron and phonon propagation. Thus, this kind of Hamiltonian will be used through all the article, although most of the conclusions can be applied to other Hamiltonians. The Schrödinger equation for a 1D tight-binding Hamiltonian, defined on a chain of n sites, with an on-site potential V_n at site n, and hopping integral t_n between sites n and $n+1$ is

$$t_n\psi_{n-1}+t_{n+1}\psi_{n+1}+V_n\psi_n=E\psi_n, \tag{1}$$

where ψ_n is the value of the wave function at site n. Usually, for this equation two cases are considered: the on-site or diagonal problem, where t_n is a constant that does not depend on the site, and the off-diagonal, where V_n is the same for all sites. In this paper, both cases are considered, although in the applications we will study the on-site for simplicity.

As is well known, Eq. (1) can be rewritten in terms of the transfer matrix $M(n)$,

$$\mathbf{\Psi}_n=\begin{pmatrix}(E-V_n)/t_n & -t_{n-1}/t_n\\ 1 & 0\end{pmatrix}\mathbf{\Psi}_{n-1}\equiv M(n)\mathbf{\Psi}_{n-1}, \tag{2}$$

where Ψ_n stands for

$$\mathbf{\Psi}_n=\begin{pmatrix}\psi_n\\ \psi_{n-1}\end{pmatrix}. \tag{3}$$

A successive application of Eq. (2), gives the wave function at site n as a function of the value at the beginning of the chain

$$\mathbf{\Psi}_n=M(n)M(n-1)M(n-2)M(n-3)\cdots M(2)\Psi_1 \equiv T(n)\mathbf{\Psi}_1. \tag{4}$$

The allowed values for the energies are those for which the norm of trace of the matrix $[\tau_n\equiv trT(n)]$ is less than 2.[12] Furthermore, in many cases one can obtain a recurrence relation of the type

$$\tau_n=f(\tau_{n-1},\tau_{n-2},\tau_{n-3},\ldots,\tau_{n-j}), \tag{5}$$

which allows us to compute the spectrum without calculating the full product of matrices, and thus reduces the complexity of the problem. Such a relation is a trace map. Our aim is to use this map to determine the nature of localization in a chain.

A starting point toward this goal is to use a parameter for characterizing the localization of a wave function. Usually, a parameter to estimate the growth of the wave function as the excitation goes along the chain is the Lyapunov exponent, defined as[10,12]

$$\gamma(E)\equiv\lim_{n\to\infty}\gamma_n(E)\equiv\lim_{n\to\infty}\frac{1}{n}\ln\|T(n)\|, \tag{6}$$

where the norm $\|T(n)\|$ is

$$\|T(n)\|=\sup\|T(n)\mathbf{\Psi}\|/\|\mathbf{\Psi}\|. \tag{7}$$

In the last definition, $\mathbf{\Psi}$ is any vector that maximizes $\|T(n)\|$. In the case of exponentially localized functions, $\gamma(E)$ is the inverse of the localization length (ξ), since $\|T(n)\mathbf{\Psi}\|\sim e^{n/\xi}$. The growth of the wave function is determined by the greatest eigenvalue of the transfer matrix,[13] denoted by $\lambda_{\max}$,

$$\gamma(E)=\lim_{n\to\infty}\frac{1}{n}\ln|\lambda_{\max.}|. \tag{8}$$

The next step is to obtain this maximum eigenvalue of $T(n)$ using the characteristic equation of $T(n)$

$$\det[\lambda-T(n)]=\lambda^2-\lambda\tau_n+1=0, \tag{9}$$

where we used that the determinant of the transfer matrix is one, since it is the product of matrices with the determinant one. By solving Eq. (9) we found the two eigenvalues of $T(n)$,

$$\lambda_\pm=\frac{\tau_n\pm\sqrt{\tau_n^2-4}}{2}. \tag{10}$$

For energies which satisfies $\|\tau_n\|>2$, the eigenvalues are real and the Lyapunov exponent is

$$\gamma(E)=\lim_{n\to\infty}\frac{1}{n}\ln(|\tau_n|+\sqrt{\tau_n^2-4}). \tag{11}$$

Inside the spectrum $\|\tau_n\|\leqslant 2$, $\lambda_\pm$ are complex, both with unitary norm, and thus the Lyapunov exponent is zero, since $\|T(n)\|$ is always 1. At first sight, it seems to be strange that for states inside the spectrum the Lyapunov exponent is zero, whatever the shape of the wave function, since for a localized state we would like to find its corresponding localization length.

