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On the multifractal spectrum of the Fibonacci chain

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Abstract. We consider the multifractal properties of a quasiperiodic tight binding Hamiltonian where the hopping elements are arranged according to the Fibonacci chain. By using the trace map approach and an assumption relating the cycles of the trace map to the integrated density of states, it is shown that the maximal scaling of the spectrum does not always occur at the edges or the centre of the spectrum, which is confirmed by numerical simulations. A good description of the multifractal spectrum $f(\alpha)$ is obtained by applying the $3z$ -model which was recently developed for the Harper model.

Despite their conceptual and formal simplicity one-dimensional quasiperiodic Hamiltonians display a complex hierarchical behaviour concerning both energy spectrum and wavefunctions. We consider in the following the Hamiltonian

$$H = \sum_i t_{i+1}|i\rangle\langle i+1| + t_i|i\rangle\langle i-1| \quad (1)$$

where the hopping elements $t_i \in \{t_A, t_B\}$ are arranged according to the Fibonacci chain. This quasiperiodic chain can be obtained by the substitution rule ($A \mapsto B, B \mapsto BA$). After n iterations a chain of f_n letters is obtained, where f_n are the Fibonacci numbers ($f_n = f_{n-1} + f_{n-2}, f_0 = f_1 = 1$). Asymptotically f_n grows like ω^{-n} , where $\omega = (\sqrt{5}-1)/2$ is the golden number. The spectral measure of the quasiperiodic Hamiltonian (1) has been proven to be singular continuous for all $t_A \neq t_B$ [1, 2]. Moreover, the spectrum is a Cantor set of zero Lebesgue measure. The most powerful method to characterize spectra of this kind quantitatively is the multifractal analysis, yielding a multifractal spectrum $f(\alpha)$ [3, 4]. The function $f(\alpha)$ which can numerically be calculated by means of the thermodynamic formalism gives the fractal dimension of the set of energies where the spectral measure scales with the local exponent α . Furthermore, $f(\alpha)$ is via its Legendre transform $\tau(q)$ directly related to the generalized (Rényi) dimensions $D_q = \tau(q)/(q-1)$. These have been shown to play an important role in explaining the anomalous diffusion properties found in the quantum dynamics of quasiperiodic systems [5–9]. In this paper we address the following two related issues: the local scaling of the spectral measure at certain energies and the global scaling function $f(\alpha)$.

As for the local scaling, the exponents at the edges and centre of the spectrum have been calculated by means of a renormalization analysis based on the trace map approach in a series of pioneering articles [10–15]. It was conjectured that these exponents were the minimal and maximal ones [12]. In the following the Fibonacci trace-map has been

extensively investigated as a dynamical system and deep results on the structure of its cycles have been found [16, 17]. These results, however, have not yet been used for calculating the local scaling at other points than centre or edges of the spectrum. We will give a method linking the scaling at any rational value of the integrated density of states (IDOS) to the period of the cycle which governs the scaling at this point of the spectrum. By these means we find an exact result for the scaling at one third of the IDOS, which disproves the conjecture about the occurrence of maximal scaling at the centre or the edges of the spectrum.

Concerning the multifractal spectrum, a first approximation of $f(\alpha)$ based on the scaling of the edges and the centre of the spectrum was given in [18]. By including further scaling properties as we did for the Harper model [19] we overcome a principal drawback of this simple approximation and arrive at a description of the multifractal spectrum which agrees well with numerical simulations.

The rest of the paper consists of two parts: First we consider the scaling properties of the spectrum by means of the trace-map approach, second we discuss the multifractal properties in the framework of the $3z$ -model.

An important step towards the understanding of the scaling properties of the spectrum of the Fibonacci chain was achieved by means of the trace map. We describe the main points that are important for the following, a detailed discussion can be found in [12]. The first step to the trace map is the reformulation of the eigenvalue equation $t_{i+1}\psi_{i+1} + t_i\psi_{i-1} = E\psi_i$ in terms of transfer matrices. Due to the inflation properties of the Fibonacci chain and the fact that the transfer matrices are elements of $SL(2, R)$ one can find a simple recursion relation for the traces of the transfer matrices T_n , which describe the mapping of (ψ_1, ψ_0) to $(\psi_{f_n}, \psi_{f_n-1})$. With $x_n := \frac{1}{2}\text{Tr} T_n$ this recursion is given by [11, 14]

$$x_{n+1} = 2x_n x_{n-1} - x_{n-2} \quad (2)$$

with initial conditions

$$x_{-1} = \frac{1}{2} \left(\frac{t_A}{t_B} + \frac{t_B}{t_A} \right) \quad x_0 = \frac{E}{2t_B} \quad x_1 = \frac{E}{2t_A}. \quad (3)$$

