Analytical Results for Scaling Properties of the Spectrum of the Fibonacci Chain

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We solve the approximate renormalization group found by Niu and Nori for a quasiperiodic tight-binding Hamiltonian on the Fibonacci chain. This enables us to characterize analytically the spectral properties of this model.

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Much theoretical effort has gone into the study of one-dimensional Schrödinger equations with quasiperiodic (QC) or incommensurate (IC) potentials [1]. Such models are invoked to describe a variety of experimental situations [1,2]. These include, for example, charge density wave systems, semiconductor superlattices with quasiperiodic stacking sequence, two-dimensional crystals in a magnetic field, and superconducting networks in magnetic field. This family of models are neither periodic nor random, but in some sense lie in between. For example, a quantum particle moving on an infinite chain and subjected to a QC or IC modulation can exhibit critical localization properties. Depending on the modulation strength, and in contrast to the case of a random modulation, the particle wave function is not necessarily strongly localized (insulating); it can also be extended (metallic) as in a translationally invariant system or in a critical localization regime at the metal-insulator transition. Typical models where these peculiar localization properties occur are Harper-like models (IC) or tight-binding Hamiltonians associated with a quasiperiodic sequence such as the Fibonacci sequence (QC). In general, these models have two important parameters: an irrational ω which is responsible for the absence of periodicity, and a parameter K which determines the strength of the QC or IC modulation. The usual procedure to characterize the localization properties of these Hamiltonians $H_{\omega,K}$ is to study the scaling of the spectral properties of a sequence of periodic Hamiltonians $H_{\omega_n,K}$ which converge to $H_{\omega,K}$ as n goes to infinity. If the widths of the q_n individual bands that compose the spectrum of $H_{\omega_n,K}$ decrease exponentially with the period (q_n) of $H_{\omega_n,K}$, then $H_{\omega,K}$ is in an insulating regime and has a *pure point* spectrum. In the case when the widths decrease only inversely proportionally to q_n, then $H_{\omega,K}$ is in the metallic regime and has an *absolutely continuous* spectrum. In contrast with these two cases, the critical localization regime of $H_{\omega,K}$ is expected to have a *singular continuous* spectrum with multifractal (MF) properties in the spectral measure. In fact, in this latter case, the scaling found by many numerical simulations [1] is that the bandwidths decrease like $\sim q_n^{-1/\alpha}$ where the exponent α (< 1) varies from band to band so that there are typically $\sim q_n^{+g(\alpha)}$ bands with the same exponent. Because of these peculiarities, the critical regime has been extensively studied by both numerical simulations and analytic techniques [1]. However, as yet, an analytical quantitative determination of the exponents α and $g(\alpha)$ has not been achievable for even one irrational ω.

The purpose of this paper is to show a QC tight-binding model for which we are able to analytically characterize all the spectral properties. Our work starts from the approximate renormalization group (RG) found by Niu and Nori [3] for a QC model on the Fibonacci chain and other hierarchical chains. By reformulating and solving the RG of Niu and Nori, we derive constructive and transparent recurrence schemes for both the energy levels and the bandwidths. From these two schemes we deduce new recurrence relations for the spectral measure, the large time average return probability of particles defined in [4], the spectrum Lebesgue measure, the MF partition function [5], and the bandwidth distribution. For most of these relations, a natural fixed point solution is a power law, in either size or time. By comparing with the fixed point equation of the MF partition function, it appears that the exponents associated to these power laws are related to a subset of the *anomalous* dimensions which characterize the MF properties of the spectral measure. A direct calculation of the function $g(\alpha)$ vs α confirms these MF properties. To complete the analysis of the spectral properties, we also study the gap properties. We find that there are two types of gaps: *transient* and *stable*. For the first type, their properties are like those of the bandwidths. In contrast, for the *stable* gaps, the distribution of their widths g is a *stable* power law $P(g) \sim g^{-(1+D_F)}$, where D_F is the Hausdorff dimension of the spectrum measure.

These results complete and correct a previous MF analysis of the spectral measure of this model [6]; our work also unifies many partial results obtained by other methods, for both this model [7–9] and the Harper model [10].

