

Gap states and localization properties of one-dimensional Fibonacci quasicrystals

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Localization lengths of electronic states on one-dimensional Fibonacci quasicrystals are calculated exactly within a decimation-renormalization scheme. A self-similar pattern is obtained for the localization lengths along the spectrum as the numerical resolution is improved. Properties of the states in the spectrum are inferred from the scaling of the gap states as the gap width approaches zero. No exponential localization is present for any type of model (diagonal and/or off-diagonal quasiperiodicity). Power-law-type localization has also been investigated and not found, at least in a standard form.

I. INTRODUCTION

The concept of a quasicrystal is a natural extension of that of a crystal, in which *translational periodicity* is relaxed, preserving *quasiperiodic order*. The discovery¹ and successful growth² of materials exhibiting quasiperiodic ordering has enhanced theoretical interest in the electronic properties of quasicrystals. One-dimensional (1D) quasicrystals are particularly interesting with regard to localization properties, since for disordered chains almost all states are exponentially localized,³ while the Bloch states associated to periodic chains are delocalized. The localization properties of quasiperiodic chains constitute a question of current interest, regarding which some controversy exists in the literature.

Localized, critical and extended states have been reported to exist and/or coexist in some model 1D quasicrystals.⁴⁻⁷ For models involving quasiperiodic incommensurate *modulated* potentials, a transition between localized and extended states is obtained as a function of the potential strength.^{4,5,7}

Another class of model 1D quasicrystals is best described by a tight-binding Hamiltonian, whose matrix elements are taken to assume two values, disposed successively along the chain according to a quasiperiodic sequence. The potential in this case is then a piecewise continuous function along the chain. Among the quasiperiodic binary sequences, the Fibonacci one has received the most attention, since the works of Kohmoto *et al.*⁸ and Ostlund *et al.*⁹. The Fibonacci sequence is particularly well suited for experimental realization in superlattices due to the rule which connects successive generations: $S_r = S_{r-1}S_{r-2}$. Therefore a Fibonacci superlattice of generation r may be directly grown over generation $r-1$ by deposition of the sequence corresponding to generation $r-2$, a procedure implemented in molecular-beam epitaxial growth by Merlin *et al.* up to $r=13$, and by Dharma-wardana *et al.* for $r=11$.²

It has been proved by Delyon and Petritis¹⁰ for a class of binary quasiperiodic tight-binding Hamiltonians that the eigenfunctions cannot decay at infinity, which excludes exponentially localized states from the spectrum.

The Fibonacci sequence, however, does not belong to this class of operators, leaving open the question of localization in this model. To our knowledge, no rigorous results about localization exist for this case. Evidence has been found for a mobility edge in a non-Fibonacci binary quasicrystal,⁶ which shows that the validity of the above theorem¹⁰ is indeed restricted.

The localization properties of Fibonacci tight-binding models have been studied by several authors. Renormalization-group (RG) studies^{8,11-13} present evidence that the spectrum is purely singular continuous, which uniquely corresponds to critical (neither localized nor extended) wave functions, irrespective of the potential strength. It should be noticed that the RG approach is only exact in some limiting cases, and usually the study is restricted to a few energies in the spectrum belonging to special cycles. Numerical studies of conductance by Liu and Riklund¹⁴ report three kinds of behavior (extended, localized and critical) for the wave functions. However, similar studies by Das Sarma and Xie¹⁵ show evidence for power-law localization (critical states) for the whole spectrum. There has also been some controversy in the literature¹⁶ about the existence of extended states on a Fibonacci superlattice.

A major difficulty in characterizing the nature of the eigenstates of a Fibonacci quasicrystal is that the spectrum seems to be a Cantor set of zero Lebesgue measure: The total bandwidth is zero.^{13,17} Therefore, a numerical study for a state at any chosen energy will almost certainly correspond to a *gap state*. The relevance of gap states in this kind of system has been stressed by several authors:^{12,17,18,19} They are always present due to surfaces and impurities in real samples. Theoretically, gap states are known to be exponentially localized, and the scaling behavior of their localization length may provide some insight about *global* properties of the spectrum.

In this paper we present a numerical study of the localization properties of Fibonacci-chain quasicrystals, based on the exact decimation-renormalization scheme used by Ashraff and Stinchcombe²⁰ for the determination of the Green's functions of this system. Previous works using this scheme have mainly concentrated on the average

(global)²⁰ or local²¹ properties of the electronic density of states.

