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Spectrum and Extended States in a Harmonic Chain with Controlled Disorder: Effects of the Thue–Morse Symmetry

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Along the lines of previous work, we give the general framework together with a detailed and rigorous study of the spectrum and Born–von Karman eigenstates of a 1D harmonic chain with controlled disorder determined by the Thue–Morse sequence. The spectrum is a Cantor-like set; we prove numerically that its measure is zero and calculate its Bouligand–Minkowski dimension (box dimension). We prove that the value of the IDS on each of the gaps is $(2k+1)/(3 \cdot 2^p)$, with k and p integers. Finally, we also prove that points in a dense subset of the spectrum give rise to extended states, an exceptional property due to the symmetry of the Thue–Morse substitution which can have important applications to multilayered structures, and we illustrate this situation.

KEY WORDS: Controlled disorder; Thue–Morse sequence; spectrum; extended states; localization.

1. INTRODUCTION

The discovery of quasicrystals by Schechtman *et al.*[(1)] has opened a large new field of interest for both experimentalists and theoreticians. For the theoreticians there has been, for one, a renewed interest in the role of geometry in the description of quasicrystal order, somewhat along the lines of what had been done in the case of amorphous structures, using curved space models.[(2)] Also, this discovery raised anew the question of the

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possible existence, stability, and properties of a kind of order intermediate between crystallographic order and random disorder. Around quasicrystals soared a number of models having quasiperiodic controlled disorder, for example, using Fibonacci-type sequences, for reasons which are well known. Indeed, the word quasiperiodic does refer to both the Fourier spectrum of the Fibonacci sequence, generated by the substitution σ acting on the two-letter alphabet (0, 1),

$$\sigma(0) = 1$$
$$\sigma(1) = 10$$

and the X-ray diffraction spectra found in certain quasicrystalline samples.

Previous work[3,4] raised for the first time the question of the properties of a nonperiodic, nonquasiperiodic system having controlled—non-random—disorder described by sequences generated by substitutions or automata.[6] Underlying our choice of the Thue–Morse sequence[4,5]

$$\sigma(0) = 01$$
$$\sigma(1) = 10$$

was also the question of the possible role of the sequence Fourier transform, which, in the case of the Thue–Morse sequence, is singular continuous, at variance with the Fibonacci situation. This question, which is of great interest to experimentalists studying X-ray spectra of multilayer superlattices, is not addressed here.[7–10]

We now give a careful wording—although perhaps scholarly—of work which has been presented by both authors in various invited seminars and conferences in Europe and the USA during 1987 and 1988.[4,5]

In Section 2 we establish the rigorous framework of our study. In Section 3 we demonstrate certain properties of the general "quasi-alloy" chain and of the Thue–Morse situation. The associated dynamical system is studied in Section 4, where we prove that the value of the IDS on the gaps is $(2k+1)/(3 \cdot 2^p)$, k and p integers.

In Section 5 we calculate the Bouligand–Minkowski dimension (box dimension) of the spectrum for various mass ratios, and numerically demonstrate that it has zero Lebesgue measure. In Section 6 we give examples of the extended states, whose existence is rigorously proven in Section 3, and explain the role of the symmetry of the Thue–Morse substitution in their generation.

We now remind the reader that the study of our elastic chain trivially maps onto the study of (among others) the Schrödinger, tight-binding, and hopping conduction equations, whose properties have been investigated in controlled disorder situations, including the Thue–Morse sequence, by various authors.[11–14]

2. FRAMEWORK OF THE STUDY

2.1. Vibrations of Cyclic (or Born–von Karman) Chains

Let n be an integer larger than 1 and m a mapping from $\mathbb{Z}/nZ$ to $]0, +\infty[$. Let us consider the differential system

$$m(j)\frac{d^2X_j}{dt^2} = X_{j+1} + X_{j-1} - 2X_j \qquad (j \in \mathbb{Z}/n\mathbb{Z}) \tag{1}$$

where the unknown is a function X defined on $\mathbb{R}$ and which assumes its values in $l^2(\mathbb{Z}/n\mathbb{Z})$. This equation describes the vibrations of the masses $m_1,..., m_n$ linked by springs of identical strength which we can take equal to 1, forming a chain of length n.

Let $Y_j = X_j m_j^{1/2}$. We then get the equivalent system

$$\frac{d^2Y_j}{dt^2} = \frac{Y_{j+1}}{(m_j m_{j+1})^{1/2}} - 2\frac{Y_j}{m_j} + \frac{Y_{j-1}}{(m_{j-1}m_j)^{1/2}}, \qquad (j \in \mathbb{Z}/n\mathbb{Z}) \tag{2}$$

Thus we are led to study the operator T on $l^2(\mathbb{Z}/n\mathbb{Z})$ so defined

$$(Ty)_j = -\frac{y_{j-1}}{(m_{j-1}m_j)^{1/2}} + \frac{2y_j}{m_j} - \frac{y_{j+1}}{(m_j m_{j+1})^{1/2}}$$

It is easily checked that T is a Hermitian operator. Moreover, it is positive because the scalar product

$$\langle Ty, y\rangle = \sum_{j \in \mathbb{Z}/n\mathbb{Z}} \left| \frac{y_j}{m_j^{1/2}} - \frac{y_{j+1}}{(m_{j+1})^{1/2}} \right|^2$$

is positive.

Any solution of the system (2) is therefore a linear combination of solutions of the form $ye^{i\omega t}$, where ω^2 (λ in our notation) is an eigenvalue of T, and y a corresponding eigenvector.

Here is an equivalent formulation of the problem: to determine a nonnegative number λ such that there exists a nonzero vector in $l^2(\mathbb{Z}/n\mathbb{Z})$ satisfying

$$-\lambda m_j x_j = x_{j+1} - 2x_j + x_{j-1} \qquad (j \in \mathbb{Z}/n\mathbb{Z}) \tag{3}$$

which can be written in the following way (transfer matrix formalism):

$$\begin{pmatrix} x_{j+1} \\ x_j \end{pmatrix} = \begin{pmatrix} 2-\lambda m_j & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_j \\ x_{j-1} \end{pmatrix} \quad (j \in \mathbb{Z}/n\mathbb{Z}) \tag{4}$$

Let us denote by $P_n(\lambda)$ the following product:

$$\begin{pmatrix} 2-\lambda m_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2-\lambda m_{n-1} & -1 \\ 1 & 0 \end{pmatrix} \cdots \begin{pmatrix} 2-\lambda m_2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2-\lambda m_1 & -1 \\ 1 & 0 \end{pmatrix} \tag{5}$$

Then, for Born–von Karman or cyclic boundary conditions, λ is a solution to the problem if and only if 1 is an eigenvalue of $P_n(\lambda)$. Then

$$\begin{pmatrix} x_1 \\ x_0 \end{pmatrix}$$

is a corresponding eigenvector. But, as the determinant of $P_n(\lambda) = 1$, the condition on λ can be written $\operatorname{Tr} P_n(\lambda) = 2$ (where, as usual, $\operatorname{Tr} A$ stands for the trace of the matrix A).

Moreover, for any fixed λ, the space of x's satisfying (3) has dimension 2 at most. As a consequence, the eigenvalues of T have a multiplicity 2 at most and λ is a double eigenvalue if and only if $P_n(\lambda) = I$.

2. Infinite Chains

We are given the sequence $(m(j))_{j \in \mathbb{Z}}$ of masses linked as previously by springs of strength 1 and want to study the vibrations of this system. In other words, we want to study the spectrum of the following operator T on $l^2(\mathbb{Z})$:

$$(Tx)_j = -\frac{x_{j+1}}{(m_j m_{j+1})^{1/2}} + \frac{2x_j}{m_j} - \frac{x_{j-1}}{(m_j m_{j-1})^{1/2}} \quad (j \in \mathbb{Z}) \tag{6}$$

As previously, T is a positive Hermitian operator.

The purpose of this paper is to determine the spectrum and modes of T when the sequence $\{m_j\}$ has the particular form of the Thue–Morse sequence. This will be done by approximating T by operators associated with cyclic chains as described above.

2.3. An Approximation Property

Let $\{l_n\}_{n \geqslant 1}$ be an increasing sequence of integers larger than 2. For any $n \geqslant 1$ we are given two sequences $\{a_{n,j}\}_{j \in \mathbb{Z}}$ and $(b_{n,j})_{j \in \mathbb{Z}}$ of real numbers, both periodic with period l_n. Besides, we suppose that there is a uniform bound M for these sequences: for any j and n, $|a_{n,j}| \leqslant M$ and $|b_{n,j}| \leqslant M$.

Furthermore, we suppose that there exists an increasing sequence $\{t_n\}_{n \geqslant 1}$ of nonnegative integers such that $l_n - t_n$ tends to infinity and such that, for any $j \in \mathbb{Z}$, both sequences $\{a_{n,j+t_n}\}_{n \geqslant 0}$ and $\{b_{n,j+t_n}\}_{n \geqslant 0}$ have limits, which we denote by a_j and b_j, respectively.

Let us denote by T_n and T the following operators of $l^2(\mathbb{Z}/l_n\mathbb{Z})$ and $l^2(\mathbb{Z})$ respectively:

$$(T_n x)_j = a_{n,j} x_{j-1} + b_{n,j} x_j + a_{n,j+1} x_{j+1} \qquad (j \in \mathbb{Z}/l_n\mathbb{Z}) \tag{7}$$

$$(Tx)_j = a_j x_{j-1} + b_j x_j + a_{j+1} x_{j+1} \qquad (j \in \mathbb{Z}) \tag{8}$$

It is easily checked that these operators are Hermitian. Let us denote by Λ_n and Λ their respective spectra. We have the following result.

Lemma:

$$\Lambda \subset \bigcap_{n \geqslant 1} \overline{\bigcup_{m \geqslant n} \Lambda_m}$$

Proof. Let S_n be the following operator from $l^2(\mathbb{Z})$ to $l^2(\mathbb{Z}/l_n\mathbb{Z})$:

$$(S_n x)_j = x_{j-t_n} \qquad \text{for} \quad 0 \leqslant j < l_n$$

Obviously, we have $\|S_n x\| \leqslant \|x\|$ and $\lim_{n \to \infty} \|S_n x\| = \|x\|$.

Let J_n be the operator from $l^2(\mathbb{Z}/l_n\mathbb{Z})$ to $l^2(\mathbb{Z})$ so defined,

$$(J_n(x))_j = \begin{cases} 0 & \text{if} \quad j < -t_n \text{ or } j \geqslant l_n - t_n \\ x_{j+t_n} & \text{if} \quad -t_n \leqslant j < -t_n + l_n \end{cases} \tag{9}$$

Obviously, we have $\|J_n x\| = \|x\|$. A simple but tedious calculation shows that we have

$$\begin{aligned} &\|(T - J_n T_n S_n)\, x\|^2 \\ &\quad \leqslant 6M^2 \Bigg(\sum_{j \leqslant 2 - t_n} |x_j|^2 + \sum_{j \geqslant l_n - t_n - 2} |x_j|^2 \Bigg) \\ &\quad + \sum_{-t_n < j < l_n - t_n - 1} |(a_j - a_{n,j+t_n})\, x_{j-1} \\ &\quad + (b_j - b_{n,j+t_n})\, x_j + (a_{j+1} - a_{n,j+1+t_n})\, x_{j+1}| \end{aligned} \tag{10}$$

Therefore the operators $T - J_n T_n S_n$ and $Id - J_n S_n$ tend strongly to 0.