All energies for which $x_n \leq 1$ are in the spectrum of the n th approximant. The dynamical map $R^3 \rightarrow R^3$ which is given by the recursion shows a remarkable invariant $I = x_{n+1}^2 + x_n^2 + x_{n-1}^2 - 2x_{n+1}x_nx_{n-1} - 1$ [14] which has been interpreted as Fricke character [21]. Due to the initial condition the invariant is fixed by the parameters of the Hamiltonian to be $I = (\rho - \rho^{-1})^2/4$, where $\rho = t_A/t_B$.

The importance of the trace map lies in the fact that its periodic orbits correspond to special points in the spectrum [12]. Furthermore the minimal eigenvalue of the linearized map λ_p gives the local scaling exponent

$$\alpha = \frac{p \ln \omega}{\ln \lambda_p} \quad (4)$$

where p denotes the length of the periodic orbit. The exponent α describes the shrinking of the band widths $\Delta^{(n)}$ as a function of the length of the approximant: $\Delta^{(n)} \sim f_n^{-1/\alpha} \sim \omega^{n/\alpha}$.

The first orbits to be identified were the 6-cycle

$$C_6 : \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} 0 \\ 0 \\ -a \end{pmatrix} \mapsto \begin{pmatrix} 0 \\ -a \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} -a \\ 0 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix} \mapsto \begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} \quad (5)$$

where $a = \sqrt{I+1}$, governing the scaling of the centre of the spectrum and the 2-cycle

$$C_2 : \begin{pmatrix} a \\ b \\ b \end{pmatrix} \mapsto \begin{pmatrix} b \\ a \\ a \end{pmatrix} \mapsto \begin{pmatrix} a \\ b \\ b \end{pmatrix} \quad (6)$$

where $a = J + \sqrt{J^2 - J}$, $b = J - \sqrt{J^2 - J}$, $J = \frac{1}{8}(3 + \sqrt{25 + 16I})$, governing the scaling at the edge of the spectrum. The corresponding local exponents are given by (4) with

$$\lambda_6 = (-2(I+1) + \sqrt{4(I+1)^2 + 1})^2 \quad (7)$$

and

$$\lambda_2 = \frac{1}{2}(8J - 1 - \sqrt{(8J - 1)^2 - 4}). \quad (8)$$

It has been conjectured that these two local exponents are the extreme exponents found in the spectrum. For simplicity we define contraction factors z which determine the scaling of the bandwidth with respect to two inflation steps[†]. Therefore, $z_6 = \lambda_6^{1/3}$, $z_2 = \lambda_2$. These two contraction factors are shown in figure 3. For the periodic limit $\rho = 1$ the expected behaviour is obtained: $z_6 = \omega^2$, $\alpha_6 = 1$, i.e. the bands at the centre scale inversely to the length of the chain, and $z_2 = \omega^4$, $\alpha_2 = \frac{1}{2}$, i.e. the bands at the edges of the spectrum scale inversely to the length squared due to the van Hove singularities.

The question arises whether these two scaling exponents are really the extremal ones. If this were the case the spectrum would be monofractal for $\rho_c \approx 0.094\,408$, where $z_2 = z_6$. In order to answer this question, we investigate the connection between cycle and energy by considering the trace map in the limit of the periodic chain $t_A = t_B = 1$. In this special case, the recursion (2) can be solved explicitly yielding

$$x_n = \cos \left(f_n \arccos \frac{E}{2} \right). \quad (9)$$

For rational values of $\frac{1}{2\pi} \arccos \frac{E}{2} =: Q/N$ the sequence x_n is necessarily periodic with the period depending (*a priori*) on Q and N . In the following table the values of the period are given for $N \leq 10$. The period does not depend on Q , provided N and Q are coprime. Due to (9) the periods of the trace map for $I = 0$ are related to those of the modified Fibonacci rule $f_{n+1} = f_n + f_{n-1} \bmod N$ [‡]

N	1	2	3	4	5	6	7	8	9	10
Period	1	3	4	6	10	12	8	12	12	30.