We consider the tight-binding Hamiltonian H_n defined on an approximant of period F_n of the Fibonacci chain by the following equation:

$$H_n = \sum_{i=1}^{F_n} V_i c_i^\dagger c_i + t_{i,i+1} c_i^\dagger c_{i+1} + t_{i-1,i} c_i^\dagger c_{i-1} . \qquad (1)$$

The on-site potential V_i is taken to be uniform $(V_i = V)$. In contrast, the hopping amplitude $t_{i,i+1}$ from site i to site $i+1$ is given by $t_{i,i+1} = t_w[1 - \chi(\omega_n i)] + t_s \chi(\omega_n i)$,

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where $\omega_n = F_{n-1}/F_n$ tends to the golden mean $\omega = (\sqrt{5}-1)/2$ ($F_{n+1} = F_n + F_{n-1}$ and $F_n \simeq \omega^{-n}$). The characteristic function $\chi(\omega i)$ takes the value 0 or 1 according to the Fibonacci sequence, and, correspondingly, the bond $t_{i,i+1}$ will take the value t_w or t_s. For finite n the density of weak bonds (t_w) is ω_n and tends to ω in the quasiperiodic limit. For the strong bonds (t_s) the density is $\omega_n^2 = F_{n-2}/F_n$ and tends to ω^2. The periodicity of the Hamiltonian $H_n(V, t_s, t_w)$ allows us to define Bloch boundary conditions of the form $c_{j+F_n} = e^{ik}c_j$. For a fixed k, the energy spectrum of $H_n(V, t_s, t_w)$, which we define as $W_n(V, t_w, t_s)$, consists of F_n levels $E_n^i(k)$ ($i = 1, \ldots, F_n$ and $E_n^i \leq E_n^{i+1}$ by convention). Varying k from 0 to π allows the association of an energy band of width $\Delta_n^i = |E_n^i(\pi) - E_n^i(0)|$ to each of these levels.

Using a perturbative approach, Niu and Nori have shown that in the strong modulation regime ($t_w/t_s \ll 1$) the spectrum $W_n(0, t_w, t_s)$ is the union of three subspectra $W_{n-2}(V^+, t_s^+, t_w^+)$, $W_{n-3}(V^0, t_s^0, t_w^0)$, and $W_{n-2}(V^-, t_s^-, t_w^-)$, which correspond to three sub-Hamiltonians with periods F_{n-2}, F_{n-3}, F_{n-2}, and renormalized parameters $V^{\pm,0}, t_s^{\pm,0}, t_w^{\pm,0}$, respectively. A representation of this perturbative RG, with the explicit value of the renormalized parameters, is schematically given by the following :

$$W_n(0, t_s, t_w) \rightarrow \left| \begin{array}{l} W_{n-2}\left(t_s, \frac{+t_w}{2}, \frac{+t_w^2}{2t_s}\right), \\ W_{n-3}\left(0, \frac{-t_w^2}{t_s}, \frac{t_w^3}{t_s^2}\right), \\ W_{n-2}\left(-t_s, \frac{-t_w}{2}, \frac{-t_w^2}{2t_s}\right). \end{array} \right. \tag{2}$$

In principle, the scheme (2) simplifies the problem, since it relates the spectral properties of a Hamiltonian of period F_n to those of three sub-Hamiltonians of smaller period. However, it is clear that upon l iterations of (2) the difficulty which is initially due to the large period F_n is replaced by the problem of an increasing number (3^l) of different Hamiltonians to be solved. As we now describe, certain properties of the Hamiltonian and the RG (2) allow us to overcome this difficulty. First, it is clear that the spectrum of $H_n(0, t_s, t_w)$ is independent of the sign of t_s and t_w, thus we have $W_n(0, t_s, t_w) = W_n(0, |t_s|, |t_w|)$ [11]. Second, we see that the spectrum $W_{n-2}(V^\pm, t_s^\pm, t_w^\pm)$ is just uniformly translated from $W_{n-2}(0, t_s^\pm, t_w^\pm)$ by a factor $V^\pm$. Third, the renormalized parameters have the following property:

$$|t_s^\pm| = zt_s, \qquad |t_w^\pm| = zt_w, \qquad |t_s^0| = \overline{z}t_s,$$
$$|t_w^0| = \overline{z}t_w, \qquad z = \frac{t_w}{2t_s} \ll 1, \qquad \overline{z} = \frac{t_w^2}{t_s^2} \ll 1. \tag{3}$$