Let us now consider a number λ outside the set

$$\bigcap_{n \geqslant 1} \overline{\bigcup_{m \geqslant n} \Lambda_m}$$

We have to show that λ does not belong to Λ. There exists $n_0 > 0$ and $\varepsilon > 0$ such that dist $(\lambda, \bigcup_{m \geqslant n_0} \Lambda_m) \geqslant \varepsilon$. Therefore, for any $n \geqslant n_0$, we have $\|(T_n - \lambda)^{-1}\| \leqslant \varepsilon^{-1}$.

Let us first show that $T - \lambda$ is one-to-one. Let us consider $x \in l^2(\mathbb{Z})$ such that $Tx - \lambda x = 0$. As we have noted, $\|Tx - \lambda x - J_n(T_n - \lambda) S_n x\|$ tends to zero as n tends to infinity. We thus have

$$\lim_{n \to \infty} \|J_n(T_n - \lambda) S_n x\| = 0, \qquad \text{i.e.,} \qquad \lim_{n \to \infty} \|(T_n - \lambda) S_n x\| = 0 \quad (11)$$

But $\|S_n x\| \leqslant \varepsilon^{-1} \|(T - \lambda) S_n x\|$; therefore $\|x\| = \lim \|S_n x\| = 0$.

We can now complete the proof. Let y be an element of $l^2(\mathbb{Z})$. For each nonnegative integer n, let us set $x^{(n)} = J_n(T_n - \lambda)^{-1} S_n y$. If $n \geqslant n_0$, we have $\|x^{(n)}\| \leqslant \varepsilon^{-1} \|y\|$. Therefore, one can extract from the sequence $\{x^{(n)}\}$ a subsequence which converges weakly toward a vector x. It results from the definition of $x^{(n)}$ that, for $-t_n < j < l_n - t_n - 1$, one has

$$a_{n,j+t_n} x_{j-1}^{(n)} + (b_{n,j+t_n} - \lambda) x_j^{(n)} + a_{n,j+1+t_n} x_{j+1}^{(n)} = y_j \qquad (12)$$

Taking the limit as n goes to infinity, we get $(T - \lambda) x = y$. This shows that $T - \lambda$ is invertible and that $\|(T - \lambda)^{-1}\| \leqslant \varepsilon^{-1}$. QED

3. THE "QUASI-ALLOY" CHAIN PROPERTIES

3.1. Substitutions

Let A be a finite set called an alphabet. A word constructed over A is a finite sequence $x = x_1 x_2 \cdots x_n$ of elements of A. The length n of the word x is also denoted by $|x|$. The set of words over A is denoted A^* (notice that, unlike the usual situation, the empty word is not considered, because it is not needed in the sequel). The concatenation of two words is the operation, denoted multiplicatively, consisting in putting these words end to end. Endowed with this operation, A^* is a semigroup.

A substitution over the alphabet A is a mapping σ from A to A^*. Such a mapping σ defines an endomorphism of A^*, still denoted by σ, in the following way:

$$\sigma(x_1, x_2, \ldots, x_n) = \sigma(x_1)\, \sigma(x_2) \cdots \sigma(x_n)$$

More complex substitution rules have been studied in [15].

A substitution is said to be irreducible if, for any a and b in A, there exists an integer n such that the word $\sigma^n a$ contains the letter b. In the sequel we will be dealing only with irreducible substitutions such that, for one letter a (and therefore for any letter) the length of $\sigma^n a$ goes to infinity with n.

If $x = x_1 x_2 \cdots x_n$ is a word and if t is a nonnegative integer, $\tau_t x$ stands for the sequence $\{x_{j+t}\}_{1-t \leqslant j \leqslant n-t}$.

A sequence $x = \{x_j\}_{j \in \mathbb{Z}} \in A^{\mathbb{Z}}$ is said to be substitutive if there exists a substitution σ over the alphabet A, a letter a in A, and two increasing sequences $\{t_n\}_{n \geqslant 0}$ and $\{p_n\}_{n \geqslant 0}$ of positive integers such that:

1. $\lim_{n \to \infty}(|\sigma^{p_n} a| - t_n) = +\infty$.
2. For any $j \in \mathbb{Z}$, $(\tau_{t_n} \sigma^{p_n} a)_j = x_j$ as soon as n is large enough. In other words, the sequence x is the weak limit of $\tau_{t_n} \sigma^{p_n} a$.

3.2. Definition of the "Quasi-alloy" Chain

We are given an alphabet A, a mapping m from A to the positive real numbers, and a substitutive sequence $\{\varepsilon_j\}_{j \in \mathbb{Z}}$. At each site j in $\mathbb{Z}$ is a mass $m(\varepsilon_j)$; neighboring masses are linked by springs of constant strength 1. We study the spectrum and the corresponding eigenstates of the chain operator T so defined

$$(Tx)_j = -\frac{x_{j-1}}{[m(\varepsilon_{j-1})\, m(\varepsilon_j)]^{1/2}} + \frac{2x_j}{m(\varepsilon_j)} - \frac{x_{j+1}}{[m(\varepsilon_j)\, m(\varepsilon_{j+1})]^{1/2}} \tag{13}$$

If we have $\varepsilon = \lim_{n \to \infty} \tau_{t_n} \sigma^{p_n} a$, we shall denote by T_n the operator on $l^2(\mathbb{Z}/|\sigma^{p_n} a|\, \mathbb{Z})$ associated with the sequence

$$\{m((\sigma^{p_n} a)_j)\}_{1 \leqslant j \leqslant |\sigma^{p_n} a|}$$

extended by periodicity (with period $|\sigma^{p_n} a|$) to the whole $\mathbb{Z}$).

Let us denote by Λ the spectrum of T and by Λ_n the spectrum of T_n. We have already shown that we have

$$\Lambda \subset \bigcap_{n \geqslant 1} \overline{\bigcup_{m \geqslant n} \Lambda_m}$$

We are going to show that, for the Thue–Morse substitution defined below, we have

$$\Lambda = \bigcap_{n \geqslant 0} \overline{\bigcup_{m \geqslant n} \Lambda_m}$$

Before doing that, we give some clues on the general case.

3.3. Renormalization of Traces: The General Trace Mapping

For each $\alpha \in A$ and $\lambda \in \mathbb{R}$, let us denote by $M(\alpha, \lambda)$ the matrix

$$\begin{pmatrix} 2-\lambda m(\alpha) & -1 \\ 1 & 0 \end{pmatrix}$$

and by $P_n(\lambda)$ the product

$$P_n(\lambda) = M((\sigma^n a)_{|\sigma^n a|}, \lambda)\, M((\sigma^n a)_{|\sigma^n a|-1}, \lambda) \\ \times \cdots M((\sigma^n a)_2, \lambda)\, M((\sigma^n a)_1, \lambda) \tag{14}$$

As we have already explained, the elements of Λ_n are the roots of the equation $\operatorname{Tr} P_{p_n}(\lambda) = 2$, because of the Born–von Karman boundary conditions.

Computing this trace in the general case is not an easy task: one has to iterate a polynomial mapping from the space $\mathbb{R}^{4\#A}$ into itself. Nevertheless, in the case where the cardinality $\#A$ of A is 2, it suffices to iterate a polynomial mapping from $\mathbb{R}^3$ into $\mathbb{R}^3$, as shown in ref. 16. Besides, in certain cases, including the one we are going to study, everything can be done in $\mathbb{R}^2$.

In view of an easier reading, let us recall the result of ref. 16. Let σ be a substitution on the two-letter alphabet $A = \{0, 1\}$, and $M = (M_0, M_1)$ a couple of 2×2 matrices with determinant 1. Let J_M denote the mapping from A^* to the set of 2×2 matrices defined by the properties

$$J_M(0) = M_0, \qquad J_M(1) = M_1$$

and, if w_1 and w_2 are two words,

$$J_M(w_1 w_2) = J_M(w_2)\, J_M(w_1) \tag{15}$$

When $M_0 = M(0, \lambda)$ and $M_1 = M(1, \lambda)$ one has $J_M(\sigma^n a) = P_n(\lambda)$. Let us also denote by $\sigma(M)$ the couple $(J_M(\sigma(0)), J_M(\sigma(1)))$. Then, for any word w, we have

$$J_M(\sigma w) = J_{\sigma M}(w) \tag{16}$$

In ref. 16 it is proved that there exists a polynomial mapping χ from $\mathbb{R}^3$ to $\mathbb{R}^3$ such that, for any M, we have

$$(\tfrac{1}{2}\operatorname{Tr} J_M(\sigma(0)), \tfrac{1}{2}\operatorname{Tr} J_M(\sigma(1)), \tfrac{1}{2}\operatorname{Tr} J_M(\sigma(01))) \\ = \chi[\tfrac{1}{2}\operatorname{Tr} J_M(0), \tfrac{1}{2}\operatorname{Tr} J_M(1), \tfrac{1}{2}\operatorname{Tr} J_M(01)] \tag{17}$$

Therefore, one has

$$\begin{aligned}&(\tfrac{1}{2}\operatorname{Tr} J_M(\sigma^n(0)); \tfrac{1}{2}\operatorname{Tr} J_M(\sigma^n(1)), \tfrac{1}{2}\operatorname{Tr} J_M(\sigma^n(01)))\\ &\qquad = \chi^n(\tfrac{1}{2}\operatorname{Tr} J_M(0), \tfrac{1}{2}\operatorname{Tr} J_M(1), \tfrac{1}{2}\operatorname{Tr} J_M(01))\end{aligned} \tag{18}$$

In other terms,

$$\begin{aligned}&\operatorname{Tr}(J_A\sigma^n(0))\\ &\qquad = \text{twice the first component of}\\ &\qquad\quad \chi^n(\tfrac{1}{2}\operatorname{Tr} J_M(0), \tfrac{1}{2}\operatorname{Tr} J_M(1), \tfrac{1}{2}\operatorname{Tr} J_M(01))\end{aligned} \tag{19}$$

The trace mapping found in the Fibonacci case[17] is a particular case of this theorem.

3.4. The Thue–Morse Case

This is the case, which we shall consider from now on, of the substitution σ defined as

$$\begin{aligned}\sigma(0) &= 01\\ \sigma(1) &= 10\end{aligned} \tag{20}$$

There exist two kinds of masses m_0 and m_1 and we shall work at fixed mass ratio $m_1/m_0 = \rho$ (with $\rho < 1$ without loss of generality).