The decimation-renormalization technique for calculating Green's functions was originally developed for the study of disordered chains,²² and has shown itself to be particularly suitable for studies of the localization properties of these systems.²³ The technique consists in projecting the Green's function (G) onto alternate (or any reduced number of) sites of the chain, and then eliminating the dependence of G on the decimated sites by performing a configurational average over the occupations of these sites. This last step cannot be performed exactly for a disordered chain,^{22,23} and approximate results for G are obtained in this case. When applied to the Fibonacci sequence chain, however, a decimation transformation removing appropriate sites²⁰ maps the Fibonacci chain of generation n into the previous generation sequence, eliminating the need to perform any kind of configurational average. In this way exact results are obtained for G and, as discussed here, for the localization length of exponentially localized wave functions.

In Sec. II we briefly review the decimation approach for the Fibonacci chain, and describe its application to the calculation of localization lengths. In Sec. III we present our results concerning gap states. The final section gives a summary and conclusions.

II. DECIMATION-RENORMALIZATION APPROACH

The procedure developed by Ashraff and Stinchcombe²⁰ for the Green's function of Fibonacci chains starts from a tight-binding Hamiltonian:

$$\mathcal{H} = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{i,j}^{\text{nearest neighbors}} |i\rangle V_{ij} \langle j|, \quad (2.1)$$

where the nearest-neighbor hopping matrix elements, V_{ij} , are allowed to assume two different values, V_A and V_B , arranged according to the Fibonacci sequence. This sequence can be generated by repetition of the following inflation rule:

$$\begin{aligned} A &\rightarrow AB, \\ B &\rightarrow A, \end{aligned} \quad (2.2)$$

so that starting from element A , a Fibonacci sequence of arbitrary length may be constructed ($ABAABABAABAAB \dots$).

The diagonal elements $\{\varepsilon_i\}$ may assume three different values, depending on the local environment of site i :

$$\varepsilon_i = \begin{cases} \varepsilon_\alpha & \text{if } V_{i-1,i} = V_{i,i+1} = V_A, \\ \varepsilon_\beta & \text{if } V_{i-1,i} = V_A \text{ and } V_{i,i+1} = V_B, \\ \varepsilon_\gamma & \text{if } V_{i-1,i} = V_B \text{ and } V_{i,i+1} = V_A. \end{cases} \quad (2.3)$$

Suitable choices of the parameters $V_A, V_B, \varepsilon_\alpha, \varepsilon_\beta, \varepsilon_\gamma$ can cast the model into the particular cases of purely off-diagonal quasiperiodicity ($V_A \neq V_B, \varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma$), and purely diagonal quasiperiodicity ($V_A = V_B, \varepsilon_\alpha = \varepsilon_\beta \neq \varepsilon_\gamma$), as well as more general cases.

The Green's function corresponding to the operator \mathcal{H}

is defined in the usual form $G(z) = (z - \mathcal{H})^{-1}$, and its matrix elements in the tight-binding basis set, $G_{ij}(z) = \langle i | G(z) | j \rangle$, yield information on the electronic properties of the system. In particular, the average density of states (DOS) is readily obtained:

$$\bar{\rho}(E) = -\frac{1}{\pi} \text{Im} \lim_{\eta \rightarrow 0} \bar{G}(E + i\eta), \quad (2.4)$$

where

$$\bar{G}(z) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N G_{ii}(z). \quad (2.5)$$

A decimation procedure, which consists in reverting the inflation rule (2.2) through the elimination of " β -sites" in a chain, generates a Fibonacci chain of the preceding generation with a length rescaling factor equal to the golden mean $\tau = (\sqrt{5} + 1)/2$. As shown by Ashraff and Stinchcombe,²⁰ this procedure is directly applicable to the exact determination of \bar{G} through successive renormalizations of the Hamiltonian.²² We call $V_A^{(n)}, V_B^{(n)}, \varepsilon_\alpha^{(n)}, \varepsilon_\beta^{(n)}, \varepsilon_\gamma^{(n)}$ the n -times renormalized Hamiltonian matrix elements, so $V_A^{(n)}$ denotes the effective interaction between two sites a distance τ^n apart, measured in units of the original lattice spacing: for $n \rightarrow \infty, V_A^{(n)} \rightarrow 0$.