The solution to this problem is related with the Borland conjecture,[14] and to the appearance of bands when using the transfer matrix even for isolate eigenvalues. In order to explain this point, let us consider the problem of an impurity in a periodic linear chain (we set $V_0=\delta$ and $V_n=0, n\neq 0, t_n=t$). As is known, the spectrum of this chain is the original band of the periodic chain (the set $-2\leqslant E\leqslant 2$), plus a localized impurity mode at $E_c=\sqrt{4+\delta^2}$.[3] How can we obtain the localization length of this mode from the transfer matrix?

Quite generally, in the method of the transfer matrix, if we put an excitation at the left of the chain in a spectral gap of the periodic chain, the excitation grows exponentially with a speed determined by the greatest eigenvalue of the transfer matrix, unless we start with a vector that corresponds to the lower eigenvalue eigenvector; in such a case the excitation decreases. Now, if we traverse the chain from right to left, we obtain the opposite result, since the excitation grows from right to left.[10] At first sight, this seems quite paradoxical for the impurity mode, because we need to satisfy fixed boundary conditions at both ends of the chain, with a maximum at the impurity site.

The solution to this problem is that the growing solution from left to right, is the same that decreases from right to left.[14] For an energy that corresponds to an eigenvalue of the *whole* chain, the excitation can be matched at the impurity site to satisfy the boundary conditions on both sides of the chain.[14] This matching is achieved by making zero the growing solution at the impurity site.

Thus, if we define the Lyapunov exponent only in one half of the chain $[\gamma_\pm(E)]$, from the left (right) of the impurity site, the Lyapunov exponents are given by

$$\gamma_\pm(E_c)\equiv\lim_{n\to\pm\infty}\ln\frac{1}{n}\|T(n)\|=\ln\left(\frac{|E_c|+\sqrt{E_c^2-4}}{2}\right), \tag{12}$$

but if we consider the whole chain, the exponent is zero since the excitation does not grow in order to satisfy the boundary conditions. This is in agreement with the previous result which showed that, whenever we have an allowed state, $\gamma(E)$ of the whole chain is zero.

Figure 1 illustrates this point. The Lyapunov exponent of the whole chain (solid line) and half of it (dashed line) when $\delta=1.5(E_c=2.5)$ are shown. Calculations were carried out using the norm of the product of successive transfer matrices for a given initial excitation. The Lyapunov of half of the chain gives the correct localization length, while the corre-

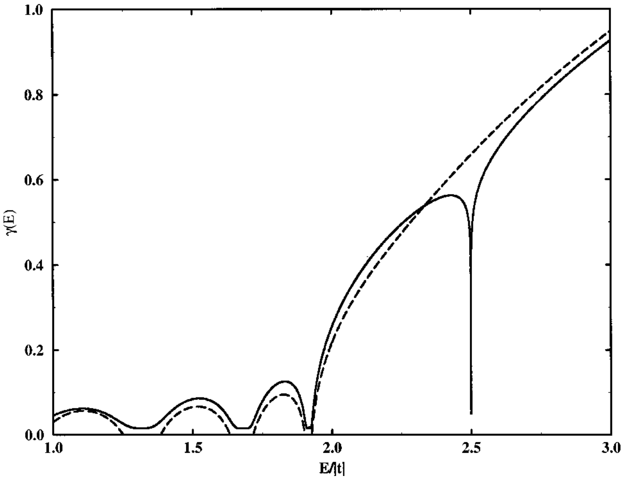

FIG. 1. Lyapunov exponents for a periodic chain with an impurity ($\delta=1.5$, $E_c=2.5$) near the upper band edge. The solid line corresponds to the exponents of the whole chain, while the exponents calculated by dividing the chain in 2 are shown by dots. Observe the pronounced dip of the Lyapunov at the impurity mode, which gives a value similar to the states inside the band of the periodic chain (energies from 1 to 2 in the figure).

sponding to the full chain has a pronounced dip that approaches zero at the energy that corresponds to the impurity mode.

