Unusual scaling of the spectrum in a deterministic aperiodic tight-binding model

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Local and global scaling properties of the integrated density of states of the tight-binding Rudin-Shapiro model are numerically derived by investigating the dependence of the bandwidths of its periodic approximants on the size of the unit cells. Scaling relations intermediate between the power and exponential laws are found for various values of the energy and amplitude of the on-site potential V. An analysis of the global properties of the spectrum performed in the case when V is equal to the hopping integral t points out its multifractal structure. Multifractal arguments together with earlier results concerning the nature of the wave functions indicate a pure point spectrum for $V \geq t$, while for smaller values of the amplitude V the spectrum reveals a mixed character.

I. INTRODUCTION

The elucidation of the influence the atomic distribution has on the nature of the electronic states in multicomponent structures is one of the fundamental problems of solid-state physics. The nature of the states and spectra in models of noninteracting electrons with periodic or disordered atomic potentials is well known. The electronic wave functions in periodic solids are extended (Bloch states) and the spectrum is absolutely continuous, while the electrons are exponentially localized and the spectrum is pure point in one-dimensional disordered models. Also, the structural disorder favors the localization in higher dimensions.[1] Much less is known about the intermediate class of aperiodic ordered structures, where it is not clear what is the minimum deviation from periodicity that is necessary to localize the electrons. Earlier studies have shown that localization can occur in incommensurate systems provided the amplitude of the atomic potential is strong enough.[2] On the other hand, the absence of localization was proven in one-dimensional binary alloys of quasicrystalline type, which display singular continuous spectra[3] and critical states[4] (i.e., states which are not normalizable but which are "less extended" than the Bloch states in the sense that the distribution of the charge density could present large fluctuations). Also, sufficient conditions for the absence of the absolutely continuous and pure point parts in the spectra of systems generated through substitutions have been derived.[5]

Recently, a tight-binding model with two types of atoms ordered according to the Rudin-Shapiro (RS) sequence has been proposed as a candidate for the study of the electron localization in a deterministic aperiodic medium.[6,7] Numerical studies suggested that the electronic states of the model are generically localized (i.e., normalizable) and a detailed investigation of some particular cases indicated that the rate of spatial decay of the wave functions is intermediate between the power and exponential laws. This means that the charge distribution is less spread in space than in the case of the critical states, but the localization is weaker than in a random medium. These features make the RS chain a unique example of an aperiodic ordered system whose atomic distribution generates properties in between those of the quasiperiodic and disordered structures.

This paper reports numerical results regarding the nature of the spectrum of the RS model. The method is based on the investigation of the scaling of the integrated density of states (IDS), that can be inferred from the asymptotic dependence of the bandwidths of the periodic approximants of the system on the size of their unit cells. The IDS of periodic systems is known to scale locally with the energy as a power law, with power 1 (inside the bands) or $\frac{1}{2}$ (at the Van Hove singularities). Studies on deterministic aperiodic systems such as Harper-Aubry[8,9] and Fibonacci[4] models led to the conclusion that the scaling with powers smaller than 1 is generally associated to the singular continuous spectra, while the power 1 is the signature of absolutely continuous spectra. In the case of localized states perturbational arguments suggest that the size of the shift of the energy levels caused by the change of the boundary conditions depends on the rate of spatial decay of the wave functions.[10] Thus, if the states are exponentially localized, the widths of the bands of the periodic approximants decrease following an exponential law when the length of the unit cell increases. Also, exact results indicate in the case of the Maryland model that the bandwidths scale exponentially when the states are exponentially localized.[11]

One can expect that the existence of localized states with a decay rate intermediate between the power and exponential laws in the RS model would have some important consequences on the scaling of the bandwidths, leading to a qualitatively new behavior. Here it is shown by means of numerical arguments that the IDS of the RS chain generically scales following a logarithmic law. The various types of scaling which occur for different energy

values are investigated in Sec. II. Moreover, a multifractal analysis performed in Sec. III will permit the extraction of some important conclusions regarding the nature of the spectrum of the RS model.