Let us show in this particular case how one can determine the function χ. Let us set

$$a = \tfrac{1}{2}\operatorname{Tr} M_0, \qquad b = \tfrac{1}{2}\operatorname{Tr} M_1, \qquad c = \tfrac{1}{2}\operatorname{Tr} M_1 M_0 \tag{21}$$

Then,

$$\begin{aligned}J_M(\sigma(0)) &= M_1 M_0\\ J_M(\sigma(1)) &= M_0 M_1\\ J_M(\sigma(01)) &= M_0 M_1 M_1 M_0\end{aligned} \tag{22}$$

Therefore we have

$$\tfrac{1}{2}\operatorname{Tr} J_M(\sigma(0)) = \tfrac{1}{2}\operatorname{Tr} J_M(\sigma(1)) = c \tag{23}$$

But $M_0 M_1 M_1 M_0$ has the same trace as $M_0^2 M_1^2$, which is equal to $(2aM_0 - I)(2bM_1 - I)$, in virtue of the Cayley–Hamilton theorem. So

$$\tfrac{1}{2}\operatorname{Tr} M_0 M_1 M_1 M_0 = 4abc - 2a^2 - 2b^2 + 1 \tag{24}$$

It means exactly that $\chi(a, b, c) = (c, c, 4abc - 2a^2 - 2b^2 + 1)$. In this particular case, to compute χ^{n+1} $(n \geqslant 1)$, one has in fact to iterate a function of two variables:

$$\tilde{\chi}(x, y) = (y, 1 - 4x^2(1 - y)) \tag{25}$$

Indeed, if we set $(x, x, y) = \chi(a, b, c)$, we have

$$\chi^{n+1}(a, b, c) = (u, u, v) \tag{26}$$

where $(u, v) = \tilde{\chi}^n(x, y)(n \geqslant 0)$.

In fact, it will be more convenient to use, instead of $\tilde{\chi}$, one of its conjugates: by changing variables (y changed into $1 - y$), $\tilde{\chi}$ becomes the following function:

$$\Phi(x, y) = (1 - y, 4x^2 y) \tag{27}$$

Therefore, if we set $(x, x, 1 - y) = \chi(a, b, c)$, we have

$$\chi^{n+1}(a, b, c) = (u, u, 1 - v) \tag{28}$$

where $(u, v) = \Phi^n(x, y)$.

In the present case,

$$M_i = \begin{pmatrix} 2 - \lambda m_i & -1 \\ 1 & 0 \end{pmatrix} \qquad \text{for} \quad i = 0, 1$$

Let us set

$$\begin{aligned} a_i(\lambda) &= 1 - \lambda m_i/2 \text{ or } a_i(\lambda) \\ &= \tfrac{1}{2} \operatorname{Tr} M_i \qquad \text{for} \quad i = 0, 1 \\ \xi(\lambda) &= \tfrac{1}{2} \operatorname{Tr} M_1(\lambda)\, M_0(\lambda) \\ &= 2a_0(\lambda)\, a_1(\lambda) - 1 \\ \eta(\lambda) &= 1 - \tfrac{1}{2} \operatorname{Tr}[M_0(\lambda)\, M_1(\lambda)\, M_1(\lambda)\, M_0(\lambda)] \\ &= 2[a_0(\lambda) + a_1(\lambda)]^2 - 8[a_0(\lambda)\, a_1(\lambda)]^2 \end{aligned} \tag{29}$$

Then, for any $n \geqslant 0$, we have the trace mapping

$$\tfrac{1}{2} \operatorname{Tr} P_{n+1}(\lambda) = \text{first component of } \Phi^n(\xi(\lambda), \eta(\lambda)) \tag{30a}$$

or, as already written in ref. 2, with $x_n = \frac{1}{2} \operatorname{Tr} P_n(\lambda)$,

$$x_{n+1} = 4x_n x_{n-1}^2 - 4x_{n-1}^2 + 1 \qquad (n > 2) \tag{30b}$$

Let us now define a parametrized curve Ω: $x=\xi(\lambda)$, $y=\eta(\lambda)$ $(\lambda \geqslant 0)$. It is shown on Fig. 1 in the case $\rho = m_1/m_0 = 0.6$. The parabola $\mathscr{P}$ which also appears on this figure corresponds to $m_0 = m_1$ or $\rho = 1$ and has the equation $y = 2(1-x^2)$. Let us set $E_n = \Phi^{-n}(x=1)$ (the inverse images, under Φ^n, of the straight line the equation of which is $x=1$).

Then Λ_{n+1} is the set of parameters corresponding to the intersection points of Ω and E_n.

Let us now state the results.[5]

Theorem. In the Thue–Morse case we have

1. For $n \geqslant 2$, $\Lambda_{n+1} \supset \Lambda_n$.

2. If $\lambda \in \bigcup_{n \geqslant 3} \Lambda_n \backslash \Lambda_2$, then the operator T has a dimension 2 vector space of extended states associated with λ. And if $\lambda \in \Lambda_2$, there is one extended state.

3. $\Lambda = \overline{\bigcup_{n \geqslant 3} \Lambda_n}$

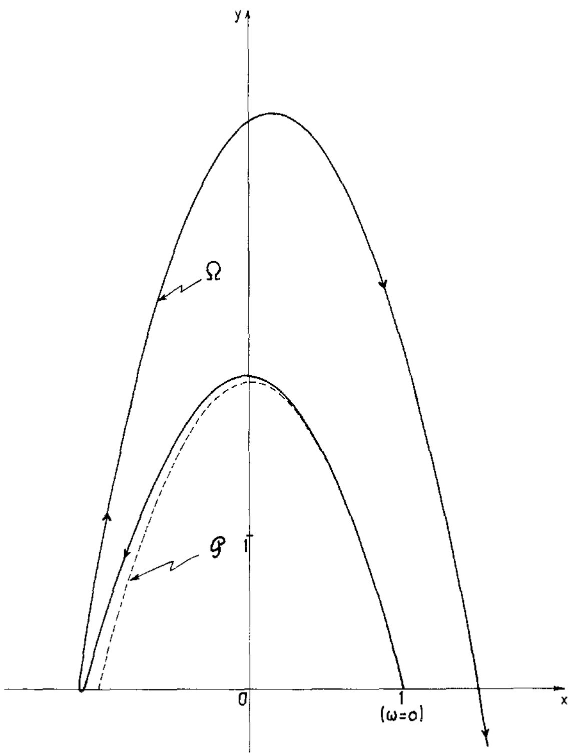


Fig. 1. The curve Ω in the (xy) plane as defined in the text for $\rho = 0.6$. The parabola $\mathscr{P}$ has equation $y = 2(1-x^2)$.

Furthermore, when $t_n = 2^{2n}$ and $p_n = 2n+2$ (see Section 3.1), Delyon[18] has proved that the corresponding operator T has no eigenvalue, a situation also found in ref. 19.

The proofs are organized as follows. Assertions 1 and 2 will be proved in the next paragraph. Then, assertion 3 follows from 2 and the lemma of Section 2.3.

3.5. Study of Λ_n

We have $E_1 = \Phi^{-1}(x=1) = \{y=0\}$ and $E_2 = \Phi^{-1}(E_1) = \{x=0\} \cup \{y=0\}$.

Therefore, we have, for $n \geqslant 0$,

$$E_{n+2} = \Phi^{-n}(E_2) = \Phi^{-n}(E_1) \cup \Phi^{-n}(x=0) = E_{n+1} \cup \Phi^{-n}(x=0)$$

So the first assertion is proved.

But, in fact, the equation of E_2 is $4x^2y=0$, which means that when decomposing the algebraic manifold E_2, the component E_1 is simple, while the component $\{x=0\}$ has multiplicity 2. By taking successive inverse images under Φ, we get that any eigenvalue in $\Lambda_n \backslash \Lambda_2$ (the complement of Λ_2 in Λ_n) has multiplicity 2. This therefore means that if $\lambda \in \Lambda_n \backslash \Lambda_2$, we then have $P_n(\lambda) = I$ (for $n \geqslant 3$).

Let us denote by $\tilde{P}_n(\lambda)$ the product of matrices obtained from the word $\sigma^n 1$ instead of $\sigma^n 0$ (this just means flipping 0's and 1's). In the terms of Section 3.3,

$$\tilde{P}_n(\lambda) = J_m(\sigma^n(1)) \tag{31}$$

As noted in that section, for $n \geqslant 2$, one has

$$\operatorname{Tr} \tilde{P}_n(\lambda) = \operatorname{Tr} P_n(\lambda) \tag{32a}$$

[because $\chi(a, b, c) = (u, u, v)$]. Therefore, when $\lambda \in \Lambda_n \backslash \Lambda_2$ we also have $\tilde{P}_n(\lambda) = I$. Also, it trivially follows from the definition of $\tilde{P}_n(\lambda)$ that

$$P_{n+1}(\lambda) = P_n(\lambda)\, \tilde{P}_n(\lambda) \tag{32b}$$

Let λ be in $\Lambda_n \backslash \Lambda_2$ for one $n > 2$. The sequence $\{\varepsilon_j\}_{j \in \mathbb{Z}}$ we are considering is built up out of the two blocks $\sigma^n 0$ and $\sigma^n 1$ which repeat according to a sequence of the same kind. We have just proved that the products of matrices $P_n(\lambda)$ and $\tilde{P}_n(\lambda)$, which are associated with $\sigma^n 0$ and $\sigma^n 1$, are both equal to unity. So, if we consider any sequence $\{x_j\}_{j \in \mathbb{Z}}$ satisfying the recursion relations,

$$\lambda m_{\varepsilon_j} x_j = 2x_j - x_{j+1} - x_{j-1} \qquad (j \in \mathbb{Z}) \tag{33}$$

it is built up out of two sequences of length 2^n which repeat in the same way as the blocks $\sigma^n 0$ and $\sigma^n 1$ do. *Therefore, such a sequence is bounded, so λ is in the spectrum of T and the corresponding eigenstates are extended.* This will be developed and illustrated below.

Let us now suppose that λ is in Λ_2. We then have

$$\operatorname{Tr} P_2(\lambda) = \operatorname{Tr} \tilde{P}_2(\lambda) = \operatorname{Tr} P_1(\lambda)\, \tilde{P}_1(\lambda) = 2 \tag{34}$$

Any of these matrices has determinant 1, has 1 for a double eigenvalue, and is not diagonalizable. It is then easy to show that the matrices $P_2(\lambda)$ and $\tilde{P}_2(\lambda)$ share their eigendirection. So the above analysis applies, but this time there is only one, up to a multiplicative constant, bounded sequence satisfying (33). So, assertion 2 is proved.

4. STUDY OF THE DYNAMICAL SYSTEM ASSOCIATED WITH THE TRACE MAPPING

4.1. Reduction of the Domain

Obviously, the x axis as well as both closed half-planes it delimits are invariant sets under Φ [recall that $\Phi(x, y) = (X, Y) = (1 - y, 4x^2 y)$, Eq. (27)].

If we set $X = 1 - y$ and $Y = 4x^2 y$, we get

$$Y - 2(1 - X^2) = 2y[y - 2(1 - x^2)]$$

So the parabola $\mathscr{P}$, the equation of which is $y = 2(1 - x^2)$, is also invariant under Φ (see Fig. 1). Moreover, the closed set

$$\mathscr{E} = \{(x, y) \in \mathbb{R}^2;\ y \geqslant 0 \quad \text{and} \quad y \geqslant 2(1 - x^2)\} \tag{35}$$

is also invariant under Φ. It is represented in Fig. 2.

The curve Ω lies outside $\mathscr{P}$. Indeed, we have

$$\eta_1(\lambda)^2 - 2[1 - \xi_1(\lambda)^2] = 2[a_0(\lambda) - a_1(\lambda)]^2$$

[see formulas (29)], which is positive for $m_0 \neq m_1$ and $\lambda \neq 0$.