(10)

Can this connection between the energy and the period of the corresponding cycle of the trace map, which is valid for the periodic chain ($\rho = 1$), be extended on the quasiperiodically modulated chain ($\rho < 1$)? For the cycle governing the edge of the spectrum, the corresponding energy changes as a function of the parameter ρ , whereas the IDOS of this energy is independent of ρ . We now make the natural assumption that this behaviour is not only valid for the edges and the centre of the spectrum, but also for the general case, i.e. we assume that a given cycle governs the scaling at an energy the IDOS of which is independent of ρ . As for the periodic chain (with odd length q and Bloch vector $k = 0$) the energy levels are given by $E_j = 2 \cos(\pi j/q)$ and as for this case $E = 2 \cos(2\pi Q/N)$, we find that the cycle (Q/N) corresponds to the scaling of the energy level with IDOS = $j/q = 2Q/N$.

[†] Referring to *two* inflation steps is arbitrary, but makes visualization simple.

[‡] A generalization of this rule is known as a Fibonacci random number generator. We refer the reader to Parker [22] for details on the structure of the cycles. A related question is the structure of the Fibonacci orbits in $SU(2)$ which is treated in Wagner and Kramer [22].

As an illustration we consider first the cycles corresponding to the centre and edge of the spectrum. Take for example the energy at the centre, $E = 0$, i.e. $Q/N = \frac{1}{4}$, then $x_n = \cos(f_n\pi/2)$, which is periodic with period 6 and is the special case of (5) for $I = 0$. In general, however, the generic cycle (for $\rho \leq 1$) can be degenerated for $\rho = 1$. Then the period of the generic cycle is an integer multiple of the one for $\rho = 1$. This is the case for the edges of the spectrum. Consider the upper edge of the spectrum, $E = 2$, $Q/N = \frac{0}{1}$, $x_n = 1$, which is the degenerated case of (6) for $I = 0$. More interesting is the lower edge, $E = -2$, $Q/N = \frac{1}{2}$, i.e. $x_n = \cos(f_n\pi)$, which is periodic with period three. Since there is no 3-cycle of the trace map which depends on one free parameter, we are looking for a 6-cycle that reduces for $I = 0$ to $x_n = \cos(f_n\pi)$. This cycle can be found to be

$$C'_6 : \begin{pmatrix} a \\ b \\ a \end{pmatrix} \mapsto \begin{pmatrix} b \\ a \\ -b \end{pmatrix} \mapsto \begin{pmatrix} a \\ -b \\ -a \end{pmatrix} \mapsto \begin{pmatrix} -b \\ -a \\ -b \end{pmatrix} \mapsto \begin{pmatrix} -a \\ -b \\ a \end{pmatrix} \\ \mapsto \begin{pmatrix} -b \\ a \\ b \end{pmatrix} \mapsto \begin{pmatrix} a \\ b \\ a \end{pmatrix} \quad (11)$$

with $a = -(J + \sqrt{J^2 - J})$, $b = a/(2a + 1)$, $J = \frac{1}{8}(3 + \sqrt{25 + 16I})$. As expected from the symmetry of the spectrum the local exponent calculated by linearization around this 6-cycle is the same as for the upper edge (8). We remark that two cycles corresponding to E and $-E$ are related by a symmetry property of the trace map [16]. It can be shown that the periods of the two cycles are either equal or related by a factor three [16], the latter being the case for the upper and lower edge of the spectrum.

Apart from these cycles describing the scaling at the centre and the edges of the spectrum, the next simple ones are those with $N = 3$, corresponding to a cycle of length four and $N = 7$, corresponding to a cycle of length eight.

In order to find the 4-cycle governing the scaling at the IDOS $= \frac{2}{3}$, we take the (unique) one which reduces in the periodic limit to the known solution $x_n = \cos(2\pi f_n/3)$. It is given by

$$C_4 : \begin{pmatrix} -\frac{1}{2} \\ a \\ -\frac{1}{2} \end{pmatrix} \mapsto \begin{pmatrix} a \\ -\frac{1}{2} \\ \frac{1}{2} - a \end{pmatrix} \mapsto \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} - a \\ -\frac{1}{2} \end{pmatrix} \mapsto \begin{pmatrix} \frac{1}{2} - a \\ -\frac{1}{2} \\ a \end{pmatrix} \mapsto \begin{pmatrix} -\frac{1}{2} \\ a \\ -\frac{1}{2} \end{pmatrix} \quad (12)$$