As shown by Robbins and Koiller,²³ the scaling of $V_A^{(n)}$ to zero is related to localization properties: For an exponentially localized state, $\psi(L) \sim \exp(-\lambda L)$ at large L , the inverse localization length λ is given by

$$\lambda = \lim_{n \rightarrow \infty} -\frac{\ln V_A^{(n)}}{\tau^n}. \quad (2.6)$$

Note that, contrary to Ref. 23, no configurational averaging is involved here. The limit $n \rightarrow \infty$ guarantees that our results are the same as for an infinite chain.

One of the characteristics of the renormalization procedure is the *tunability* of the energy resolution for quantities obtained from the Green's function. Decreasing the imaginary part η added to the energy [see Eq. (2.4)], more structure is revealed,^{20,22,24} which allows a "magnification" effect in the energy scale. In Fig. 1 we present results for the DOS of a chain with $\varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma = 0$ and $V_A = 1, V_B = 2$ on three energy ranges. Figure 1(a) corresponds to the whole spectrum, $\eta = 5 \times 10^{-3}$ while 1(b) and 1(c) concentrate at smaller regions around the center ($E = 0$), $\eta = 1 \times 10^{-3}$ and 2×10^{-4} , respectively. A self-similar nature of the DOS is clearly noted by comparison of the figures, a behavior already encountered in some fractal lattices.²⁴ The trifurcating structure of the spectral region, typical for this purely off-diagonal tight-binding sequence is also illustrated in Fig. 1.

Results for λ calculated from (2.6), for the same model and the respective energy resolutions as above, are given in Figs. 1(d), 1(e) and 1(f). It can be seen that λ also exhibits a self-similar pattern. In the wide gap regions λ converges to well-defined values, however small η is, indicating that the gap states are exponentially localized. In regions near energy eigenstates (peaks in the DOS), λ has minima corresponding to very small but nonzero values. Reducing η further reduces the minimum value of λ . A

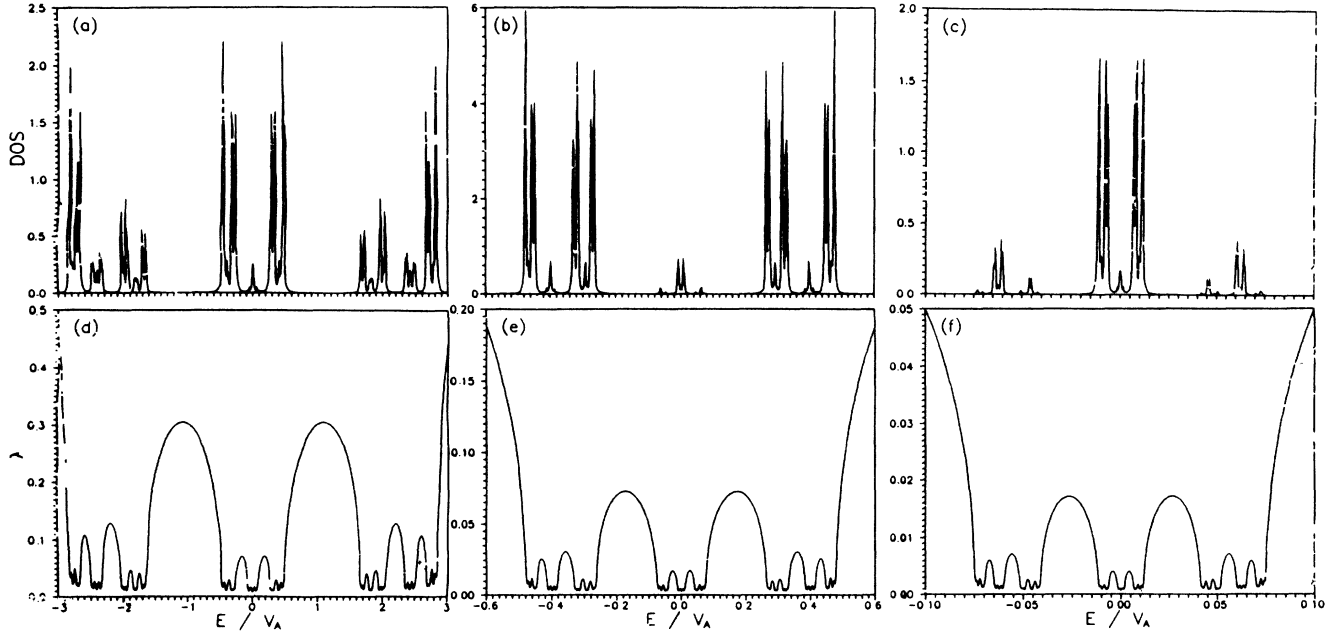


FIG. 1. Values of the DOS (upper frames) and λ (lower frames) for a Fibonacci chain with $\epsilon_\alpha = \epsilon_\beta = \epsilon_\gamma = 0$ and $V_A = 1$, $V_B = 2$ on three energy ranges.