II. LOCAL SCALING

The system investigated in this article is a one-orbital tight-binding model composed of two kinds of atoms distributed aperiodically on the sites of a regular chain with unit spacing. The potential on the atom located on the site j is given by

$$V_j = V \exp[i\pi S(j)] , \quad V > 0 , \tag{1}$$

where $S(j)$ denotes the number of occurrences of "11" in the dyadic representation of j. The electron can hop between nearest-neighbor atoms according to the equation of motion

$$\psi_{j-1} + \psi_{j+1} + V_j \psi_j = E \psi_j , \quad j \geq 0 , \tag{2}$$

where ψ_j denotes the amplitude of the wave function on site j, E is the energy of the electron, and the hopping integral is set to 1. The distribution of the on-site potentials V_j given by Eq. (1) is in a one-to-one correspondence with the RS sequence[12] which gains distinction among the binary sequences through some peculiar statistical properties. Namely, the distribution of $\pm V$ is ordered enough to prevent the occurrence along the chain of most of the possible finite clusters that can be built up by arbitrary concatenation of the two types of atoms, but is at the same time far enough from periodicity to generate an absolutely continuous Fourier measure like a disordered chain.

The first purpose of this study is the derivation of local scaling relations of the type

$$N(E+\Delta E) - N(E) \propto F(\Delta E) , \quad \Delta E \to 0 , \tag{3}$$

where $N(E)$ represents the value of the IDS at the energy E, and F denotes some function to be derived. In practice the model is approximated by periodic systems with unit cells given by the successive generations of the chain containing 2^n atoms each, whose spectra $\sigma^{(n)}$ are composed of 2^n bands of widths $w_i^{(n)}$, $i = 1, \ldots, 2^n$. The number of states is normalized to unity, therefore the fraction of states contained in each band (i.e., the variation ΔN of the IDS along the band) is equal to the inverse of the cell size. Then, if $w^{(n)}(E)$ denotes the width of the band which contains E at generation n, a relation of the type $w^{(n)}(E) = g(\Delta N)$ can be numerically derived, where g is expected to become equal to the inverse of the scaling function F from Eq. (3) in the limit of large n. [For instance, in the case of the disordered systems the exponential law $w^{(n)} = \exp(-\text{const} 2^n)$ implies $g(\Delta N) = \exp(-\text{const}/\Delta N)$ and therefore $F(\Delta E) = -\text{const}/\ln(\Delta E)$.]

The above formalism was successfully applied to some deterministic aperiodic models, where power-law scaling was found of the type

$$N(E+\Delta E) - N(E) \propto (\Delta E)^{\alpha(E)} , \quad \Delta E \to 0 , \tag{4}$$

with spectral indices $\alpha(E)$ in the range $]0,1]$. Thus, studies of the scaling at the center of the spectrum of the Harper-Aubry model indicated a jump of the index α from 1 to a smaller value when passing from the subcritical regime to the critical value of the strength of the on-site potential.[8] Also, further numerical evidence for the Harper-Aubry[9] and Fibonacci[4] models revealed scaling of the power-law type whenever the states are extended or critical.

We have performed a numerical study of the scaling of the bandwidths $w^{(n)}(E, V)$ of periodic approximants of the RS model for various values of the energy and potential amplitudes. In general, if some energy belongs to the spectrum of the mth approximant, its occurrence in the spectra of approximants with $n > m$ is not guaranteed. The convergence of the procedure being faster at the energies which recur more frequently in the spectra of the periodic approximants, we are interested to first apply the method to those energy values for which the frequency of recurrence has been derived analytically. This is the case with the energies to which a general statement proven in a previous paper[7] applies, ensuring their recurrence in the spectra of the periodic approximants given by each second generation. The energies here investigated can be classified in three groups. The first one contains energies located at the center of the spectrum,[13] whose existence was proven[7] for some decreasing sequence of values of the potential strength $V = V^{(2m+1)}$, $m = 0, 1, 2, \ldots$ ($V^{(1)} = \sqrt{2}$, $V^{(3)} \approx 0.6071$, etc.). The second class refers to the energies[6] $E = \pm[2 \pm (2 + V^4)^{1/2}]^{1/2}$ for the particular value $V = 1$. The third class consists of the energies $E = \pm E_c(V)$, $E_c(V) = (V^2 + 2)^{1/2}$, whose associated wave functions were shown[6] to be non-normalizable for some infinite set of "critical" values of the amplitude $V = V_c^{(m)} < 1$, $m = 1, 2, \ldots$. The bandwidths at the nth generation were computed by looking for those energies for which the absolute value of the trace of the transfer matrix is less than or equal to 2 after $n-1$ iterations of the trace map[14] of the model.