The problem with this method is that we need to know in advance where the maximum of the wave function is, and then proceed to study the Lyapunov exponent. Clearly, in many cases this information is difficult to obtain, so the method is hard to apply. However, as we shall see in the next section, the problem can be avoided by using the scaling of the spectrum bandwidth.

III. LOCALIZATION AND STABILITY OF THE TRACE MAP

A. Scaling of bands

A second approach toward the use of the trace map as a diagnostic tool, is to adapt a qualitative argument similar to the one introduced by Thouless[15] and Sire[16] in the localization problem to explain the scaling of bands. Consider a piece of chain with n sites. For the moment we do not care about its internal structure, which may be periodic, disordered, or quasiperiodic. Now we construct a crystal by a periodic repetition of the chosen piece, which acts as an unitary cell of this crystal.

Let us first consider that the cell is also a crystal. As usual, the width of the band (W_n) of this crystal is $W_n \sim t_n$. This width also can be seen as the overlap between two similar states $|\psi_1\rangle$ and $|\psi_2\rangle$ at two contiguous unit cells. This overlap is given by

$$W_n \sim \langle \psi_1 | H | \psi_2 \rangle \sim t_n, \tag{13}$$

where it was assumed that the fact that extended states do not decrease with n, and thus their overlap is n independent. This shows that the size of the band is clearly n independent.

Next, we consider that the unit cell is disordered, with eigenstates that are exponentially localized with a length $\xi(n \gg \xi)$. The overlap leading to W_n is then of the order,

$$W_n \sim <\psi_1|H|\psi_2> \sim t_n e^{-n/\xi}, \tag{14}$$

due to the decay of the wave function. Here the band width depends on n, i.e., the band-width is reduced exponentially as $n \to \infty$. Thus, it is natural to define the inverse of the localization length as

$$\gamma_n(E) \equiv \frac{1}{\xi} = \lim_{n\to\infty} -\frac{1}{n}\ln\left(\frac{W_n}{t_n}\right). \tag{15}$$

When the cell is a quasicrystal, the wave functions are critical (self-similar in real space) and scale with an exponent $\beta(E,n)$ as $|\psi(n)| \sim n^{-\beta(E,n)}$. This leads to an overlapping and a bandwidth scaling with the size of the system as $W_n \sim tn^{-2\beta(E,n)}$. From Eq. (15), $\lim_{n\to\infty}\gamma_n(E) = \beta(E,n)\ln(n)/n = 0$. In this case, however, much more information can be obtained if we define an scaling exponent through

$$\beta(E) = \lim_{n\to\infty} -\frac{\ln(W_n/t_n)}{\ln(n)}, \tag{16}$$

which remains finite for power law-localized states. Observe that $\beta(E)$ has the form of a fractal dimension. In general, we can expect small oscillations of $\beta(E)$ as the system size increases, since critical states can display a multifractal nature.[17–20]

B. Stability of the trace map

Once the relation between localization and band width is established, the scaling properties of the bands are easily found from the trace map, since W_n is determined by the energies that are the roots of $\tau_n^2(E) - 4 = 0$, which also satisfies

$$\frac{d\tau_n^2}{dE} \neq 0, \tag{17}$$

in order to assure that the trace crosses the line defined by 2 or -2 (observe that sometimes in this article we will consider the square of the trace, instead of the trace, in order to avoid making differences between the points 2 and -2). If we arrange the band edges in decreasing order (denoted by E_i^n), the width of each band is $W_i = (E_{2i}^n - E_{2i-1}^n)$.

For those energies that are in the spectrum of H_n, the inverse localization length of these states can be estimated using Eq. (15),

$$\gamma_n(E) = \lim_{n\to\infty} -\frac{1}{n}\ln\left(\frac{E_{2i}^n - E_{2i-1}^n}{t_n}\right)$$

$$= \lim_{n\to\infty} -\frac{1}{n}\ln[\tau_{n,2i}^{-1}(\pm 2) - \tau_{n,2i-1}^{-1}(\pm 2)].$$

In the last step it was assumed that $E_{2i}^n = \tau_{n,2i}^{-1}(\pm 2)$, where $\tau_{n,2i}^{-1}$ is the branch $2i$ of the inverse of τ_n, and that t_n does not grow faster than n. Due to Eq. (17), at the points E_{2i}^n, we must require that the derivative of $\tau_{n,2i}^{-1}$ must be finite.