typical trend is illustrated in Fig. 2, where we give results for the converged value of λ , for decreasing values of η , at energy $E = 2.831\,908\,746\,762\,43$. This is the energy of a peak on the rightmost cluster in Fig. 1(a), as determined with our higher numerical resolution. This result does not imply that λ is zero, as for a strictly extended Bloch state. In the present scheme η sets the accuracy scale down to which the outcome of calculation is defined. Studying a periodic chain state in the continuum for example, the calculated value of λ would always be of the order of η , however here it is orders of magnitude larger. This confirms that the ansatz

$$\psi(L) \sim \exp(-\lambda L)$$

is not suitable to describe the present situation.

We have also tried to investigate a possible power-law

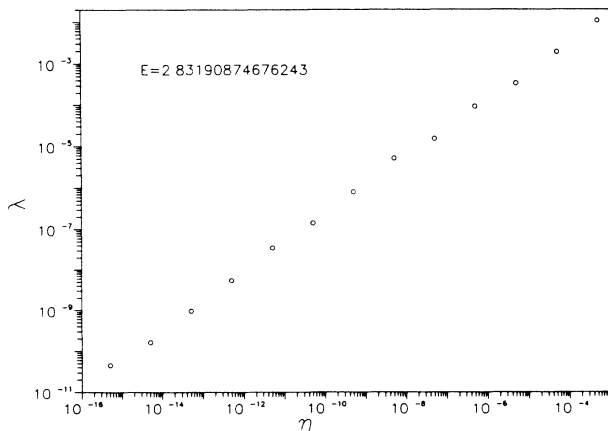


FIG. 2. Value of λ calculated at a maximum of the DOS as a function of the imaginary part, η , added to the energy.

behavior of the eigenstates, $\psi(L) \sim L^p$, introducing a localization exponent similarly to (2.6).

$$p = \lim_{n \rightarrow \infty} \frac{-\ln V_A^{(n)}}{n \ln \tau}. \quad (2.7)$$

However, no numerical convergence was obtained for this quantity at any of the investigated values of the energy. Thus, although the states are somewhere in-between Bloch-like and exponentially localized as regards their localization properties (i.e., *critical*), according to our results they do not seem to fit into a power-law decay description, even on an average sense. Note that Das Sarma and Xie¹⁵ have been able to unveil a power-law behavior for the average electrical resistance of a Fibonacci lattice; this does not imply that the associated wave functions behave exactly in the same way. Rather, if one is to take a clue from results for a particular energy, as given in Ref. 11, the overall shape of a critical wave function seems to consist of a quasiperiodic structure of “bursts” and “zeros,” with at most a power-law-type behavior governing the highest peaks.

In the next section we take advantage of the fact that numerically defined energies almost certainly belong to a gap, so that properties of the eigenstates for general types of quasiperiodicity are indirectly investigated from the limiting behavior of gap states as a function of gap widths.

III. SCALING BEHAVIOR OF THE LOCALIZATION LENGTH IN GAP STATES

Results in Figs. 1(d), 1(e), and 1(f) show that λ attains a maximum value (we call it λ_{\max}) in gap regions, and this value decreases for smaller gaps. We investigate quanti-

tatively the relation between the maximum value of λ in a gap and the gap width (E_g). The expected behavior, if the allowed states were exponentially localized, would be that λ_{\max} should tend to some finite value in the limit $E_g \rightarrow 0$. The relevant parameter driving localization in quasicrystals is the potential strength or discontinuity, as a function of which transitions from localized to nonlocalized states have been obtained.^{4,7} A mobility edge, separating localized from nonlocalized states, might also be expected in analogy with the results of Refs. 4 and 6. In this case different energy regions should yield different limiting behaviors.