Combining these properties and using (2), we deduce the renormalization scheme (4), where now both sides of the arrow refer to the spectrum of Hamiltonians with the same parameter $(0, t_s, t_w)$ but distinct periods:

$$W_n(0, t_s, t_w) \rightarrow \left| \begin{array}{l} -t_s + zW_{n-2}(0, t_s, t_w), \\ \overline{z}W_{n-3}(0, t_s, t_w), \\ +t_s + zW_{n-2}(0, t_s, t_w). \end{array} \right. \tag{4}$$

Although this RG scheme is exact in the limit $|t_w/t_s| \ll 1$ [3], from the last equation we can give a minimal condition for its validity. That is, t_s has to be sufficiently strong so that the spectrum $W_{n-2}(0, t_s, t_w)$, which is contracted by a factor z and centered around $\pm t_s$, is not mixed with the spectrum $W_{n-3}(0, t_s, t_w)$, which is contracted by $\overline{z}$. More precisely, calling Δ_n the width of the spectrum $W_n(0, t_s, t_w)$, this nonoverlapping condition becomes $z\Delta_{n-2} + \overline{z}\Delta_{n-3} \leq 2t_s$. Under this condition, relation (4) gives the following recurrence scheme between the energy levels E_n^i, E_{n-2}^i, and E_{n-3}^i:

$$\begin{array}{lll} E_n^i & = -t_A + zE_{n-2}^i & (i = 1, F_{n-2}), \\ E_n^{i+F_{n-2}} & = \overline{z}E_{n-3}^i & (i = 1, F_{n-3}), \\ E_n^{i+F_{n-1}} & = t_A + zE_{n-2}^i & (i = 1, F_{n-2}). \end{array} \tag{5}$$

Similarly, the associated recurrence for the bandwidths is given by

$$\begin{array}{ll} \Delta_n^i & = z\Delta_{n-2}^i, \\ \Delta_n^{i+F_{n-2}} & = \overline{z}\Delta_{n-3}^i, \\ \Delta_n^{i+F_{n-1}} & = z\Delta_{n-2}^i. \end{array} \tag{6}$$

We now give the quantitative consequences of the last three relations (4)–(6) upon the spectral properties.

As noted before [3] and as relation (5) makes evident, there is a natural coding of individual energy levels. Using relation (5), we can assign a set of indices $\{+\}$, $\{0\}$, or $\{-\}$ to each level according to its *path of trifurcations.* Therefore a typical level E_n^i has n_+, n_0, and n_- indices $(+,0,-)$; with the constraint $2(n_+ + n_-) + 3n_0 = n(\pm 1)$. For example, the lowest level is indexed by $\{-- -\cdots\}$ ($n_- = [n/2]$, $n_+ = n_0 = 0$) and the central level by $\{000\cdots\}$ ($n_- = n_+ = 0$, $n_0 = [n/3]$) [1,12]. From the indexation and relation (6), we see that the band associated with a level $E_n^i(n_+, n_0, n_-)$ has a width $\Delta_n^i(p,q) \approx z^p\overline{z}^q$ with $p = (n_+ + n_-)$ and $q = n_0$. Consequently, the number of bands of width $\Delta_n(p,q)$ is given by $N_n(p,q) = 2^p\binom{p+q}{p}$. These last two results allow us to calculate the exponents α and $g(\alpha)$ defined in the introduction [$\Delta_n^i = F_n^{-1/\alpha_i}$ and $N_n(p,q) = F_n^{g(\alpha)}$]. As shown in relation (7), in the quasiperiodic limit ($n \rightarrow \infty$), these exponents are functions of the parameter $x = p/n$, which varies continuously in $[0, 1/2]$ [6]:

$$\alpha(x) = \ln\omega/(x\ln z/\overline{z}^{2/3} + \ln\overline{z}^{1/3}),$$
$$g(\alpha(x)) = [x\ln 3x/2 - (1+x)\ln(1+x)^{1/3} + (1-2x)\ln(1-2x)^{1/3}]/\ln\omega. \tag{7}$$