Also note that the set $\{(x, y);\ y < 0 \text{ and } x \neq 0\}$ is invariant under Φ; so it does not intersect the inverse image of $\{y = 1\}$ by Φ^n for any n.

It results from the above that the intersection of Ω and of $\Phi^{-n}\ (x = 1)$ is contained in $\mathscr{E}$ for any $n \geqslant 0$.

So, from now on, we shall consider the mapping $\tilde{\Phi}$ from $\mathscr{E}$ to $\mathscr{E}$ which Φ defines by restriction.

Set

$$A_t = (\cos \pi t,\ 2 \sin^2 \pi t) \tag{36}$$

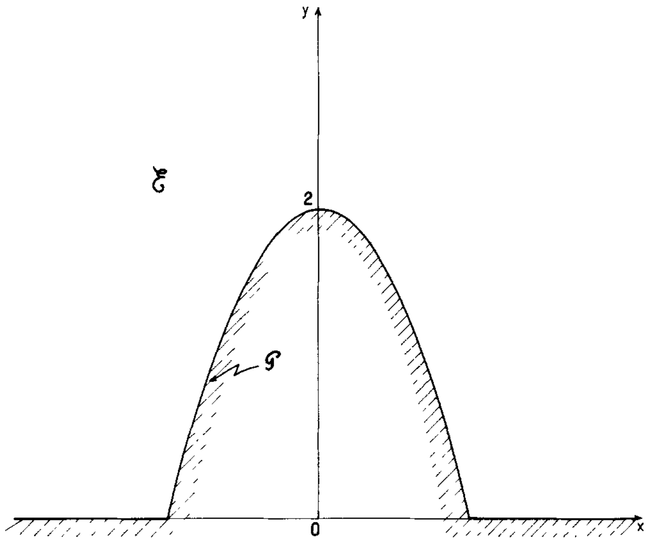


Fig. 2. The invariant closed set $\mathscr{E}$ as defined by Eq. (35).

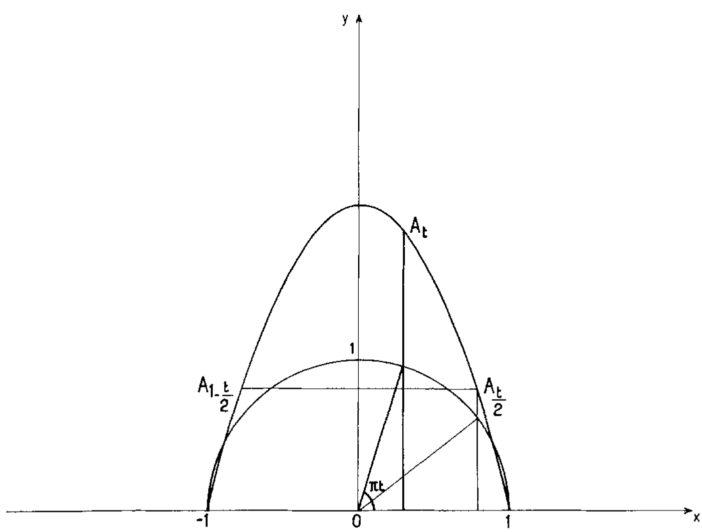


Fig. 3. Definition of the parametrization of the parabola $\mathscr{P}$ by A_t and the effect of ψ_0 and ψ_1 (see text).

When t varies from 0 to 1, A_t goes along the arc of parabola $\mathscr{P}$ which is part of the boundary of $\mathscr{E}$ (Fig. 3). Also note that the change of variables $X = 1 - y$ and $Y = 4x^2 y$ yields

$$(X, Y) = \tilde{\Phi}(x, y) = (\cos 2\pi t, 2\sin^2 2\pi t)$$

$$\Phi(A_t) = \begin{cases} A_{2t} & \text{if} \quad 0 \leqslant t \leqslant 1/2 \\ A_{2-2t} & \text{if} \quad 1/2 \leqslant t \leqslant 1 \end{cases} \tag{37}$$

of course,

$$\tilde{\Phi}^n(\cos \pi\tau, 2\sin^2 \pi t) = (\cos 2^n\pi t, 2\sin^2 2^n\pi t)$$

4.2. Inversion of $\tilde{\Phi}$

The following facts are easily checked:

$$\Phi(\mathscr{E}) = (\mathscr{E} \cap \{x < 1\}) \cup \{(1, 0)\}$$

$$\tilde{\Phi}^{-1}(1, 0) = \{y = 0\}$$

Moreover, if $(a, b) \in \mathscr{E} \cap \{x < 1\}$, then (a, b) has two inverse images by $\tilde{\Phi}$, $(\pm 1/2[b/(1-a)]^{1/2}, 1-a)$. So the two branches of the inverse map of $\tilde{\Phi}$ are so defined on $\mathscr{E} \cap \{x < 1\}$:

$$\begin{aligned} \psi_0(a, b) &= \left(\frac{1}{2}\left(\frac{b}{1-a}\right)^{1/2}, 1-a\right) \\ \psi_1(a, b) &= \left(-\frac{1}{2}\left(\frac{b}{1-a}\right)^{1/2}, 1-a\right) \end{aligned} \tag{38a}$$

On the parabola $\mathscr{P}$, one has, with $(a, b) = (\cos \pi t, 2\sin^2 \pi t)$,

$$\begin{aligned} \psi_0(a, b) &= \left(\cos\frac{\pi t}{2}, 2\sin^2\frac{\pi t}{2}\right) \\ \psi_1(a, b) &= \left(-\cos\frac{\pi t}{2}, 2\sin^2\frac{\pi t}{2}\right) \\ &= \left(\cos \pi\left(1 - \frac{t}{2}\right), 2\sin^2 \pi\left(1 - \frac{t}{2}\right)\right) \\ &\ \ \vdots \end{aligned} \tag{38b}$$

Let us now summarize the properties of ψ_0 and ψ_1:

$$\begin{aligned}
&\tilde{\Phi}(\psi_i(a,b)) = (a,b) \qquad \text{for} \quad i=0,1 \\
&\psi_0(a,b) \neq \psi_1(a,b) \qquad \text{if} \quad b \neq 0 \\
&\tilde{\Phi}(x,y) = (a,b) \qquad \text{for} \quad (a,b) \in \{\mathscr{E} \cap \{a<1\}\} \\
&\qquad \text{means} \quad (x,y) = \psi_0(a,b) \quad \text{or} \quad (x,y) = \psi_1(a,b) \\
&\psi_0(\tilde{\Phi}(x,y)) = (|x|, y) \\
&\psi_1(\tilde{\Phi}(x,y)) = (-|x|, y) \\
&\psi_0(A_t) = A_{t/2} \\
&\psi_1(A_t) = A_{1-t/2}
\end{aligned} \tag{39}$$

These properties are shown in Fig. 3.

4.3. The Polynomials Q_n

Let us define a sequence of polynomials in two variables by the recursion

$$\begin{aligned}
Q_0(x,y) &= 1-x \\
Q_1(x,y) &= y \\
Q_{j+2}(x,y) &= 4[1-Q_j(x,y)]^2\, Q_{j+1}(x,y) \qquad \text{for} \quad j \geqslant 0
\end{aligned} \tag{40}$$

It is easy to check that

$$\tilde{\Phi}^j(x,y) = (1-Q_j(x,y), Q_{j+1}(x,y)) \qquad \text{for} \quad j \geqslant 1 \tag{41}$$

By induction one can obtain

$$\begin{aligned}
d^\circ Q_j &= [2^{j+1} + (-1)^j]/3 \\
d_x^\circ Q_j &= [2^j + 2(-1)^j]/3 \\
d_y^\circ Q_j &= [2^j - (-1)^j]/3
\end{aligned} \tag{42}$$

where d°, d_x°, and d_y° stand, respectively, for the total degree, the degree with respect to x, and the degree with respect to y.

In the same way, if we define the polynomial $\tilde{Q}_j$ by the formula $\tilde{Q}_j(\lambda) = Q_j(\eta_1(\lambda), \xi_1(\lambda))$, we have

$$d^\circ \tilde{Q}_j = 2^{j+1} \tag{43}$$

Considering this polynomial is natural since we have

$$\tfrac{1}{2} \operatorname{Tr} P_{j+1}(\lambda) = 1 - \tilde{Q}_j(\lambda) \tag{44}$$

4.4. The curves $C_{\epsilon_1,\dots,\epsilon_n}$

Let us denote by C, C', and C'' the following half straight lines contained in $\mathscr{E}$ (Fig. 4):

$$\begin{aligned} C &= \{(x, 0); x \geqslant 1\} \\ C' &= \{(x, 0); x \leqslant -1\} \\ C'' &= \{(0, y); y \geqslant 2\} \end{aligned} \tag{45}$$

We have (recall that $x = 1$ corresponds to the Born–Von Karman situation)

$$\begin{aligned} \tilde{\Phi}^{-1}(x=1) &= \{y=0\} \cap \mathscr{E} = C \cup C' \\ \tilde{\Phi}^{-1}(C) &= C \cup C' \\ \tilde{\Phi}^{-1}(C') &= C'' \end{aligned} \tag{46}$$

It follows then that we have

$$\begin{aligned} \tilde{\Phi}^{-2}(x=1) &= C \cup C' \cup C'' \\ \tilde{\Phi}^{-3}(x=1) &= C \cup C' \cup C'' \cup \tilde{\Phi}^{-1}(C'') \\ \tilde{\Phi}^{-4}(x=1) &= C \cup C' \cup C'' \cup \tilde{\Phi}^{-1}(C'') \cup \tilde{\Phi}^{-2}(C'') \end{aligned} \tag{47}$$

and so on.

So we are led to study the sets $\tilde{C}_n = \tilde{\Phi}^{-n}(C'')$. Note that $\tilde{C}_n$ is contained in the algebraic manifold, the equation of which is $Q_n(x, y) = 1$ [by (41)]. Let us define a sequence $C_{\varepsilon_1,\dots,\varepsilon_n}$ of subsets of $\mathbb{R}^2$, indexed by the finite sequences of 0's and 1's, by the following recursion:

$$\begin{aligned} C_0 &= \psi_0(C'') \\ C_1 &= \psi_1(C'') \\ C_{\varepsilon_1,\dots,\varepsilon_n,0} &= \psi_0(C_{\varepsilon_1,\dots,\varepsilon_n}) \\ C_{\varepsilon_1,\dots,\varepsilon_n,1} &= \psi_1(C_{\varepsilon_1,\dots,\varepsilon_n}) \end{aligned} \tag{48}$$

The sets C_0 and C_1 are nothing but half straight lines, as shown on Fig. 4, which shows the results of three iterations of $\tilde{\Phi}^{-1}$:

$$C_0 = \{(x, 1); x \geqslant 1/\sqrt{2}\}, \qquad C_1 = \{(x, 1); x \leqslant -1/\sqrt{2}\} \tag{49}$$

Figure 5 shows C_{00}, C_{01}, C_{10}, and C_{11} (four iterations of $\tilde{\Phi}^{-1}$), which are connected smooth curves, and their corresponding intersections with the parabola $\mathscr{P}$. In the same way, Fig. 6 shows C_{000}, C_{001},..., C_{111}, which are connected smooth curves also (five iterations of $\tilde{\Phi}^{-1}$).