where $a = (1 + \sqrt{9 + 8I})/4$. The linearization around this cycle yields

$$z_4 = \sqrt{\frac{16I + 7 - \sqrt{(16I + 7)^2 - 4}}{2}}. \quad (13)$$

In figure 1 this result is compared with data from numerical simulations. The agreement is good in the whole range $0 < \rho < 1$. The consequences of this new contraction factor are obvious from figure 3, where the three analytically known contraction factors are plotted: the contraction factor corresponding to the IDOS $= \frac{2}{3}$ is always bigger than the one at the edges of the spectrum. Therefore in a certain range of the parameter $0 < \rho < 0.135366$ the maximal contraction factor, corresponding to the minimal shrinking of the bands and to the maximal local exponent of the spectral measure is neither at the centre nor at the edges of the spectrum. Furthermore, for $\rho = \rho_c$, where edges and centre scale in the same way, the spectrum is not a monofractal since $z_4 > z_2 = z_6$.

We consider now the next more complicated case, $N = 7$ corresponding to an 8-cycle of the trace map. In this case the orbit corresponding to the IDOS $= \frac{2}{7}$ is given by the

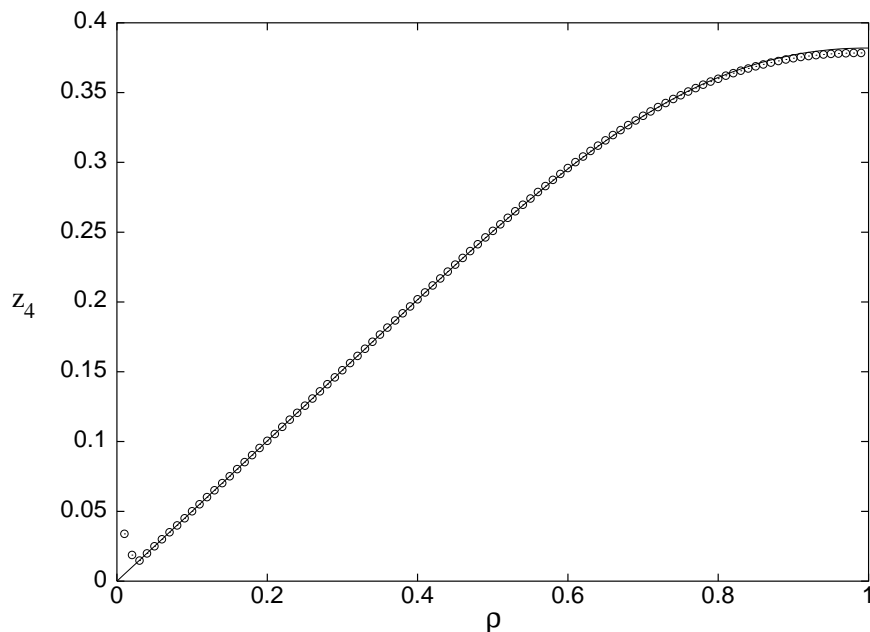


Figure 1. The scaling of the bands at the IDOS = $\frac{2}{3}$ compared with the analytical result by linearizing around the 4-cycle. The numerical results were obtained with the approximants $f_7 = 21$ and $f_{15} = 987$. The corresponding bands were those with index 14 and 658, respectively.

initial condition $x_{-2} = a$, $x_{-1} = c$, $x_0 = a$, where a and c as a function of the invariant I are given by the following equations:

$$64a^2(2a-1)^2(2a+1)^2I^2 - 16a(2a-1)(8a^3+4a^2-4a-1)(8a^3+2a^2-5a-1)I \\ + (1+8a-16a^2-8a^3+16a^4)(8a^3+4a^2-4a-1)^2 = 0$$