Figure 3(a) shows, in a log-log scale, the variation of λ_{\max} with the gap width for purely off-diagonal quasiperiodicity and different values of V_B , keeping $V_A = 1$. The gaps are taken equally from all regions of the spectrum, and the straight lines are power-law approximations. None of the possibilities mentioned above concerning a transition from localized to nonlocalized behavior is obtained. In fact, these results suggest a relationship of the type $\lambda_{\max} \sim E_g^\delta$, where the exponent δ is a function of

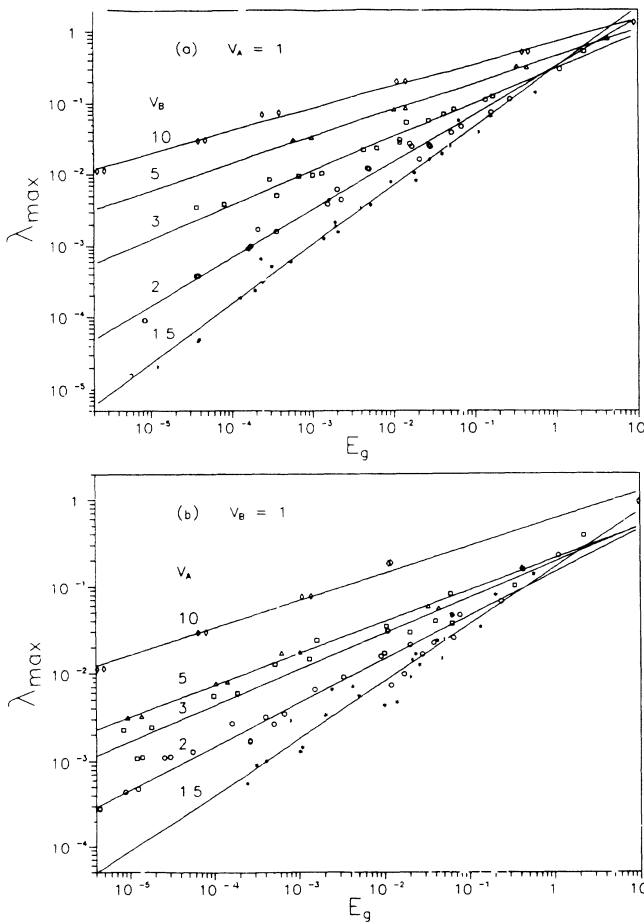


FIG. 3. Maximum of λ within a gap vs gap width for cases of purely off-diagonal quasiperiodicity: $\varepsilon_\alpha = \varepsilon_\beta = \varepsilon_\gamma = 0$ and V_A, V_B as indicated. Straight lines are best fits corresponding to a power-law behavior, $\lambda_{\max} \sim E_g^\delta$.

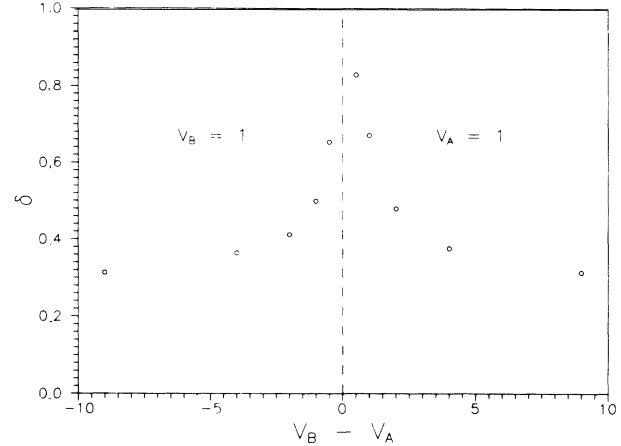


FIG. 4. Power-law exponents for the fits in Fig. 3.

the disorder strength $|V_B - V_A|$. Figure 3(b) shows the same study for several values of V_A and keeping $V_B = 1$. All results indicate that $\lambda_{\max} \rightarrow 0$ in the limiting case $E_g \rightarrow 0$, that is, if the properties of allowed states are faithfully represented by this limit we conclude that none of these states is exponentially localized. Besides, we note that the smaller the disorder strength the faster the convergence to $\lambda_{\max} \rightarrow 0$, that is, δ is a decreasing function of $|V_B - V_A|$.

The variation of δ with $V_B - V_A$ is plotted in Fig. 4. Although no simple function could describe this variation for all $V_B - V_A$, it is clear that δ will not be equal to zero for any finite disorder strength. In the limit $|V_B - V_A| \rightarrow \infty$, the chain decouples into monomers, dimers and, if $V_B < V_A$, trimers, so that extreme localization with no exponential tails would occur. In this case the $E_g \rightarrow 0$ limit is not physical, so our procedure is not well defined. On the other hand, for all situations of interest, we find $\delta > 0$, which means absence of exponential localization.