It results from the above construction that

$$\tilde{C}_n = \bigcup_{\varepsilon_1,\ldots,\varepsilon_n} C_{\varepsilon_1,\ldots,\varepsilon_n} \qquad \text{for} \quad n \geqslant 1$$

It is easy to show by induction that none of the sets $\tilde{C}_n$ (for $n \geqslant 1$) intersects C''. From this, it follows that $C_{\varepsilon_1,\ldots,\varepsilon_n}$ (for $n \geqslant 1$ and $\varepsilon_j = \pm 1\}$, C, C', and C'' are disjoint.

As C'' contains the point $A_{1/2}$, the set C_0 contains $A_{2^{-2}} = A_{1/4}$ and C_1 contains $A_{1-2^{-2}} = A_{3/4}$. By recursion one can see that $C_{\varepsilon_1,\ldots,\varepsilon_n}$ intersects the parabola $\mathscr{P}$ at a single point A_t, where t is a number of the form $(2k+1)/2^{n+1}$ (k being an integer such that $0 \leqslant k < 2^n$). Conversely, to any such number $t = (2k+1)/2^{n+1}$ there corresponds a single sequence $\varepsilon_1,\ldots, \varepsilon_n$ such that $C_{\varepsilon_1,\ldots,\varepsilon_n}$ contains A_t.

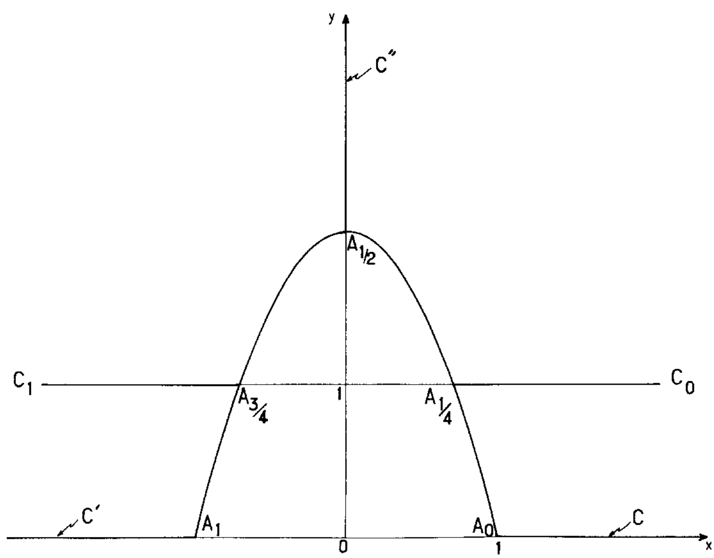


Fig. 4. Results of the first three iterations of $\tilde{\Phi}^{-1}$ on the $x = 1$ line together with the corresponding A_t points on the parabola $\mathscr{P}$.

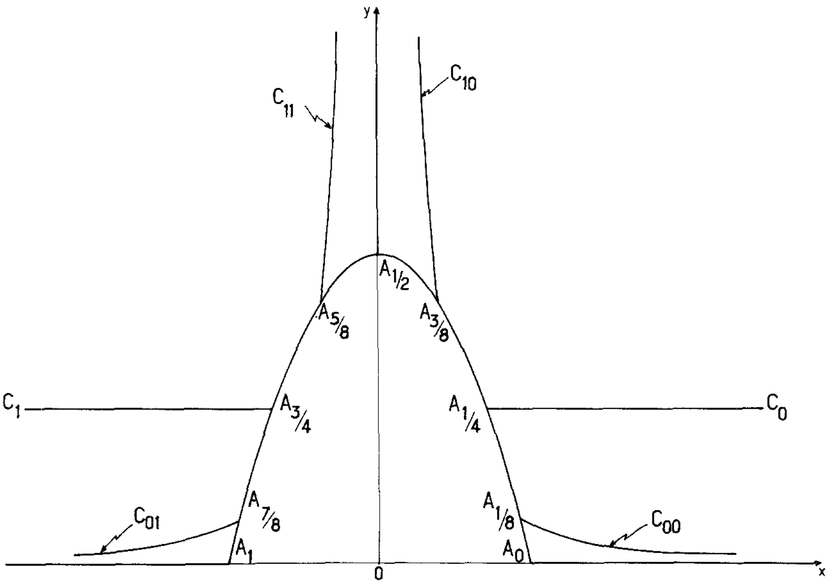


Fig. 5. Same as Fig. 4, for four iterations of $\tilde{\Phi}^{-1}$.

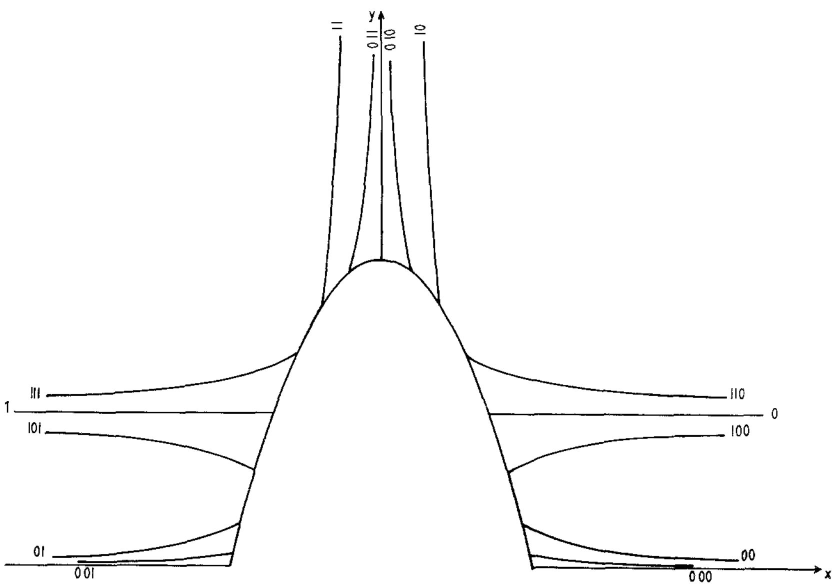


Fig. 6. Same as Fig. 4, for five iterations of $\tilde{\Phi}^{-1}$ (see text).

We are now going to prove that each $C_{\varepsilon_1,\ldots,\varepsilon_n}$ is a connected smooth curve.

Lemma. Let γ be a smooth curve in $\mathscr{E}$.

1. If γ has an infinite branch which is asymptotic to C_1, then the corresponding infinite branches of $\psi_0(\gamma)$ and of $\psi_1(\gamma)$ are asymptotic to C''.

2. If γ has an infinite branch asymptotic to C'', then the corresponding branches of $\psi_0(\gamma)$ and $\psi_1(\gamma)$ are asymptotic, respectively, to C_0 and C_1.

3. If γ has an infinite branch asymptotic to C', then the corresponding branches of $\psi_0(\gamma)$ and $\psi_1(\gamma)$ are asymptotic to C''.

4. If γ is contained in $\mathscr{E} \cap \{x<1\}$ and if $\lim_{t\to t_0} \gamma(t) = (1, a)$, with $a>0$, then, as $t\to t_0$, $\psi_0(\gamma(t))$ and $\psi_1(\gamma(t))$ have infinite branches asymptotic, respectively, to C and C'.

Proof. These assertions result from the relations $4X^2Y = y$ and $Y = 1-x$ if $\gamma(t) = (x, y)$ and $(X, Y) = \psi_0(x, y)$ or $(X, Y) = \psi_1(x, y)$.

It is then easy to prove by induction that any connected component γ of $C_{\varepsilon_1,\ldots,\varepsilon_n}$ is a smooth curve and that two alternatives may occur:

1. γ begins at a point $A_{(2k+1)2^{-(n+1)}}$ and at its other end has an asymptote which is one out of the five half straight lines C, C', C'', C_0, and C_1.

2. γ is homeomorphic to $\mathbb{R}$ and has two branches which are both asymptotic either to C or to C'.

Indeed, if γ is a component of $C_{\varepsilon_1,\ldots,\varepsilon_n}$, the components of $\psi_0(\gamma)$ and of $\psi_1(\gamma)$ correspond to the connected components of $\gamma \cap \mathscr{E} \cap \{x<1\}$, the number of which is finite because γ is algebraic.

We are going to show that the second alternative cannot occur. Let H_α and K_α be the straight lines the equations of which are $x=\alpha$ and $y=\alpha$, respectively.

In virtue of (42) and of the remark on $\tilde{C}_n$ the numbers of points of $H_\alpha \cap \tilde{C}_n$ and of $K_\alpha \cap \tilde{C}_n$ are at most $[2^n - (-1)^n]/3$ and $[2^n + 2(-1)^n]/3$, respectively. So the number of points of $(H_\alpha \cup H_{-\alpha} \cup K_\alpha) \cap \tilde{C}_n$ is at most $2[2^n - (-1)^n]/3 + [2^n + 2(-1)^n]/3 = 2^n$.

But if $\alpha \geqslant 1$, (1) H_α intersects any component of $\tilde{C}_n$ which is asymptotic to C or C_0, and (2) $H_{-\alpha}$ intersects any component of $\tilde{C}_n$ which is asymptotic to C' or C_1.

Moreover, K_2 intersects any component of $\tilde{C}_n$ which is asymptotic to C''. Therefore, if $\alpha \geqslant 1$, there are at least as many points in $(H_\alpha \cup H_{-\alpha} \cup K_2) \cap \tilde{C}_n$ as there are components of the first kind in $\tilde{C}_n$, i.e., 2^n.

Now, if there existed a component of the second kind, it would intersect H_α or $H_{-\alpha}$ for α large enough, and this would contradict the above analysis on the number of intersection points.

This analysis has a by-product which will be useful in the next paragraph: we know exactly the cardinalities of $H_\alpha \cap \tilde{C}_n$, $H_{-\alpha} \cap \tilde{C}_N$, and $K_2 \cap \tilde{C}_n$. In other terms, for n fixed:

1. The number of curves $C_{\varepsilon_1,\dots,\varepsilon_n}$ asymptotic to C or C_0 is exactly $[2^n-(-1)^n]/3$.
2. The number of curves $C_{\varepsilon_1,\dots,\varepsilon_n}$ asymptotic to C' or C_1 is exactly $[2^n-(-1)^n]/3$.
3. The number of curves $C_{\varepsilon_1,\dots,\varepsilon_n}$ asymptotic to C'' is exactly $[2^n+2(-1)^n]/3$.

Moreover, since the curves $C_{\varepsilon_1,\dots,\varepsilon_n}$ are mutually disjoint, and if they are ordered by the natural order of their intersections with $\mathscr{P}$, the $[2^n-(-1)^n]/3$ first ones are asymptotic to C or C_0, the $[2^n-2(-1)^n]/3$ following are asymptotic to C'', and the others to C' or C_1.

It follows from this analysis that any set $C_{\varepsilon_1,\dots,\varepsilon_n}$ is in fact a smooth, connected curve.