From this last relation we can obtain two interesting properties of the spectrum. First, we observe that when $z = \overline{z}^{2/3}$ ($t_w/t_s = 1/8$), the exponent α is independent of x. As a consequence, the spectrum is a pure fractal with Hausdorff dimension $D_F = \alpha = \ln\omega^3/\ln\overline{z}$. In contrast, when, for example, $z > \bar{z}^{2/3}$, we see that the exponent α varies between $\alpha_{\min} = \ln\omega^3/\ln\bar{z}$ and $\alpha_{\max} = \ln\omega^2/\ln z$. Note that these two exponents correspond to the bandwidth associated with the central and edge levels, respectively. This property allows us to compare their values with the exact analytical result of Kohmoto [8,9]. From this we observe that our shrinking factors z and $\bar{z}$ are just the dominant terms in a t_w/t_s series expansion of the two more exact values $z_{\text{ex}} = 2/[\sqrt{(J-1)^2 - 4} + J - 1]$ and $\bar{z}_{\text{ex}} = 1/[\sqrt{1 + 4(I+1)^2} + 2(I+1)]$, where $I = \frac{1}{4}(t_w/t_s - t_s/t_w)^2$ and $J = 3 + \sqrt{25 + 16I}$.

So far, we have only analyzed the properties of individual bandwidths and levels. However, it is also possible and very instructive to study integrated quantities. We start with the spectral measure and a physical quantity closely related to it. The spectral measure $d\mu_n(E)$ of the Hamiltonian H_n is $d\mu_n(E) = \rho_n(E)\,dE$ where $\rho_n(E) = (1/F_n)\sum_{i=1}^{F_n}\delta(E - E_n^i)$ is the density of states. From this definition and relation (5) we deduce the following recurrence [10]:

$$d\mu_n(E) = \omega_n^2 d\mu_{n-2}\left(\frac{E + t_s}{z}\right) + \omega_n^3 d\mu_{n-3}\left(\frac{E}{\bar{z}}\right) + \omega_n^2 d\mu_{n-2}\left(\frac{E - t_s}{z}\right). \quad (8)$$

As an example of the application of relation (8), we calculate the large time average return probability defined by $p_n(t) = |\int_{-\infty}^{+\infty} e^{-iEt}\,d\mu_n(E)|^2 = 2\pi\tilde{\mu}(t)\tilde{\mu}^*(t)$ [4]. Using (8) we first deduce that $\tilde{\mu}_n(t) = 2\omega_n^2 \cos t_s t\, \tilde{\mu}_{n-2}(zt) + \omega_n^3\tilde{\mu}_{n-3}(\bar{z}t)$. Now, in the large time limit, we have on average $\langle\cos t_s t\rangle \sim 0$ and $\langle\cos^2 t_s t\rangle \sim 1/2$, and from this we immediately get

$$p_n(t) = 2\omega_n^4 p_{n-2}(zt) + \omega_n^6 p_{n-3}(\bar{z}t). \quad (9)$$

In the limit $n \rightarrow \infty$, we see that an invariant solution of relation (9) is $p^*(t) \sim t^{-\gamma}$ where the exponent γ is determined by $2\omega^4 z^{-\gamma} + \omega^6\bar{z}^{-\gamma} = 1$. As we now show, this exponent γ is one of the anomalous dimensions D_q that characterize the MF properties of the spectral measure. In our case, these nontrivial dimensions D_q are defined by the requirement that the partition function [5] $\Gamma_n(q, \tau = (q-1)D_q) = F_n^{-q}\sum_{i=1}^{F_n}(\Delta_n^i)^{-\tau}$ be stationary in the limit $n \rightarrow \infty$. Using relation (6) we get the following recurrence for the $\Gamma_n(q,\tau)$ [6]:

$$\Gamma_n(q,\tau) = 2\frac{\omega_n^{2q}}{z^\tau}\Gamma_{n-2}(q,\tau) + \frac{\omega_n^{3q}}{\bar{z}^\tau}\Gamma_{n-3}(q,\tau). \quad (10)$$

The stationary constraint then gives a self-consistent equation for the D_q,

$$2\omega^{2q}z^{(1-q)D_q} + \omega^{3q}\bar{z}^{(1-q)D_q} = 1. \quad (11)$$

From this last relation, we immediately see that the exponent γ previously defined is, in fact, equal to D_2. A second consequence of (11) is that the Hausdorff dimension $D_F = D_0$ is the solution of $2z^{D_F} + \bar{z}^{D_F} = 1$. To see further the use of relation (11) and the role of the D_q we calculate two other quantities of interest: the Lebesgue measure $B_n = \sum_{i=1}^{F_n}\Delta_n^i$, and the number of bands of width between Δ and $\Delta + d\Delta$, $dN_n(\Delta) = \sum_{i=1}^{F_n}\delta(\Delta - \Delta_n^i)\,d\Delta$. Using relation (6) we can easily deduce a recurrence relation for each of these quantities:

$$B_n = 2zB_{n-2} + \bar{z}B_{n-3}, \quad (12)$$

$$dN_n(\Delta) = 2dN_{n-2}\left(\frac{\Delta}{z}\right) + dN_{n-3}\left(\frac{\Delta}{\bar{z}}\right). \quad (13)$$