and

$$2a^2 + c^2 - 2a^2c - 1 = I. \quad (14)$$

For the periodic case $I = 0$ one finds (as one solution) $a = \cos \frac{6\pi}{7}$, $c = \cos \frac{2\pi}{7}$ and the cycle $(\cos \frac{6\pi}{7}, \cos \frac{2\pi}{7}, \cos \frac{6\pi}{7}, \cos \frac{4\pi}{7}, \cos \frac{4\pi}{7}, 1, \cos \frac{4\pi}{7}, \cos \frac{4\pi}{7})$ in agreement with $x_n = \cos(f_n \frac{4\pi}{7})$. By solving the two equations for general values of I and keeping track of the solution which yields $x_n = \cos(f_n \frac{4\pi}{7})$ for $I \rightarrow 0$ one obtains the 8-cycle, the linearization around which describes the scaling at the IDOS = $\frac{2}{7}$. The formula of the calculated eigenvalues of the linearized map are too cumbersome to be given explicitly. Thus we have calculated the numerical values and compare them with data obtained by diagonalization in figure 2. The agreement is satisfactory but not as good as in the case of the IDOS = $\frac{2}{3}$. This is probably due to finite-size effects which are more important for $N = 7$ than for $N = 3$.

After having considered the local scaling properties we now turn to the description of the global scaling function $f(\alpha)$, defined as the Legendre transform of $\tau(q)$ which is implicitly given by requiring that the partition function

$$\Gamma(\tau, q) = \frac{1}{f_n^q} \sum_{j=1}^{f_n} \Delta_j^{-\tau} \quad (15)$$

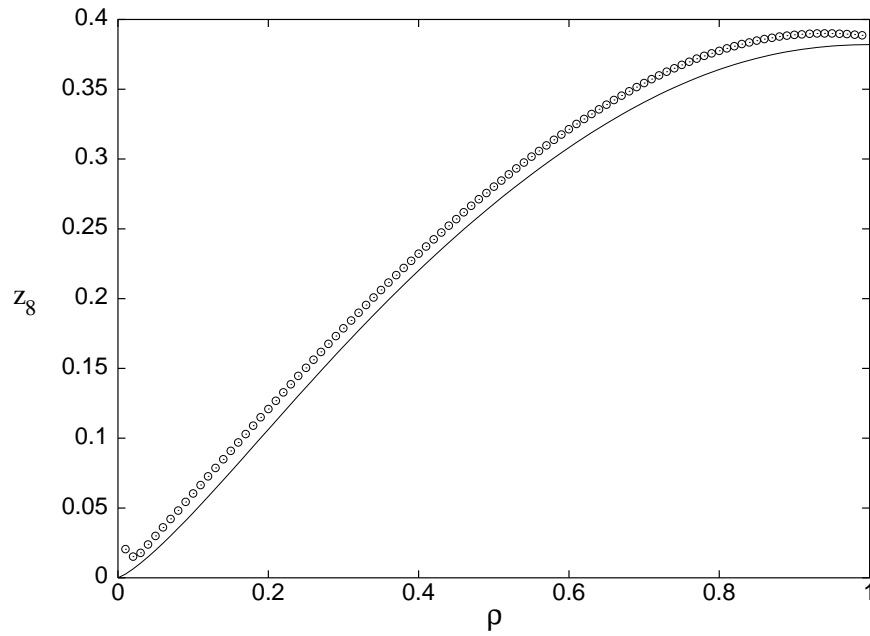


Figure 2. The scaling of the bands at the IDOS = $\frac{2}{7}$ compared with the result obtained by linearizing around the 8-cycle. The numerical results were obtained with the approximants $f_7 = 21$ and $f_{15} = 987$. The corresponding bands were those with index 6 and 282, respectively.