Using all these facts, we can classify the localization properties in terms of the trace map. We start by considering the case of a band of extended states. In the previous subsection, we showed that the band width does not depend on the system size. Then, $\tau_n(E_{2i}^n) = \pm 2, \tau_n(E_{2i-1}^n) = \pm 2$ are fixed points of the trace map, since the trace remains fixed as the map is iterated. These fixed points have the following property, if we start to iterate the map with an energy that is close to E_{2i}^n but inside the band $(E_{2i}^n-\varepsilon)$, then $\tau_n(E_{2i}^n-\varepsilon)$ is bounded since the band width is constant, but to the other side of E_{2i}^n, the corresponding orbit of the map is unbounded because $\gamma(E_{2i}^n+\varepsilon)$ is positive defined outside the band. These kinds of fixed points are called saddle points.

Around a localized eigenstate (E_c), the band shrinks in an exponential way, which means that if $\tau_n(E_{2i}^n)=\pm 2$, after some steps of growth of the chain, E_{2i}^n must lie outside of the band. Thus, the only point that satisfies $|\tau_n(E)|<2$ when n goes to infinity is E_c because, for small ε, and n large enough, $|\tau_n(E_c+\varepsilon)|>2$. Any deviation of the initial conditions, $\tau_1(E_c),\tau_2(E_c),\ldots$, of the trace map, will eventually diverge exponentially as we iterate the trace map. Thus, an exponential state corresponds to an unstable fixed point of the trace.

The width of the band can be estimated by making a Taylor expansion of the trace, or even better, the square of it, to simplify the number of cases under consideration. This expansion is

$$4=\tau_n^2(E_{2i}^n)\simeq\tau_n^2(E_c)+\frac{1}{2}\left(\frac{W_n}{2}\right)^2\left[\frac{d^2\tau_n^2}{dE^2}\right]_{E=E_c}, \qquad (18)$$

where it was used that the first derivative is zero at $E=E_c$, and that $W_n\simeq 2(E_c-E_i^n)$.

The inverse localization length is then obtained using Eq. (15), when $n\to\infty$,

$$\gamma_n(E)=\lim_{n\to\infty}\frac{1}{2n}\ln\left|\left[\frac{d^2\tau_n^2}{dE^2}\right]_{E=E_c}\right|. \qquad (19)$$

This general formula can be reduced in the cases when $\tau_n^2(E_c)=0$ (this is the case of a linear chain with an impurity, as we shall see in the next section) to get

$$\gamma_n(E)=\lim_{n\to\infty}\frac{1}{n}\ln\left|\left[\frac{d\tau_n}{dE}\right]_{E=E_c}\right|. \qquad (20)$$

The sensitivity to the initial conditions of the trace map can be also characterized by its Lyapunov exponents, now in the sense used in *chaos theory* for the study of dynamical systems. This exponents are defined as[21]

$$\sigma(E)=\lim_{n\to\infty,\varepsilon\to 0}\frac{1}{n}\ln\left|\frac{\tau_n(E+\varepsilon)-\tau_n(E)}{\varepsilon}\right|, \qquad (21)$$

which measures how different the orbits of two different but very close initial conditions are, as they are iterated by the map. If we compare last equation with Eq.(20), it is clear that they are equal. Then, the inverse localization length is given by the Lyapunov exponent of the trace map, used in the same sense of chaos theory.