The states at the center of the spectrum were found to be weaker-than-exponentially localized, the amplitude ψ_i of a state localized on some site i_0 decaying according to a law of the type

$$|\psi_i| \propto \exp(-\text{const}|i - i_0|^{1/2})$$

[see Eq. (4.4) in Ref. 7]. Assuming on the basis of the Edwards-Thouless argument[10] that the shrinking with n of the associated bandwidths is governed by a similar expression $w^{(n)} \propto \exp(-\text{const} 2^{n/2})$, then the IDS should scale at these energies following the logarithmic law

$$N(E+\Delta E) - N(E) \propto [-\ln(\Delta E)]^{-\nu} , \quad \Delta E \to 0 , \tag{5}$$

with $\nu = 2$. The numerical computations confirmed this type of behavior for the first two classes of energies mentioned above with the index $\nu = 2.00 \pm 0.02$ in both cases (see Fig. 1 for the data concerning the first class of states when $m = 0, 1, 2, 3$, and 7). The scaling relation for the bandwidths corresponding to Eq. (5) is stronger than a power and weaker than exponential (note that the disor-

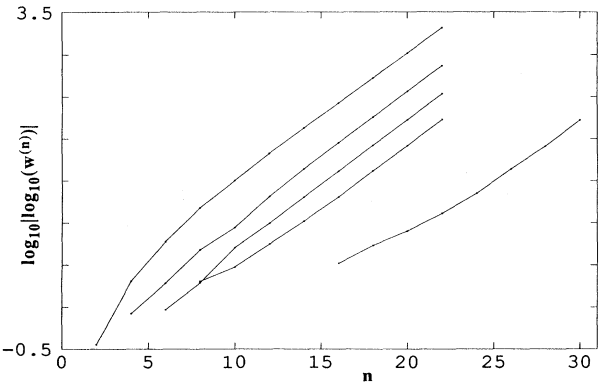


FIG. 1. Representation of $\log_{10}|\log_{10}w^{(n)}|$ for the bands closest to the center of the spectrum as a function of the generation number n. The values of the amplitude are, from top to bottom, $V^{(1)}=\sqrt{2}$, $V^{(3)}\approx 0.6071$, $V^{(5)}\approx 0.2978$, $V^{(7)}\approx 0.1483$, and $V^{(15)}\approx 0.0092$. The scaling index ν is given by $\nu=\log_{10}2/\kappa$, where κ is the slope of the asymptotic straight line resulting for large n in each case.

deredlike exponential law corresponds to the limit value $\nu=1$).

The investigation of the widths of the bands which are located in the neighborhood of the energy values $E=\pm E_c(V)$ for critical potential amplitudes revealed a qualitatively different behavior. The wave functions associated to these energies are critical and a periodic subsequence of lattice sites on which the amplitude is constant has been found analytically.[6] Also, there is an infinite subset of sites on which the amplitude scales algebraically [see Eq. (3.17) in Ref. 6]. The wave functions being not localized, the dependence of the energy shift on the boundary conditions is stronger and it is plausible to assume that the bandwidths are related to the size of the unit cell through a power law. According to the numerical computations, the IDS scales in this case following the relation (4), where the computed values of the index α are $\alpha=0.66\pm 0.02$ for $V=V_c^{(1)}=2^{-1/2}$ and $V=V_c^{(2)}=2^{-1/2}(1+2^{-1/2})^{1/2}$.