4.5. The Set Γ

It is convenient to adopt a new notation for curves $C_{\varepsilon_1,\dots,\varepsilon_n}$. If k and n are nonnegative integers such that $n \geqslant 1$ and $0 \leqslant k < 2^n$, $\Gamma_{(2k+1)2^{-(n+1)}}$ will stand for the curve $C_{\varepsilon_1,\dots,\varepsilon_n}$ which stems from the point $A_{(2k+1)2^{-(n-1)}}$. Besides, we set $\Gamma_0 = C$, $\Gamma_1 = C'$, and $\Gamma_{1/2} = C''$.

Let $\mathscr{D}_n$ be the set $\{k2^{-n};\, k \in \mathbb{N},\, 0 \leqslant k < 2^n\}$ and $\mathscr{D}$ the union of the $\mathscr{D}_n$.

We can now summarize the situation: to each $t \in \mathscr{D}$ is associated a single curve Γ_t, stemming from A_t. Moreover, the analysis at the end of the above paragraph shows that, for $t \in \mathscr{D}$:

1. If $0 \leqslant t < 1/3$, the curve Γ_t is asymptotic to either Γ_0 or $\Gamma_{1/4}$.
2. If $1/3 < t < 2/3$, the curve Γ_t is asymptotic to $\Gamma_{1/2}$.
3. If $2/3 < t \leqslant 1$, the curve Γ_t is asymptotic to either $\Gamma_{3/4}$ or Γ_1.

Applying then ψ_0 and ψ_1 (that is, $\tilde{\Phi}^{-1}$ once) gives the following results:

1. If $0 \leqslant t < 1/6$, then Γ_t is asymptotic to Γ_0.
2. If $1/6 < t < 1/3$, then Γ_t is asymptotic to $\Gamma_{1/4}$.
3. If $1/3 < t < 2/3$, then Γ_t is asymptotic to $\Gamma_{1/2}$.

4. If $2/3 < t < 5/6$, then Γ_t is asymptotic to $\Gamma_{3/4}$.
5. If $5/6 < t \leqslant 1$, then Γ_t is asymptotic to Γ_1.

We have

$$\bigcup_{t \in \mathscr{D}_n} \Gamma_t = \Gamma_0 \cup \Gamma_1 \cup \Gamma_{1/2} \cup \varphi^{-1}(\Gamma_{1/2}) \cup \cdots \cup \varphi^{-(n-1)}(\Gamma_{1/2}) \tag{50}$$

and

$$E_{n+1} \cap \mathscr{E} = \bigcup_{t \in \mathscr{D}_n} \Gamma_t \tag{51}$$

Therefore Λ_{n+2} is the set of parameters, along Ω, of the intersection points of Ω and of the curves Γ_t for $t \in \mathscr{D}_n$. But Ω meets any curve Γ_t (with $t \in \mathscr{D}$) at two points at least and these intersections have to be counted twice (eigenvalues are double, except for $t = 0$ or $t = 1$). For Λ_{n+2} it yields at least $2[2(2^n - 1) + 2] = 2^{n+2}$, which is exactly the expected number of eigenvalues of T_{n+2}, counted with their multiplicity. This means that any curve Γ_t meets Ω at exactly two points and that at the intersections these curves are transverse.

We have

$$\begin{aligned} &\tilde{\Phi}^{-1}(1, 0) = \tilde{\Phi}^{-1}(x = 1) = \Gamma_0 \cup \Gamma_1 \\ &\tilde{\Phi}^{-1}(\Gamma_0) = \Gamma_0 \cup \Gamma_1 \\ &\tilde{\Phi}^{-1}(\Gamma_1) = \Gamma_{1/2} \end{aligned} \tag{52}$$

Therefore

$$\bigcup_{t \in \mathscr{D}_n} \Gamma_t = \Phi^{-(n+1)}(1, 0) \tag{53}$$

As the point $(1, 0)$ is a fixed point for $\tilde{\Phi}$, the set $\bigcup_{t \in \mathscr{D}} \Gamma_t$ is invariant by $\tilde{\Phi}$ and $\tilde{\Phi}^{-1}$, as well as its closure, which we will denote by Γ.

The following proposition deals with the structure of Γ.

Proposition. None of the curves Γ_t ($t \in \mathscr{D}$) is isolated.

Proof. Let us consider the planar set S_v, for $v \leqslant 1$,

$$S_v = \{(x, y); \sup(0, 2(1 - x^2)) \leqslant y \leqslant v\}$$

We have

$$\psi_0(S_v) \subset S_{1-(1-v/2)^{1/2}}$$

So, if we define a sequence $\{v_n\}_{n\geq 2}$ by the recursion

$$\begin{aligned} &v_0 = 1 \\ &v_{n+1} = 1 - (1 - v_n/2)^{1/2} \qquad \text{for} \quad n \geq 2 \end{aligned} \tag{54}$$

we have

$$\psi_0^n(\Gamma_{1/2}) \subset \psi_0^n(S_1) \subset S_{v_n}$$

But the sequence v_n converges to 0. So the curve $\Gamma_{2^{-n}}$ converges to Γ_0 in the Hausdorff metric sense. By symmetry, Γ_1 is approached by the curves $\Gamma_{1-2^{-n}}$. Taking $\tilde{\Phi}^{-1}$, we see that $\Gamma_{1/2}$ is approachable by curves Γ_t on both sides. The result follows then by applying ψ_0 and ψ_1 repeatedly.

4.6. The Curves $\tilde{\Gamma}_s$

Let us define $\tilde{\Gamma}_{1/2} = \{(x, 2), x \in \mathbb{R}\}$. This straight line is tangent to the parabola $\mathscr{P}$ at $A_{1/2}$. It is also the set of points (x, y) such that the first component of $\Phi(x, y)$ is -1. Therefore we have

$$\tilde{\Phi}^{-n}(\tilde{\Gamma}_{1/2}) = \Phi^{-n-1}(x = -1) \tag{55}$$

The same analysis as before shows that $\tilde{\Phi}^{-n}(\tilde{\Gamma}_{1/2})$ consists in 2^n connected smooth curves, each of which is tangent to $\mathscr{P}$ at a point $A_{(2k+1)2^{-(n+1)}}$ $(0 \leq k < 2^n)$ and has two asymptotes out of the five half straight lines C, C', C'', C_0, and C_1. The curve tangent to $\mathscr{P}$ at point $A_{(2k+1)2^{-n-1}}$ is denoted by $\tilde{\Gamma}_{(2k+1)2^{-n-1}}$; it lies between $\Gamma_{k/2^n}$ and $\Gamma_{(k+1)/2^n}$ because the sets $\Phi^{-n-1}(x=1)$ and $\Phi^{-n-1}(x = -1)$ are disjoint. The sets $\tilde{\Phi}^{-n}(x=1)$ and $\tilde{\Phi}^{-n}(x = -1)$ are shown on Fig. 7.

As before, because we are dealing with continuous curves, one can realize that the curve Ω intersects $\tilde{\Phi}^{-n}(x = -1)$ (i.e., $\bigcup_{0 \leq k < 2^n} \tilde{\Gamma}_{(2k+1)/2^{n+1}}$) at 2^{n+2} points at least. As the corresponding parameters (on Ω) of these points are roots of the equation $\tilde{Q}_{n+1}(\lambda) = 2$, the degree of which is 2^{n+2} [see (41)], there are no more intersection points than the previous ones, and these intersections are transverse.

4.7. Integrated Density of States and Gaps

As Λ_n is an increasing sequence, the normalized counting measure μ_n on Λ_n tends to a measure μ in the weak sense. This measure μ, the limit when $n \to \infty$ of the density of states of finite chains, has Λ for a support. We are now going to describe it by giving an expression for its integral f, the integrated density of states.

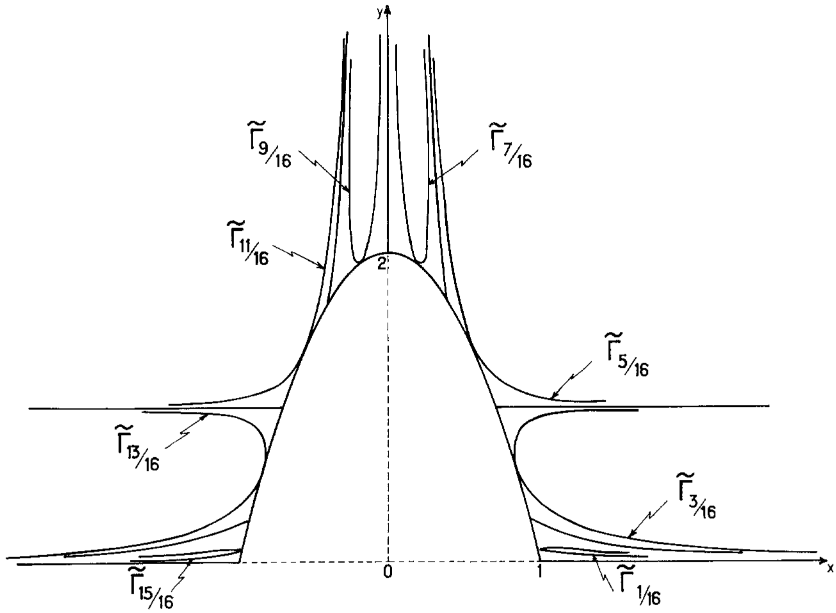


Fig. 7. The sets $\tilde{\Phi}^{-n}(x=1)$ and $\tilde{\Phi}^{-n}(x=-1)$ for $n=5$ (see text).

If $t \in \mathscr{D}$, let us denote by λ_t and λ'_t ($\lambda_t < \lambda'_t$) the parameters (on Ω) of the intersection points of Ω and Γ_t. Then f has the following properties:

$$f(\lambda_t) = t/2 \qquad \text{for} \quad t \in \mathscr{D}$$

$$f(\lambda'_t) = 1 - t/2 \qquad \text{for} \quad t \in \mathscr{D} \tag{56}$$

f is locally constant on the complement of Λ (gaps)

A way of proving the above formula is the following. Let $t = k \cdot 2^{-m}$. For $n \geqslant m$, λ_t is an eigenvalue of the chain of length 2^{n+2} with BVK boundary conditions. The value at λ_t of the integrated density of states of this chains is $2^{-(n+2)}$ times the number of eigenvalues $< \lambda_t$, $2^{-(n+2)}[1 + 2(k \cdot 2^{n-m} - 1)]$, which converges towards $k \cdot 2^{-m-1} = t/2$ when n goes to infinity. The analysis for determining the value of the integrated density of states at λ'_t is similar.