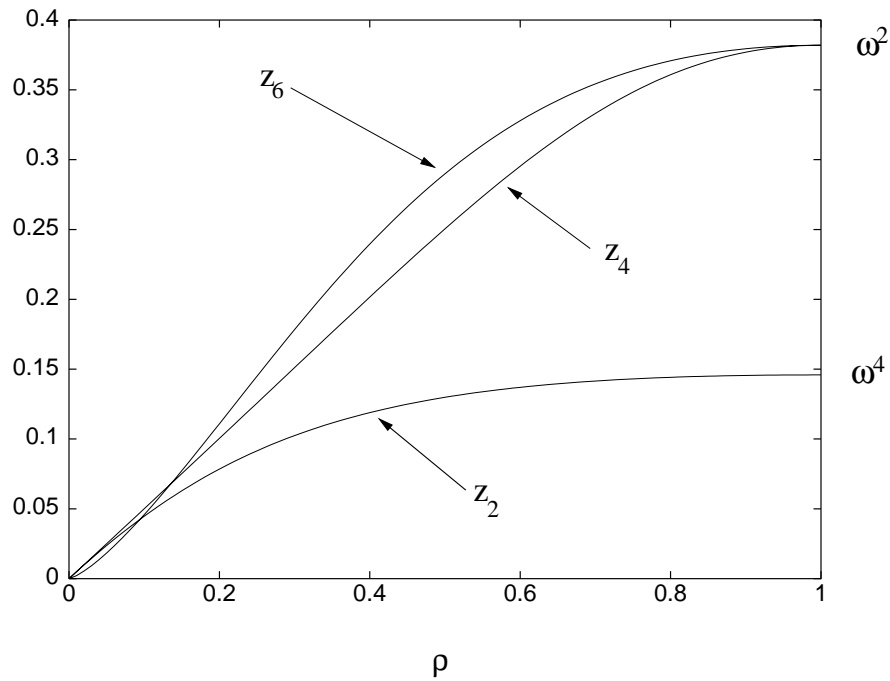


Figure 3. The analytically known contraction factors z_2 , z_6 and z_4 as a function of the quasiperiodic modulation ρ .

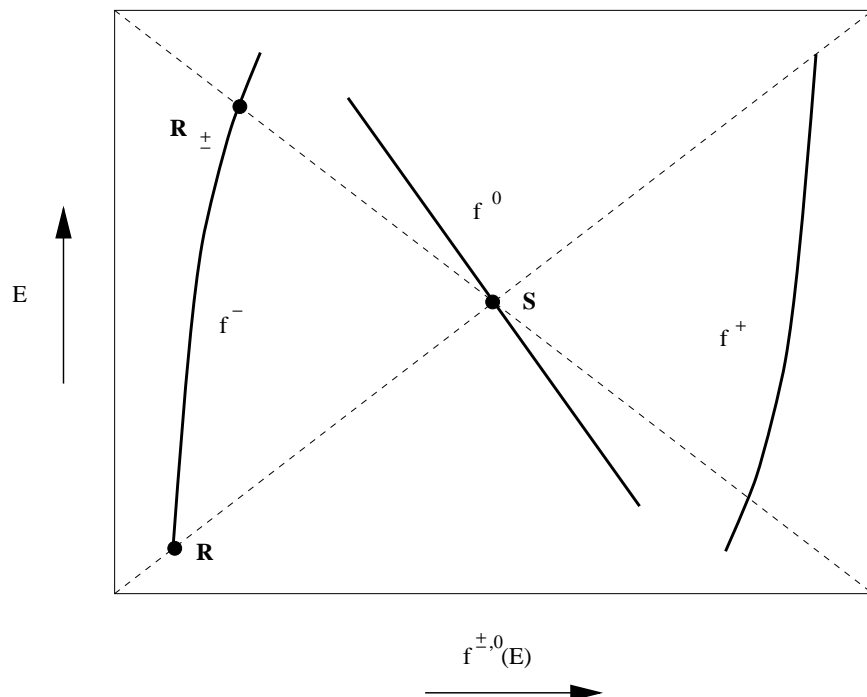


Figure 4. Quantitative version of the Hofstadter rules. The functions $f^{\pm,0}(E)$ give the mapping of the energies of an approximant of length f_{n-2} resp. f_{n-3} to those of an approximant of length f_n as described by equation (17).

be constant in the limit $n \rightarrow \infty$, where Δ_j denotes the widths of the f_n individual (nonoverlapping) bands of an approximant.

To this aim we recall that the spectrum of an approximant f_n of the Fibonacci chain can be recursively built from the spectra of the approximants f_{n-2} and f_{n-3} . This was first noticed in the limit $\rho \rightarrow 0$, where perturbative renormalization shows that the spectrum consists of three clusters, the centre cluster and two side clusters. The centre cluster is a rescaled version of the spectrum of the approximant f_{n-3} with scaling factor ρ^2 , the edges of the spectrum are rescaled versions of the spectrum of f_{n-2} with scaling factor $\rho/2$ [20, 18]. A multifractal analysis based on this observation yields [18]

$$\frac{2\omega^{2q}}{z_R^\tau} + \frac{\omega^{3q}}{z_S^\tau} = 1 \quad (16)$$

where z_R and z_S are the contraction factors at the edges and the centre, respectively. These contraction factors are exactly given by the trace map, $z_R = z_2 = \lambda_2$ and $z_S = z_6^{3/2} = \lambda_6^{1/2}$, yielding in first nonvanishing order for $\rho \rightarrow 0$ the expressions found by perturbative renormalization $z_R = \rho/2$ and $z_S = \rho^2$.