At the upper limit of critical values $V=1$ the states associated to the energies $E=\pm E_c(V)$ cease to be extended, becoming localized,[6] with a localization rate governed by the law $|\psi_i|\propto|i-i_0|^{-\text{const}\ln|i-i_0|}$ [see Eq. (3.14) in Ref. 6]. This qualitative alteration of the nature of states near $E=\pm 3^{1/2}$ implies a weaker sensitivity to the boundary conditions and the above reasoning suggests that $w^{(n)}\propto(2^n)^{-\text{const}\ln(2^n)}$, therefore the IDS should scale like

$$N(E+\Delta E)-N(E)\propto\exp\{-\text{const}[-\ln(\Delta E)]^{\xi}\}\ ,\qquad \Delta E\to 0\ , \quad (6)$$

with $\xi=\frac{1}{2}$. Numerical computations performed on periodic approximants with large unit cells give $\xi=0.50\pm 0.01$. This type of scaling is intermediate between the two previous laws Eqs. (4) and (5), and the power-law regime (4) can be obtained from it by setting $\xi=1$.

III. GLOBAL SCALING

A first step towards the global characterization of the spectrum is the study of the dependence of the total bandwidths $W^{(n)}$ of the periodic approximants on the size of the unit cells. Thus, the vanishing of $W^{(n)}$ in the limit of large n is generally credited as a proof of the absence of absolutely continuous parts in the spectra. The criterion does not exclude the existence of a dense point part, since it refers to the size of the set of eigenvalues before taking its closure. Estimations of the size of the total bandwidth have been performed for the Harper-Aubry model at the metal-insulator transition,[2,15] and in the Fibonacci case.[16] The numerical analysis of the scaling of the spectrum of the RS chain, to be exposed below, indicates the vanishing of the total bandwidth faster than a power law for $V\geq 1$.

The study is performed in the frame of the multifractal formalism,[17] whose purpose is the derivation of the scaling indices of measures defined on general sets of points that are composed of interwoven parts with different scaling properties, and to estimate the fractal dimensions of the subsets on which the measure scales with the same index. Accordingly, the spectrum $\sigma^{(n)}$ of the nth periodic approximant can be seen as a covering of the spectrum σ of the infinite chain. A probability measure is defined on every partition $\sigma^{(n)}$ of σ, by attributing to each band $w_i^{(n)}$ a weight 2^{-n}. Then a partition function is defined through

$$\Gamma_n(q,\tau,\sigma^{(n)})=\sum_{i=1}^{2^n}2^{-nq}\lambda_q(\tau,w_i^{(n)})\ , \quad (7)$$

where λ_q is a gauge function and q takes real values. The explicit form of λ_q depends on the type of scaling to be investigated. For instance, if it is assumed that the bandwidths scale algebraically with the size of the unit cell, then

$$\lambda_q(\tau,w)=w^{-\tau(q)}\ , \quad (8)$$

where $\tau(q)$ is derived from the condition[17]

$$\lim_{n\to\infty}\Gamma_n(q,\tau,\sigma^{(n)})=1\ . \quad (9)$$

It was proven[17] that the Legendre transform of $\tau(q)$, which reads

$$f(\alpha)=\alpha q(\alpha)-\tau[q(\alpha)]\ , \quad (10)$$

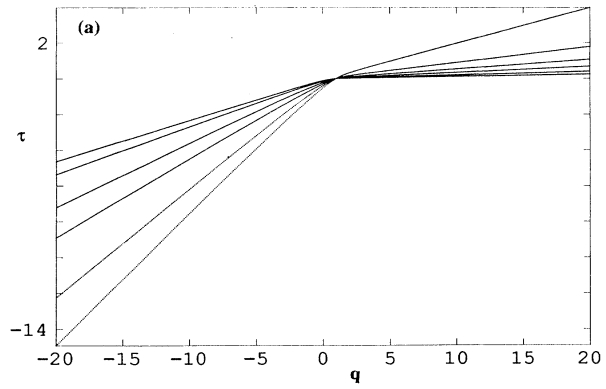
is the fractal dimension of the set of bands on which the probability scales like $(w^{(n)})^{\alpha}$ when $n\to\infty$.