It is not difficult to show by induction that the curves $C_{111\cdots 1}$ are the graphs of convex and decreasing functions of x^2. As a consequence, the curves $C_{11\cdots 1}$ with an *odd* number of 1's as indices converge increasingly toward a curve Γ^* which is the graph of a convex and decreasing function of x^2. This curve Γ^* is asymptotic to C_1 and meets the parabola $\mathscr{P}$ at the single point $(-1/2, 3/2) = A_{2/3}$, which is a fixed point for $\tilde{\Phi}$ as well as for

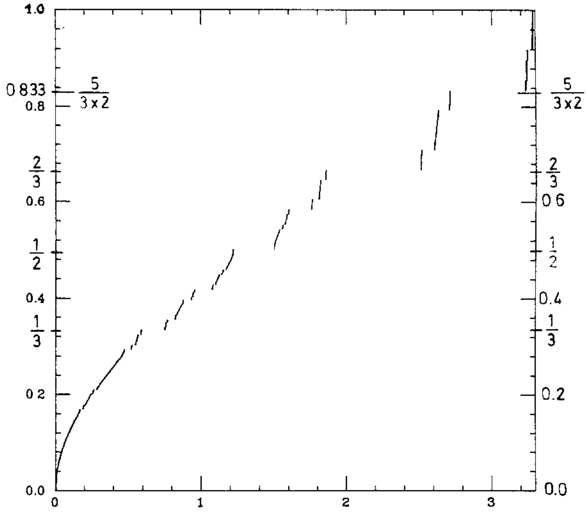


Fig. 8. The spectrum of the Thue–Morse chain for a mass ratio $\rho = 0.5$.

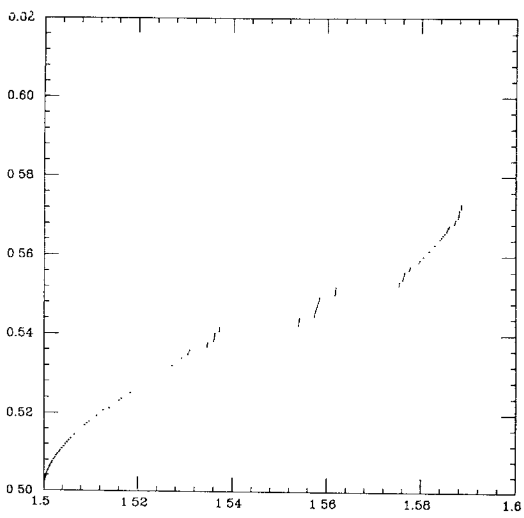


Fig. 9. An excerpt of Fig. 8 showing the envelope curve at the edge of the center gap ($\lambda = 1.5$) to be identical with the envelope curve at $\lambda = 0$.

ψ_1. In the same way the curves $C_{111\cdots 1}$ with an *even* number of 1's as indices converge decreasingly toward the curve $\psi_1(\Gamma^*)$, which is also the graph of a convex and decreasing function of x^2 and also meets $\mathscr{P}$ at $A_{2/3}$. Note that $\psi_1^2(\Gamma^*) = \Gamma^*$ and that $\Gamma^* \cup \psi_1(\Gamma^*)$ is an invariant manifold for $\tilde{\Phi}$, which is tangent at $\mathscr{P}$ at the fixed point $A_{2/3}$.

The curve Ω intersects Γ^* at two points at least. In fact, it intersects it at exactly two points. If it were not so, then there would exist a curve $C_{11\cdots 1}$ with an odd number of 1's as indices which would be intersected by Ω at three points at least, which is impossible. The same is true for the intersection of Ω and $\psi_1(\Gamma^*)$.

Then if t_1, t_2, t_3, and t_3, and t_4 are the parameters of the intersection points of Ω with Γ^* and $\psi_1(\Gamma^*)$ $(0 < t_1 < t_2 < t_3 < t_4)$, the intervals $]t_1, t_2[$ and $]t_3, t_4[$ are gaps (they are contained in the complement of Λ and their extremities are in Λ). The value of the IDS is 1/3 on $]t_1, t_2[$ and 2/3 on $]t_3, t_4[$ by the previous formula.

The other edges of the gaps are obtained as the intersections of Ω and of the successive images of Γ^* by ψ_0 and ψ_1. The value of the IDS on each of the gaps is then easily computed to be $(2k+1)/(3 \cdot 2^p)$, with p and k integers. This result can be obtained by different methods.[10,20]

Figure 8 shows the integrated density of states obtained by calculating about 5200 points of the spectrum Λ at a mass ratio of 0.5 (a calculation for the length 2^8 and $\rho = 0.8$ was given in ref. 4). Figures 9 and 10 are insets of the same. One clearly sees that (1) the envelope function is identical at

(a)

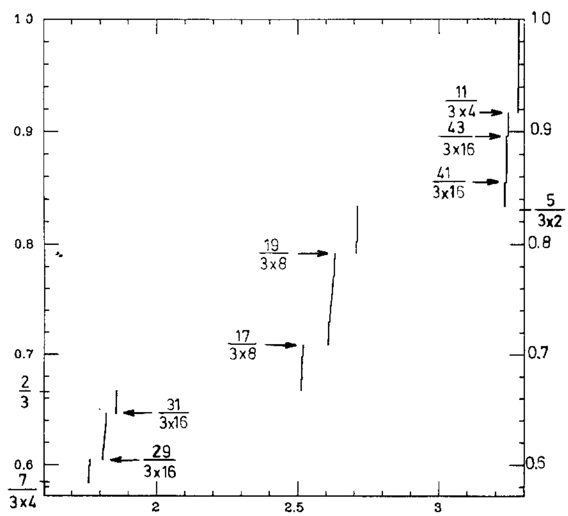


Fig. 10. Excerpts of Fig. 8 showing the fractal nature of the spectrum and the value of the IDS at the occurrences of the gaps.

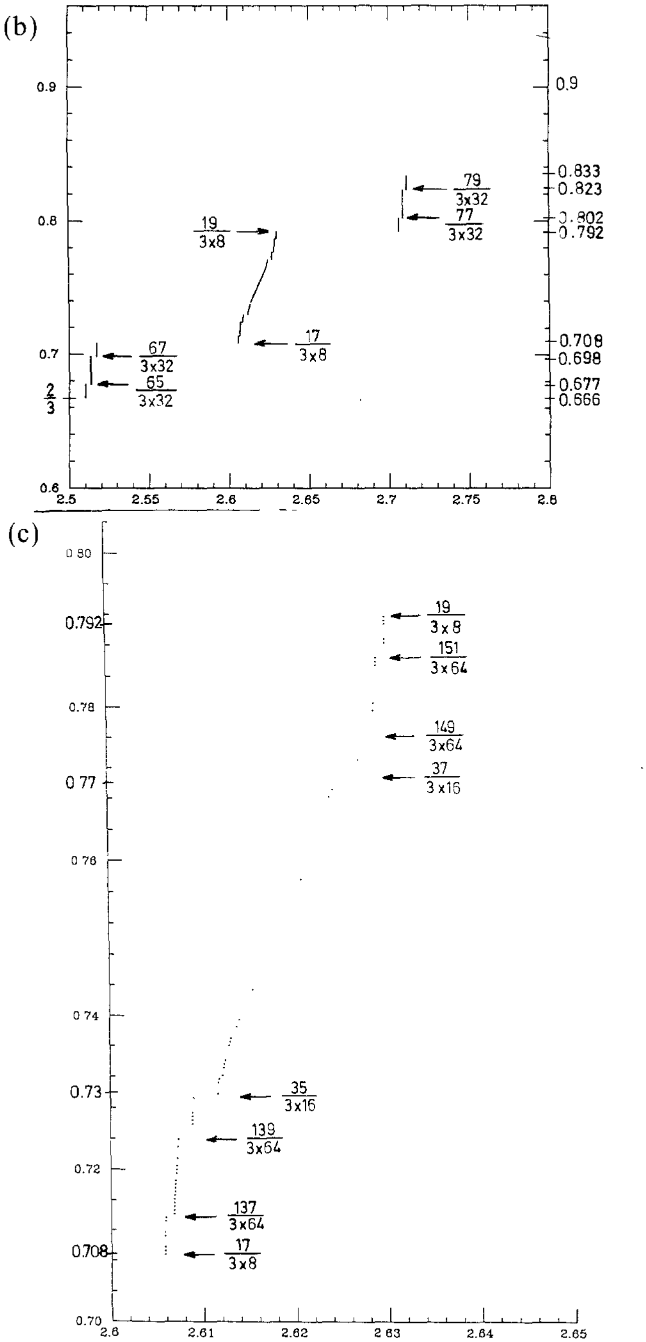


Fig. 10 (*continued*)

both edges of each gap and at the origin (Figs. 8 and 9), and (2) Fig. 10 is a "zoom" on a part of the spectrum which evidences its fractal character.[21]

The values of the integrated density of states at the occurrences of gaps are indicated in Figs. 8 and 10.

4.8. Changing Boundary Conditions

Instead of periodic boundary conditions as in Section 2.1, we could have considered antisymmetric boundary conditions. This means that we would like to determine λ in such a way that there exists a nonzero sequence $\{x_j\}_{-1 \leqslant j \leqslant 2^n}$ such that

$$\begin{aligned} x_{-1} &= -x_{2^n-1} \\ x_{2^n} &= -x_0 \\ -\lambda m_{\varepsilon_j} x_j &= x_{j+1} + x_{j-1} - 2x_j \qquad \text{for} \quad 0 \leqslant j < 2^n \end{aligned} \tag{57}$$

This means that $P_n(\lambda)$ has -1 as an eigenvalue and that (x_0, x_{-1}) is a corresponding eigenvector. Thus, the spectrum $\tilde{\Lambda}_n$ of this chain is the set of roots of the equation $1/2 \operatorname{Tr} P_n(\lambda) = -1$, i.e., $\tilde{\Lambda}_{n+1}$ is the set of parameters of the intersection points of Ω and of $\tilde{\Phi}^{-n}(x=-1)$. But we have studied this set in Section 4.6; it is the reunion of the curves $\tilde{\Gamma}_{(2k+1)/2^{n+1}}$ $(0 \leqslant k < 2^n)$. We have shown that curves Γ_s and $\tilde{\Gamma}_s$ are interleaved. From that it is easy to prove that the limit of the sets $\tilde{\Lambda}_n$, in the Hausdorff metric sense, is the same as that of Λ_n, i.e., Λ (one can nevertheless observe that the $\tilde{\Lambda}_n$ are not nested). It also implies that the integrated density of states, for finite chains with antisymmetric boundary condition, has the same limit as previously.

We have proved that all the chains associated ith the Thue–Morse substitution have the same integrated density of states. It is not clear whether they have the same spectral measure.

5. LEBESGUE MEASURE AND BOULIGAND–MINKOWSKI DIMENSION OF THE PHONON THUE–MORSE SPECTRUM

Although we found a flaw in our proof, announced in ref. 5, that the phonon spectrum of the Thue–Morse chain is of zero Lebesgue measure, we are able to give a numerical proof of this statement by calculation of its Bouligand–Minkowski dimension (box dimension), which we find inferior to 1, for various values of the mass ratio; hence, the spectrum is of zero measure.

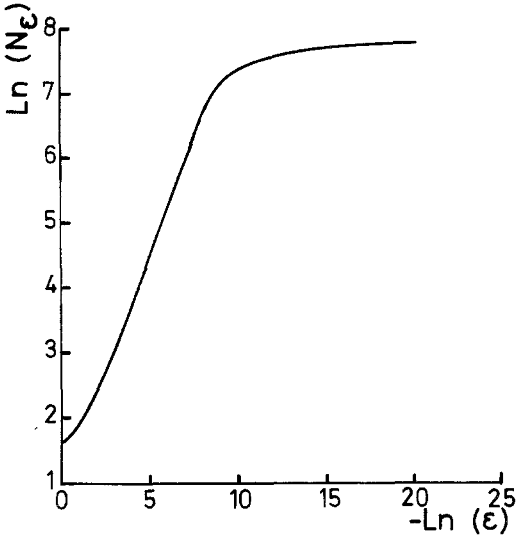


Fig. 11. Calculation of the Bouligand–Minkowski dimension d_{BM}. Graph of $\log N_\varepsilon$ versus $\log(1/\varepsilon)$ for $\rho = 0.3$ (see text).