The multifractal spectrum $f(\alpha)$ as a Legendre transformation of $\tau(q)$ obtained by equation (16) has the main drawback that $f(\alpha_{\max})$ or $f(\alpha_{\min})$ (for $\rho < \rho_c$, respectively $\rho > \rho_c$) does not vanish in contradiction to numerical results. This problem is due to the assumption that the side clusters are *uniformly* scaled versions of the spectrum of a smaller approximant. In order to remove this oversimplification we have defined in a previous work [19] scaling functions $f^{0,\pm}(E)$ (not to be confused with $f(\alpha)$) describing how the energies

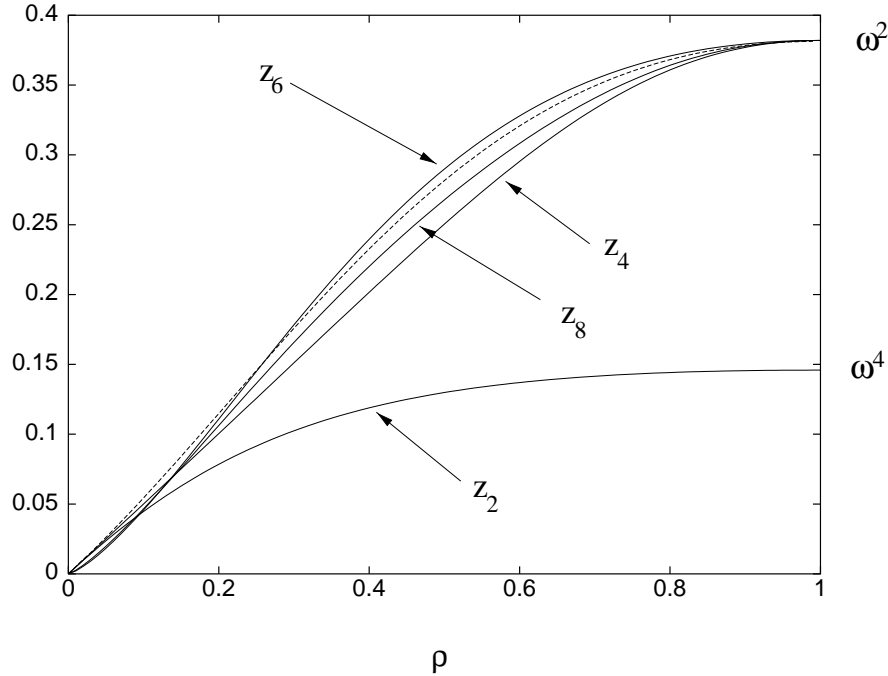


Figure 5. The contraction factors z_2 , z_4 , z_6 , z_8 and $z_{R\pm}$ (broken curve) as a function of the quasiperiodic modulation ρ . For $\rho < 0.26$ the contraction factor $z_{R\pm}$ is the maximal among the considered ones.

of an approximant f_n are obtained from those of approximants of length f_{n-2} and f_{n-3} (figure 4):

$$E_i = \begin{cases} f^-(E_i) & \text{for } i = 1, \dots, f_{n-2} \\ f^0(E_{i-f_{n-2}}) & \text{for } i = f_{n-2} + 1, \dots, f_{n-1} \\ f^+(E_{i-f_{n-1}}) & \text{for } i = f_{n-1} + 1, \dots, f_n. \end{cases} \quad (17)$$

We remark that this description is inspired by the Hofstadter rules which have been developed for the Harper equation [23–25] but also apply for other quasiperiodic Hamiltonians as the one treated here. For a general discussion of this quantitative version of the Hofstadter rules we refer the reader to [19].