The above framework was used for the investigation of the spectra of Harper-Aubry,[9] Fibonacci,[4] and Thue-Morse[18] tight-binding models. Its application to the RS case for $V=1$ led to the results displayed in Fig. 2. The tendency of vanishing of $\tau(q)$ when the size of the unit cell increases is clearly seen. This indicates the decrease of the fractal dimension of the set of bands whose widths scale algebraically with the cell site. The extrapolation of these results to the limit of the infinite cell suggests the absence of components with algebraic scaling in the spectrum σ. This leads to the conjecture that the spectrum of the RS model has no continuous part when $V=1$, in

agreement with earlier results concerning the nature of states in this case.[6]

The increase of the amplitude of the on-site potential is expected to strengthen the localization tendency, and therefore to conserve the pure point character of the spectrum. Indeed, calculations of the spectra for higher values of the potential strength show that for each fixed generation n the total bandwidth $W^{(n)}$ is a monotonous decreasing function of V. This together with previous results revealing the limited spatial spreading of the electronic wave packets[6] during their time evolution for $V \geq 1$ support the conclusion that the spectrum keeps its pure point nature in this range of amplitudes of the on-site potential.

Numerical computations performed at $V=1$ indicate that the distribution of the bandwidths is extremely sparse, the largest bands being several orders of magnitude wider than any of the other bands. Therefore, the scaling behavior of the total bandwidth is governed by the very few bands with largest width. It turns out that at $V=1$ the widest bands are those which are located in the neighborhood of the energies $E=\pm 3^{1/2}$ investigated in Sec. II. Numerical checks make plausible the assumption that the rest of the bandwidths of periodic approximants with large unit cells scale according to the law (5).



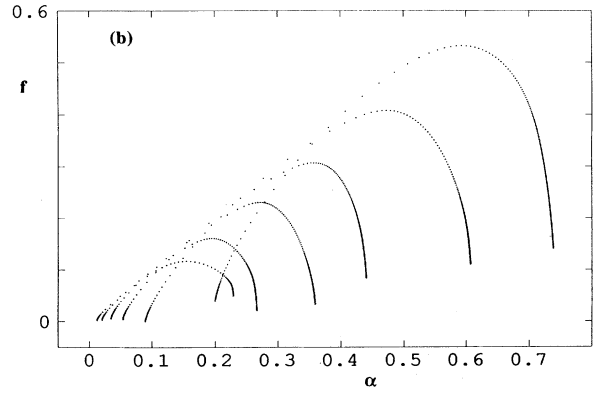


FIG. 2. (a) The functions $\tau(q)$ for the generations 5, 6, 7, 8, 9, and 10 (from top to bottom in the right half of the figure and in the opposite order in its left half); (b) the functions $f(\alpha)$ for the same generations (from right to left).

Thus, if the contributions of the type (6) are discarded, the study of the logarithmic corrections to the multifractal behavior requires a gauge function of the type

$$\lambda_q(\tau,\tau_1,w)=w^{-\tau(q)}(-\ln w)^{\tau_1(q)} . \tag{11}$$

The scaling indices ν and the associated logarithmic dimensions have been derived by means of the method from Ref. 19, that generalizes the multifractal theory to partition functions with logarithmico-exponential corrections. For a fixed q and τ the value of τ_1 at the nth generation was obtained from the normalization condition $\Gamma_n(q,\tau,\tau_1,\sigma^{(n)})=1$. Then the values of $\tau(q)$ and $\tau_1(q)$ are derived from the coordinates of the point of intersection in the plane (τ,τ_1) of the curves $\tau_1(\tau)$ corresponding to two successive generations. The logarithmic dimension is plotted in Fig. 3 as a function of the scaling index ν. The continuous set of values taken by the scaling index proves the multifractal nature of the spectrum.