The first of these equations was partially guessed in [7] for a model on the Fibonacci chain; see also [10] for a very similar relation in the case of the Harper model. From Eq. (12), we can show that the large n behavior of B_n is $B_n \simeq B_0 F_n^{-\delta}$ where the exponent δ is related to the anomalous dimensions by $D_{-\delta} = 1/(1+\delta)$. Now, considering (13), we see that in the limit $n \rightarrow \infty$ a possible *invariant* form is given by $dN^*(\Delta) = \Delta^{-(1+\beta)}\,d\Delta$ with $\beta = D_F$. In view of relation (7), this simple *invariant* solution is quite surprising, and indeed its sense is not very clear. In fact, there are many other problems, concerning the way we take the limit $n \rightarrow \infty$, with distributions related to the bandwidths. All of these come from the fact that both the individual bandwidths and their degeneracy are much too strongly fluctuating variables that totally change when going from F_{n-1} to F_n. As a consequence, even if $dN^*(\Delta)$ vs Δ is an *invariant* of (13), the *function* $dN_n(\Delta)$ does not tend to $dN^*(\Delta)$ [13].

To complete the study of the spectral properties, we also look at the statistical properties of the gaps. Roughly speaking, a gap width is the distance between two levels. As a consequence, we might expect their distribution to be quite similar to that of the bandwidths. However, there is an important difference. The number of gaps of a chain F_n is $F_n - 1$, thus, $2(F_{n-2} - 1) + F_{n-3} - 1 = F_n - 3 < F_n - 1$. Looking at Fig. 1, the last inequality means that if we take only gaps coming from $zW_{n-2}(\pm t_s, t_s, t_w)$ and $\bar{z}W_{n-3}(0, t_s, t_w)$, we miss two gaps which are, in fact, precisely the biggest. Taking this into account, we see that the number of gaps of width between g and $g + dg$, $dN_n(g) = \sum_{i=1}^{F_n}\delta(g - g_n^i)\,dg$, obeys the following recurrence ($n \geq 3$):

$$dN_n(g) = 2dN_{n-2}\left(\frac{g}{z}\right) + dN_{n-3}\left(\frac{g}{\bar{z}}\right) + 2\delta(g - g_n^0)\,dg, \quad (14)$$

where the last term reintroduces the two largest gaps of width g_n^0 at each iteration. A complete description requires two other important remarks. The first is that the initial conditions are $dN_0(g) = 0$, $dN_1(g) = 0$, and $dN_2(g) = \delta(g - g_0)\,dg$. The second is that in the limit $n \rightarrow \infty$ the width g_n^0 tends to a fixed value $g^* = t_A - \frac{1}{2}(\bar{z}\Delta^* + z\Delta^*) = t_A(1 - \bar{z} - 2z)/(1 - z)$, where Δ^* is the width of the spectrum in this limit. This last remark allows one to replace the previous recurrence for $dN_n(g)$ by the following effective equation which describes the infinite size behavior more effectively:

$$dN_n(g) \simeq 2dN_{n-2}\left(\frac{g}{z}\right) + dN_{n-3}\left(\frac{g}{\bar{z}}\right) + 2\delta(g - g^*)\,dg. \quad (15)$$