Quasiperiodic chains are much more difficult to study, because the change of the band width is usually achieved by the apparition of new gaps as the system size grows. This mechanism is similar to that used in the generation of a Cantor set. However, even in these cases the band width allows us to obtain useful information of localization. As an example, we can cite the reduction of nearly all bands in a Fibonacci chain with an impurity, due to the apparition of many localized states inside the original spectrum.[22–24]

When the band width is reduced with the scaling by the opening of new gaps, this means that there is a cascade of points E_i^n as the system grows, i.e., the number of preimages of $\tau_n=\pm 2$ grows with n. Observe that in order to have this behavior, the trace map must be nonlinear. In such maps, the orbit of the trace for the band edges can be periodic or bounded aperiodic.[6]

An estimate of the scaling of wave functions is given by using Eq. (16) and a Taylor expansion around a point E_c inside the band, with the property that the first derivative of the square of the trace is zero on it (between the two band edges, there is always a point that satisfies this condition). According to our definition (16), the scaling exponent is

$$\beta(E)=\lim_{n\to\infty}-\frac{\ln|[d^2\tau_n^2/dE^2]_{E=E_c}|}{\ln(n)}. \qquad (22)$$

Before finishing this section, we would like to mention that the stability of the trace can also be useful to explain some properties of gap states, where the states satisfy $\|\tau_n(E)\|>2$. The connection with the stability is found by taking the derivative of Eq. (11) with respect to the energy

$$\gamma_n'(E)\equiv\frac{d\gamma_n(E)}{dE}=\frac{1}{n}\left[\frac{\mathrm{sgn}(\tau_n)}{\sqrt{\tau_n^2-4}}\right]\frac{d\tau_n}{dE}. \qquad (23)$$

From this last equation it is clear that whenever the derivative of the trace map with respect to the energy is zero, we obtain a critical point for the Lyapunov exponent. We will denote these critical points by E_i^*. The nature of these points is obtained by the sign of the second derivative. $\gamma(E_i^*)$ is maximum (minimum) when $\mathrm{sgn}(\tau_n)[d^2\tau_n/d^2E]_{E=E_i^*}$ is negative (positive). In both cases, the Lyapunov exponent has a parabolic shape around these critical points,

$$\gamma(E)\simeq\gamma(E_i^*)+\gamma''(E_i^*)(E-E_i^*)^2. \qquad (24)$$

But if $(d\tau_n/dE)=0$, then, for a small perturbation ε around the critical point E_i^*, $\tau_n(E_i^*+\varepsilon)\simeq\tau_n(E_i^*)$ and thus the trace map [see Eq. (5)] must be nearly insensitive to the initial conditions at E_i^*. In the next section, we will show an example where the Lyapunov exponents of the gaps states are parabolic due to the existence of fixed points in the map.

IV. APPLICATIONS

A. Periodic chain with an impurity

In this subsection, we solve the same problem considered in Sec. II, i.e., the on-site problem in a periodic chain with an impurity ($V_0=\delta>0$, and, $V_n=0, n\neq 0, t_n=1.0$); but using the trace for calculating the localization length. For the present case, the trace of the total transfer matrix for a chain of $n+1$ sites (with n even) is given by

$$\tau_{n+1}=\mathrm{tr}(M^{n/2}DM^{n/2})$$
$$=\mathrm{tr}\left[\begin{pmatrix}E & -1\\ 1 & 0\end{pmatrix}^{n/2}\begin{pmatrix}E-\delta & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}E & -1\\ 1 & 0\end{pmatrix}^{n/2}\right], \tag{25}$$

where M is the transfer matrix which corresponds to sites where $V_n=0$, and D is the matrix at the impurity site. This expression can be evaluated by using the cyclic properties of the trace, and a matrix U that makes a unitary transformation which diagonalizes M,

$$\tau_{n+1}=\mathrm{tr}[(UMU^{-1})^n UDU^{-1}]$$
$$=\frac{1}{\sqrt{E^2-4}}\mathrm{tr}\left[\begin{pmatrix}\lambda_+(E) & 0\\ 0 & \lambda_-(E)\end{pmatrix}^n\right.$$
$$\left.\times\begin{pmatrix}(E-\delta)\lambda_+(E)-2 & -\delta/\lambda_-(E)\\ -\delta/\lambda_+(E) & -(E-\delta)\lambda_-(E)+2\end{pmatrix}\right], \tag{26}$$

where $\lambda_\pm$ are the eigenvalues of M

$$\lambda_\pm(E)=\frac{E\pm\sqrt{E^2-4}}{2}. \tag{27}$$

Finally, the trace is given by

$$\tau_{n+1}=[\lambda_+(E)]^{n+1}\left(1-\frac{\delta}{\sqrt{E^2-4}}\right)$$
$$+[\lambda_-(E)]^{n+1}\left(1+\frac{\delta}{\sqrt{E^2-4}}\right). \tag{28}$$