The Bouligand–Minkowski dimension is calculated by the "box method": let ε be the diameter of "boxes" (in fact, intervals, here) covering the spectrum and N_ε the minimum number of these "boxes" necessary to cover the spectrum Λ. Let us plot $\log N_\varepsilon$ versus $-\log \varepsilon$. The corresponding curve, shown in Fig. 11, exhibits three regimes:

Table I. Bouligand-Minkowski Dimension d_{BM} (Box Dimension) of the Thue–Morse Phonon Spectrum for Various Values of the Mass ratio ρ[a]

$\rho = m_1/m_0$	d_{BM}
0.1	0.74
0.2	0.74
0.3	0.74
0.4	0.77
0.5	0.78
0.6	0.79
0.7	0.81_8
0.8	0.84
0.9	0.87_5

[a] The error on d_{BM} is estimated to be less than ± 0.025.

1. For large values of $\log(1/\varepsilon)$, we find a horizontal part of the curve which corresponds to the effect of discretization; when ε is too small, N_ε just counts the number of points of the approximation, and does not say anything about the set itself.

2. For small values of $\log(1/\varepsilon)$ we see only the global size of the set.

3. In the intermediate regime, which is the interesting one in view of the computation of the dimension, the curve is a straight line the slope of which is a good approximation to the dimension d_{BM},

$$d_{\mathrm{BM}} = \overline{\lim} \left(\frac{\log N_\varepsilon}{\log(1/\varepsilon)} \right) \tag{58}$$

$$N_\varepsilon \approx \varepsilon^{-d_{\mathrm{BM}}} \tag{59}$$

Our results are described in Table I. We estimate the uncertainty in our calculations of d_{BM} to be inferior to ± 0.025. We find the spectrum dimension d_{BM} inferior to 1 for the indicated mass ratios, which numerically proves that its Lebesgue measure is zero.

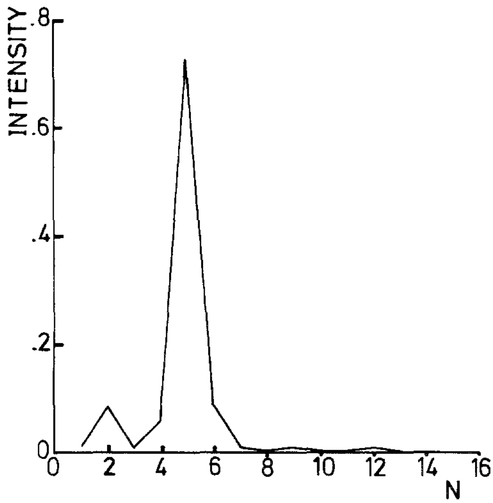
6. THE EXTENDED EIGENSTATES

In Section 3.5 we have proven that points in a dense subset of the spectrum give rise to *extended* states. Let us now give more details on this remarkable property, due to the original symmetry of the Thue–Morse substitution, by studying the example of the eigenstates corresponding to $\lambda = 5.236068$.

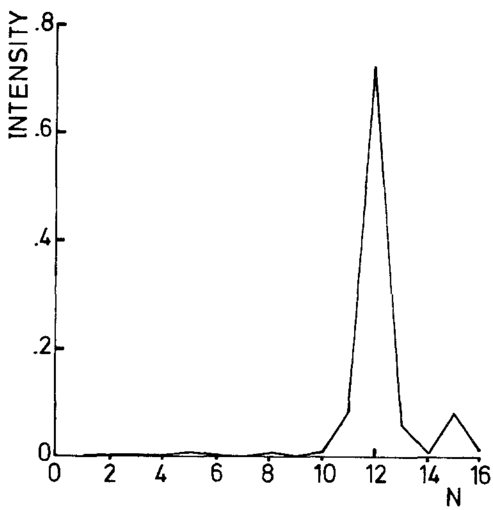
First, we recall that, as we increase the chain length (n goes to $n+1$), the spectrum Λ_{n+1} contains the spectrum Λ_n (as shown in Section 3). The point of the spectrum $\lambda = 5.236$ was "born" (appeared for the first time) at chain length $2^3 = 8$, and it is a double eigenvalue of T_3: then the conditions $P_3(\lambda = 5.236) = I$ as well as $\tilde{P}_3(\lambda = 5.236) = I$ are realized. The two corresponding Born–von Karman eigenstates are the building blocks a and b of modes 12 and 13 of the chain of length 16 (Figs. 12a and 12b) corresponding to the Thue–Morse subsequence ab and ba for the very same point $\lambda = 5.236068$, which is also a double engenvalue of T_4, since

$$P_4(5.236) = P_3(5.236)\, \tilde{P}_3(5.236) \tag{60}$$

Figures 13a and 13b show eigenmodes 22 and 23 for chain length $32 = 2^5$, corresponding to subsequences *abba* and *baab*, while Figs. 14a and 14b show eigenmodes 96 and 97 for chain length $128 = 2^7$, and the same value of λ, corresponding to subsequences *abbabaabbaababba*, and the reverse, illustrating the building process.

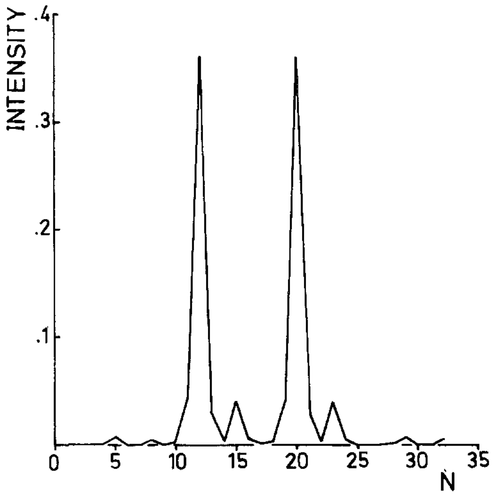


(a)

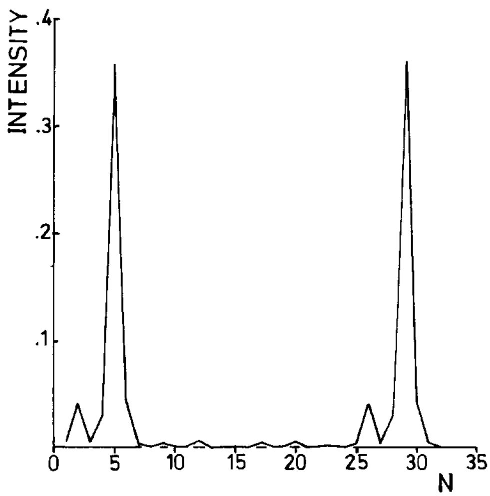


(b)

Fig. 12. Normalized eigenstates 12 and 13 (in ascending order of eigenvalues) of a Thue–Morse chain of length $2^4 = 16$ with $\rho = 1/2$ for $\lambda = 5.236068$, corresponding to subsequences *ab* and *ba*.

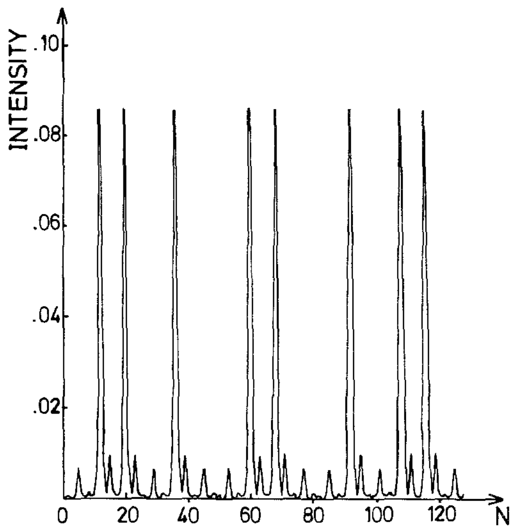


(a)

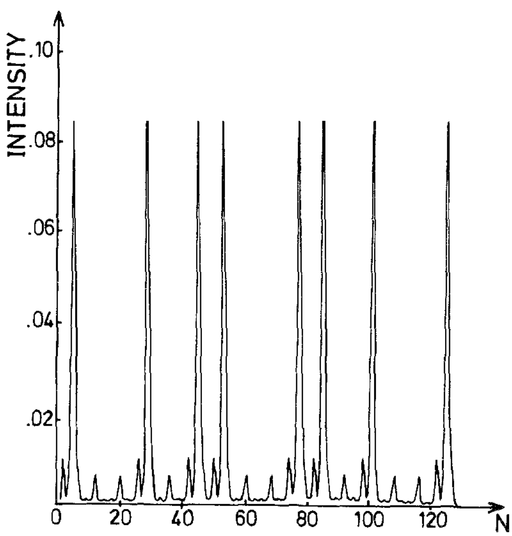


(b)

Fig. 13. Same as Fig. 12, eigenstates 22 and 23 for the same point of the spectrum and a chain of $2^5 = 32$. The corresponding Thue–Morse subsequences are *abba* and *baab* of length 4.



(a)



(b)

Fig. 14. Same as Fig. 12, eigenstates 96 and 97 for the same point of the spectrum and a chain of $2^7 = 128$. The corresponding Thue–Morse subsequences are then *abbabaabbaababba* and *baababbaabbabaab* of length 16.

Indeed, extended states have been described by other authors, but in 3D superlattices,[22-25] where they arise from a local property of the building block, at special values of the wave vector in the plane perpendicular to the controlled disorder direction, not from the intrinsic property of the sequence. Such is the fundamental Thue–Morse symmetry, which governs the existence as well as the properties of the extended states found in this chain with controlled disorder, we believe, for the first time in this situation. Applications to multilayered systems are straightforward, and might be technologically quite interesting.

NOTE ADDED IN PROOF

One of the referees brought our attention to a preprint by Kotani[26] on discrete Schrödinger operators with random potentials assuming a finite number of values. He proved that, under suitable ergodicity hypotheses, the spectral measure of such an operator is singular with respect to the Lebesgue measure, with probability 1.

Let us describe his result in our framework. Let X be the closed orbit of the Thue–Morse sequence under the shift operator S. It is known[27,28] that there exists on the compact X a unique Borel probability measure μ, invariant under S, and that the system (X, S, μ) is ergodic. Let q_0 and q_1 be two distinct real numbers and consider the Schrödinger operator H:

$$(Hx)_n = x_{n+1} + x_{n-1} + q_{\varepsilon_n} x_n$$

where the sequence $\varepsilon = \{\varepsilon_n\}_{n \in \mathbb{Z}}$ is in X.

Then, according to Kotani, for μ-almost every sequence ε, the associated Schrödinger operator has a singular spectral measure.

On the other hand, our analysis, although described for harmonic chains, is valid for these Schrödinger operators. We proved that the spectrum of such an operator does not depend on the choice of ε in X. Moreover, we have given numerical evidence that this spectrum is of zero Lebesgue measure.

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