As the example of the states located at the center of the spectrum indicates, the logarithmic law of scaling persists for amplitudes V lower than 1. However, the existence of continuous parts in the spectrum is not excluded in this range of values of V. In particular, when V takes one of the special values $V_c^{(m)}$ mentioned in the previous section, there are singular continuous parts of the spectrum characterized by the local scaling law (4) in the neighborhood of the energies $E=\pm E_c(V)$ and the states are critical. The numerical computation of the inverse participation ratio and second moment performed in Ref. 6 for $V=V_c^{(1)}$ shows that for energy values outside the neighborhoods of $\pm E_c(V)$ the states are localized, that is, the two singular continuous parts of the spectrum are surrounded by a sea of pure point spectrum. This implies the existence of four mobility edges separating the regions with critical and localized states. (Here we call mobility edge any energy value that separates regions with normalizable states from regions with non-normalizable states.) The existence of singular continuous parts in the spectrum, which is expected to take place for any critical value $V_c^{(m)}$, has important consequences on the electron

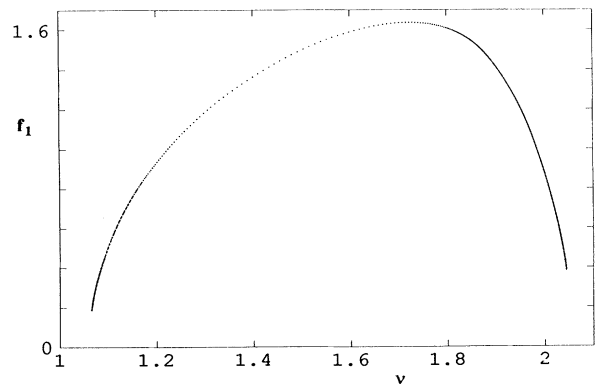


FIG. 3. Logarithmic dimension f_1 as a function of the scaling index ν computed by using the bandwidths at the generations 9 and 10.

dynamics, being shown that the states near $\pm E_c(V)$ cause the subdiffusive expansion of the electronic wave packets through the lattice (see Fig. 10 from Ref. 6 for the case $V=V_c^{(2)}$).

IV. SUMMARY

The nature of the spectrum of the Rudin-Shapiro tight-binding model was numerically investigated. A study of the scaling properties of the bands of periodic approximants performed for various values of the energy and amplitude of the on-site potential V revealed scaling relations intermediate between the power and exponential laws. The corresponding IDS was found to scale in general logarithmically, but power laws were also derived for some special values of V. A multifractal analysis of the spectrum at $V=1$ indicated the absence of the power-law scaling in the limit of the large system. This result together with numerical arguments regarding the total bandwidth and the nature of states led to the conclusion that the continuous components are absent from the spectrum of the RS chain for $V \geq 1$. Nevertheless, the existence of parts of the spectrum that scale like a power law indicated the presence at some fixed special values of $V<1$ of at least two singular continuous regions in the spectrum for which the states are critical. For such special values of V the singular continuous parts are surrounded by pure point spectrum, therefore at least four mobility edges should exist, separating the regions of localized and critical states. Finally, the insertion of logarithmic corrections to the gauge function permitted proof of the multifractal nature of the spectrum for $V=1$.

The above derived features put the RS chain in a special position among the deterministic aperiodic models as yet investigated. Namely, this is one of the very few examples[20] of a non-quasi-periodic one-dimensional model that displays mobility edges in its spectrum. Moreover, the RS case shows that at least one type of scaling law different from exponential can exist for the bandwidths of systems with pure point spectra. These results suggest that, in general, the study of complex deterministic aperiodic systems can reveal qualitatively new phenomena that enrich the physical knowledge about the mechanism of localization.

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