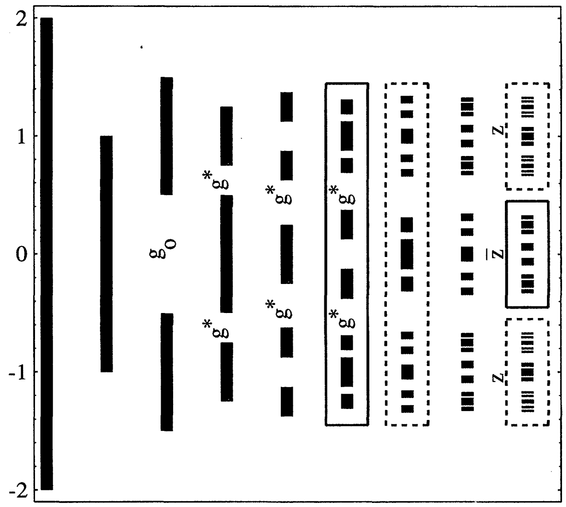

FIG. 1. Spectrum of the approximant Hamiltonian (H_n, F_n), $n \leq 8$ deduced from relation (5) for ($t_s = 1$, $t_w = 0.5$). The three initial conditions are ($H_0, F_0 = 1$, $t_i = t_s$), ($H_1, F_1 = 1$, $t_i = t_w$), and ($H_2, F_2 = 2$, $t_{2i} = t_s$, $t_{2i+1} = t_w$). z and $\overline{z}$ are the two shrinking factors. g_0 and g^* are the initial transient gap and the maximum stable gap, respectively.

As shown in Table I the iteration of relation (15), with the previous initial conditions, produces two kinds of gaps. The first kind corresponds to what we call the *transient* gaps. For a chain F_n, these gaps have widths of the form $g = z^p \overline{z}^q g_0$ with $2p + 3q = n - 2$ and $N_n(p, q) = 2^p \binom{p+q}{p}$ (the last two columns of Table I). These *transient* gaps are created by iteration of the initial condition $dN_2(g) = \delta(g - g_0)\, dg$, and their effective recurrence does not contain the last term of (15). For these reasons their distribution is strictly similar to that of bandwidths, and, in particular, the sum of their widths decreases like the spectrum Lebesgue measure B_n. In contrast, the second kind of gap is those created by the presence of the last term in relation (15) (the first two columns of Table I). As can be seen in Table I, if a gap of this kind opens for, say, a chain F_p, it persists for longer chains; it is *stable*. For such a chain F_n, these *stable* gaps have widths of the form $g = z^p \overline{z}^q g^*$ with $N_n(p, q) = 2^p \binom{p+q}{p}$, but now $2p + 3q$ takes all values between 0 and $n - 3$. Because of this difference the distribution of the *stable* gaps differs from that of the transient gaps in the following way: in a similar manner to (13), the absence of the last term yields an *invariant* solution to (15) of the form $dN^*(g) = g^{-(1+D_F)}\, dg$. However, similarly to bandwidths [13], for the *transient* gaps, $dN_n(g)$ does not tend to $dN^*(g)$. In contrast when the last term is present, that is for the *stable* gaps, then the function $dN_n(g)$ really tends to $dN^*(g) = g^{-(1+D_F)}\, dg$ over the whole interval $[0, g^*]$. Because of this property, in that case, we can also define a distribution which is of the form $P^*(g) = dN^*(g)/dg = g^{-(1+D_F)}$. An additional property of these *stable* gaps concerns the value G_n of the sum of their widths. From (15) we see that G_n obeys a recurrence relation $G_n = 2zG_{n-2} + \overline{z}G_{n-3} + 2g^*$, and from this we can deduce that, in contrast to B_n, G_n does not decrease with F_n but tends to a value G^* which is exactly equal to the spectrum width Δ^*.

TABLE I. Gap widths obtained for the first six iterations of relation (15). Stable gaps are written in the first column. Transient gaps are in the third column.

F_n	g/g^*	$N(g)$	g/g_0	$N(g)$
2	#	#	1	1
3	1	2	#	#
5	1	2	z	2
8	1 z	2 4	$\overline{z}$	1
13	1 z $\overline{z}$	2 4 2	z^2	4
21	1 z $\overline{z}$ z^2	2 4 2 8	$z\overline{z}$	4
34	1 z $\overline{z}$ z^2 $z\overline{z}$	2 4 2 8 8	z^3 $\overline{z}^2$	8 1
55	1 z $\overline{z}$ z^2 $z\overline{z}$ z^3 $\overline{z}^2$	2 4 2 8 8 16 2	z^2 $\overline{z}$	12

In conclusion, we have described as completely as possible the statistical properties of the energy spectrum of a tight-bonding Hamiltonian on the Fibonacci chain. We have compared several of the new predictions with numerical computations with satisfactory results [13]. As the text has made clear, our results qualitatively and quantitatively complete and unify previous works on similar models.

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[13] F. Piéchon (to be published).