The spectrum is the set for which $|\tau_{n+1}|$ is lower than 2, as n goes to infinity. From Eq. (28), this condition is satisfied when $\lambda_\pm$ is a complex number, and thus the set is the interval $[-2,2]$, which corresponds to the spectrum of a periodic chain. Outside this set, $|[\lambda_+(E)]^{n+1}|$ goes to infinity when $E>0$, since λ_+ is real. However, if $\delta>0$, there is an energy for which

$$\left(1-\frac{\delta}{\sqrt{E^2-4}}\right)=0, \tag{29}$$

and the trace is zero ($[\lambda_-(E)]^{n+1}\approx 0$ for $E>0$, since $\lambda_-=1/\lambda_+$). From Eq. (29), this energy corresponds exactly to the impurity mode ($E_c=\sqrt{4+\delta^2}$). Observe that for finite n, there is always a band around this point. Such a band is a natural consequence of the *continuity* of $\tau_{n+1}(E)$. The existence of a band around the impurity mode for finite n is a very important point, because it means that for finite lattices, the result is not the same as the one obtained from a direct diagonalization of the Hamiltonian, in which only one mode is found. They are only equal in the infinite limit. This fact also explains why the Lyapunov exponent is zero, because we have a continuous spectrum.[12]

Finally, the inverse localization length of the impurity mode is found using Eqs. (20) and (28):

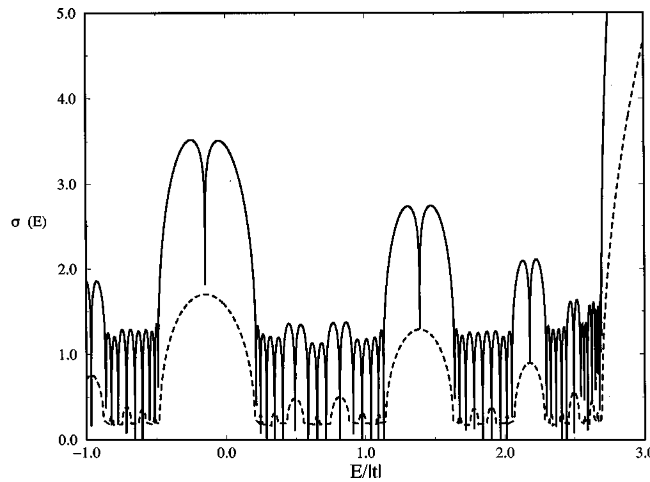

FIG. 2. Lyapunov exponents of a Fibonacci chain ($V_L=1$, $V_S=0$, $t=1$) at the gap energies. The dots correspond to the exponents of the transfer matrix norm, while the solid line corresponds to those exponents of the trace map.

$$\gamma_{n+1}(E)=\lim_{n\to\infty}\frac{1}{n+1}\ln\left|\left\{\frac{d}{dE}\left[[\lambda_+(E)]^{n+1}\times\left(1-\frac{\delta}{\sqrt{E^2-4}}\right)\right]\right\}_{E=E_c}\right|$$
$$=\ln\lambda_+(E_c). \tag{30}$$

This result is the same as the one obtained from Eq. (12).

B. Fibonacci chain

Another interesting example of a typical quasiperiodic lattice is the on-site problem in a Fibonacci chain. For this chain, Khomoto *et al.* found a nonlinear trace map[6] which allows us to compute the spectrum in a powerful way. For the on-site problem, Kohmoto *et al.* considered a chain in which the self-energy V_n has two values V_L and V_S which are ordered by a Fibonacci sequence (the results for the off-diagonal problem are similar[6]). In such a case, the transfer matrix at sites which are Fibonacci numbers [the Fibonacci number of order l is defined as $F(l)=F(l-1)+F(l-2), F(0)=1, F(1)=1$] are given by a recurrence relation, which leads to the following trace map:

$$\tau_{F(l)}=\tau_{F(l-1)}\tau_{F(l-2)}-\tau_{F(l-3)}, \tag{31}$$

with $\tau_1=(E-V_1)/t, \tau_0=(E-V_0)/t, \tau_{-1}=2$ as initial conditions. Also, it is possible to give a geometrical interpretation for the trace map, since the evolution of the trace can be visualized as a trajectory of the point $(\tau_{F(l)},\tau_{F(l-1)},\tau_{F(l-2)})$ in three-dimensional space. This trajectory occurs on a surface, because the map has an invariant (I) given by[25]

$$\tau^2_{F(l)}+\tau^2_{F(l-1)}+\tau^2_{F(l-2)}-\tau_{F(l)}\tau_{F(l-1)}\tau_{F(l-2)}-4$$
$$=(\tau_1-\tau_2)^2=I. \tag{32}$$

In Fig. 2 we show the Lyapunov exponents of the gap wave functions in a Fibonacci chain, obtained using Eq. (11) with $V_L=1, V_S=0, t=1$ for a chain with $l=4$. The results

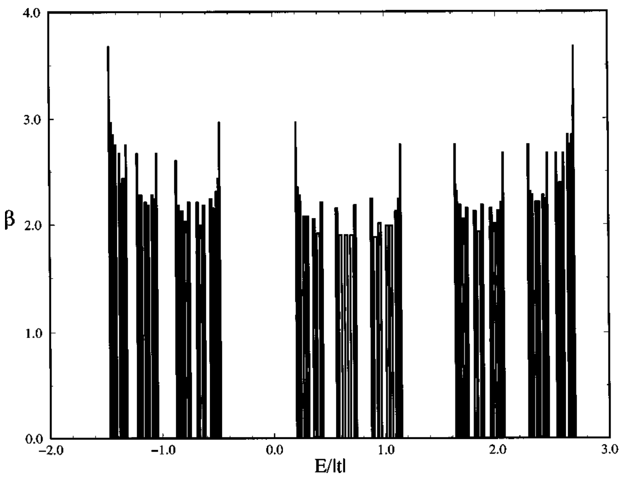

FIG. 3. Scaling exponents of a Fibonacci chain, with $V_L=1$, $V_S=0$, $t=1$, and $l=4$.

calculated via Eq. (11) are similar to those obtained in other works[26,27] using a direct evaluation of the norm of the product of matrices. The parabolic shape of the Lyapunov exponent at the middle of the spectral gaps are due to energies where the trace map is nearly insensitive to the initial conditions. This fact can be clearly seen in Fig. 2, where the solid line shows the Lyapunov exponent of the trace map, used in the sense of chaos theory. The minima for this quantity occurs at the maximum of $\gamma(E)$. Figure 2 also shows a subtle point, the difference between the Lyapunov exponents of the wave function, compared with those exponents of the trace map. Note also that at the middle of the allowed energies where $\gamma_n(E)$ is constant, there is another fixed point of the trace, which corresponds to states at the middle of the allowed bands.

Figure 3 shows an application of Eq. (22) for a Fibonacci chain, with the same parameters as those used in Fig. 2. The points E_c are in the middle of the bands, where $\tau_n(E)=0$. Observe that states at the edges of the spectrum are less extended, while the states at the center are more extended. This is in agreement with the analytical results found by Kohmoto *et al.*[6]

V. CONCLUSIONS

In this article, localization in 1D was studied by using the stability properties of the trace map. In that sense, the localization lengths are mainly determined by the Lyapunov exponents of the trace map, which are very practical, especially when the trace can be obtained by recurrence relations. These exponents have a different meaning than those defined from the norm of the transfer matrix, which have certain problems in the practice.

Using the trace map, a dynamical system can be defined, and eigenstates are classified according with the properties of the map: a localized eigenstate corresponds to energies for which $\tau_n(E)$ is a repulsive fixed point of the trace map; for an extended state, the band edges $\tau_n(E_i^n)=\pm 2$ are saddle fixed points, and for critical states, the orbit of $\tau_n(E)$ is periodic or bounded aperiodic. These critical states are always produced by nonlinear trace maps.

In these nonlinear maps, the structure of the spectrum and localization is due to the fractal structure of the attractor set of the trace map. This fact suggests the use of Feigenbaum's renormalization theory[28] to study quasiperiodic systems. This work is currently in progress.

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