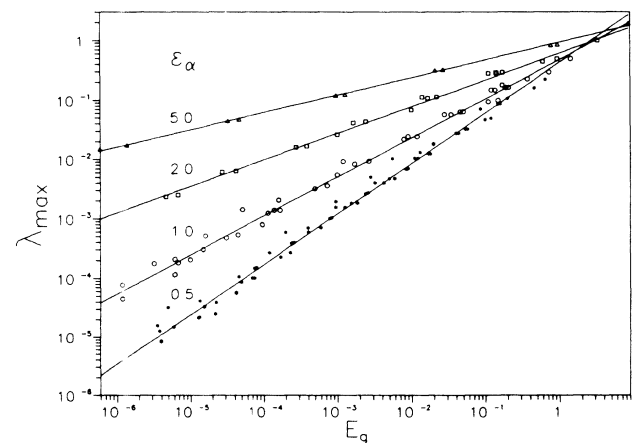


FIG. 5. Maximum of λ within a gap vs gap width for cases of purely diagonal quasiperiodicity: $V_A = V_B = 1$, $\varepsilon_\alpha = \varepsilon_\beta = -\varepsilon_\gamma$ as indicated. Straight lines are best fits corresponding to a power-law behavior, $\lambda_{\max} \sim E_g^\delta$.

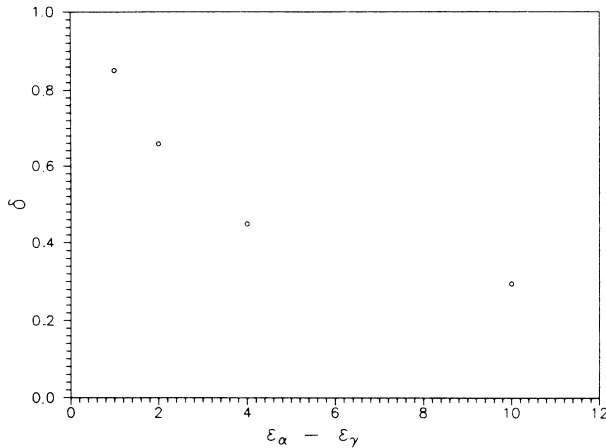


FIG. 6. Power-law exponents for the fits in Fig. 5.

Figures 5 and 6 show analogous results for purely diagonal quasiperiodicity. In this case, we keep $V_A = V_B = 1$ and $\epsilon_\alpha = \epsilon_\beta = -\epsilon_\gamma$, varying ϵ_α . The disorder strength parameter in Fig. 6 is $\epsilon_\alpha - \epsilon_\gamma$ in this case, and the results are qualitatively the same as those for purely off-diagonal quasiperiodicity.

More general models, including both diagonal and off-diagonal quasiperiodicity, have also been investigated, leading to essentially the same type of results, thus indicating the absence of exponentially localized states in all cases.

IV. SUMMARY AND CONCLUSIONS

We have presented an exact formalism for the calculation of localization lengths in 1D Fibonacci quasicrystals. The method, originally developed for exponentially localized states, was adapted to investigate power-law localization as well. Attempts to obtain conclusive information from spectral points have failed essentially due to the numerical difficulty in defining those energies belonging to the spectrum; quantities of interest are found to be sensitive to the small imaginary part added to the energy,

even if the energy is taken, for each value of the imaginary part, to correspond to a maximum in the DOS, as is the case in Fig. 2. Nevertheless, we have shown that information concerning the properties of allowed states *can* be obtained *indirectly*, through the analysis and suitable extrapolation of properties of gap states.

The decimation-renormalization scheme applied to the calculation of the DOS and exponential localization lengths of a Fibonacci chain revealed a self-similar pattern for both these quantities as the energy resolution was increased. Given that λ is a well-defined quantity in the gap regions, which cover the entire Lebesgue measure of the spectrum, the limiting behavior of λ as the individual gap widths (E_g) approach zero was used to search for exponential localization for different models and disorder strengths.

Our results show that λ goes to zero as E_g decreases, and this behavior is well described by a power law in which the exponent (δ) decreases for increasing potential discontinuity, but is always positive. This is valid for general tight-binding Hamiltonians, with diagonal and off-diagonal binary distributions, leading to the conclusion that exponential localization is not present in these models. Power-law-type critical localization has not been obtained either; however, it must be pointed out that in this latter case our negative result arises from lack of numerical convergence, rather than extrapolations from properties of gap states.

The method used here for the study of Fibonacci quasicrystals is immediately applicable for other 1D systems which may be defined in terms of inflation rules;^{6,17} work along these lines is in progress.

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