Making the simple approximation that $f^{0,\pm}$ are linear functions, $f^0(E) = -z_S E$, $f^\pm(E) = z_R E \pm \text{constant}$, one arrives again at the homogeneous scaling of the clusters and $\tau(q)$ is given by (16). The simplest improvement of this crude approximation has been developed in [19] and consists of taking into account the bands which follow an orbit of period two with respect to the Hofstadter rules (17). The corresponding self-consistent equation for $\tau(q)$ is given by [19]

$$\frac{\omega^{2q}}{z_R^\tau} + \frac{\omega^{2q}}{z_{R\pm}^\tau} + \frac{\omega^{3q}}{z_S^\tau} = 1 \quad (18)$$

where $z_{R\pm}$ is the contraction factor at the fixed point of order two:

$$z_{R\pm} = \left. \frac{df^\pm(E)}{dE} \right|_{E=-f^\pm(E)}. \quad (19)$$

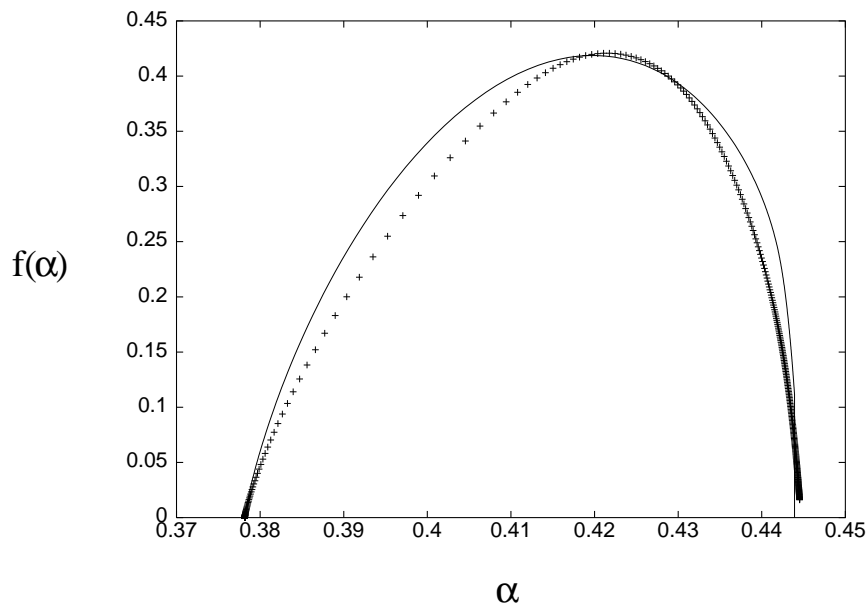


Figure 6. The multifractal spectrum $f(\alpha)$ obtained by the $3z$ -model compared with data obtained by diagonalization. The strength of the quasiperiodic modulation is $\rho = 0.2$.

How can the contraction factor $z_{R\pm}$ be determined? In the first part of this paper it has been argued that the contraction factor can be calculated by means of the trace map for special energies. In the case of the periodic chain these are given by $E = 2 \cos(2\pi Q/N)$. As for the periodic case the condition $E = -f^\pm(E)$ yields $E = \pm 2 \cos(\pi/(1 + \omega^2))$, there is no cycle in the trace map corresponding to the energy of the orbit of period two R_\pm . Having thus no method at hand to calculate $z_{R\pm}$ analytically, we determine it numerically by considering the shrinking of the corresponding bands as a function of the approximant length. The indices of these bands are given by the recursion $i_n = f_{n-2} - i_{n-1} + 1$ with $i_2 = i_3 = 1$, as can be seen from (17) and the fact that for this energy f^+ and f^- apply alternatively.

In figure 5 the contraction factors $z_{R\pm}$ are shown together with the contraction factors known from the first part of this paper. $z_{R\pm}$ is maximal in the range $0 < \rho < 0.26$ among these contraction factors. Since, however, the contraction factors cannot be calculated for all cycles of the trace map, let alone all energies in the spectrum, the question of the maximal contraction factor as a function of ρ remains still open. The comparison of the multifractal spectrum $f(\alpha)$ obtained by (18) with numerical simulations shows that the agreement is rather good, especially for relatively small values of ρ (figure 6).

Summing up, we have used the trace-map approach to calculate the scaling of the spectrum of the Fibonacci chain for certain rational values of the IDOS. Our analysis was based on the assumption that the IDOS of the energy, the scaling of which is governed by a given cycle of the trace map, does not change as a function of the strength of the quasiperiodic modulation ρ . A possible proof of this assumption could operate along the ideas of the gap labelling theorem [26, 21]. Furthermore, we have shown that the maximal scaling exponent does not always occur at the centre and never occurs at the edges of the spectrum. The multifractal spectrum $f(\alpha)$ which has been calculated approximately by a method originally developed for the Harper model is in good agreement with numerical simulations.

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