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F. AXEL*, J.P. ALLOUCHE**, M. KLEMAN*, M. MENDES-FRANCE**
and J. PEYRIERE***

*Laboratoire de Physique des Solides, (UA 2), Bâtiment 510, Université Paris-Sud, F-91405 Orsay Cedex
**Laboratoire de Mathématiques (UA 226), Université de Bordeaux I, 351, Cours de la Libération, F-33405 Talence
***Equipe d'Analyse Harmonique (UA 757), Bâtiment 425, Université Paris-Sud, F-91405 Orsay Cedex

I - INTRODUCTION

We study the effect of deterministic disorder on the vibrational density of states and modes of a one dimensional elastic chain. To this end, we use automatic sequences and sequences generated by a substitution operating on a two letter alphabet ((0,1) or (a,b)) which have been investigated and used by harmonic analysts and number theoreticians /1, 2/. We give two examples :

1) The Fibonacci sequence generating a "1D Penrose tiling" (without coloured vertices). The substitution σ is defined as

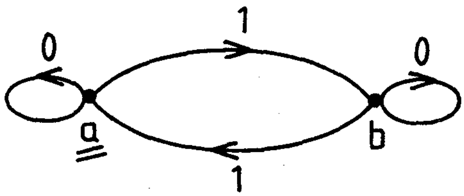
$\sigma(a) = ab$
$\sigma(b) = abb$

It has non constant length, the sequence generated by repeatedly applying σ is quasi periodic. Note that the usual 2D Penrose tiling can be generated by a substitution σ operating on a larger alphabet.

2) The Thue-Morse sequence where σ is defined by

$\sigma(a) = ab$
$\sigma(b) = ba$ and for instance
$\sigma^4(a) = abbabaabbaababba$

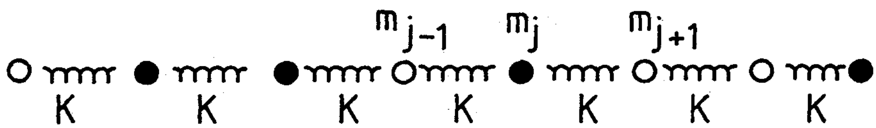
is not quasi-periodic and called automatic because it can also be generated by travelling on the following 2-automaton starting from a : the fifth term of the sequence, (which has a zeroth term) is obtained using the decomposition in base 2 of 5 : 101. (The result is a). All these sequences are completely deterministic ; they have zero entropy /3/



Recently, the effect of quasi-periodic sequences on the properties of the spectrum of certain Schrödinger operators /4/ (for a review, see /5/) and on the vibrational /6/ and electronic modes of discrete one dimensional chains has been widely investigated. We chose to concentrate, instead, on the non quasi-periodic Morse sequence.

II - THE "QUASI-ALLOY" MODEL

We study a chain of $N = 2^n$ masses and identical springs, with two different kinds of masses m_o and m_1.



The sequence of masses $\{m_j\}$ is such that the indices 0 and 1 are distributed according, here, to Morse sequence. We coined the name of "quasi-alloy" for this class of models by analogy with quasicrystal models where properties are distributed after Fibonacci or Fibonacci-like sequences. The u_j being displacements, we look for time stationary solutions of

$$(1) \quad m_j \frac{d^2u_j}{dt^2} = K(u_{j+1} - u_j - (u_j - u_{j-1})) \quad \text{hence}$$

$$(2) \quad -\frac{m_j}{K}\,\omega^2\, u_j = u_{j+1} + u_{j-1} - 2u_j$$

Let $m_j = \rho_j m$, $\omega_o^2 = \frac{K}{m}$, $x = \frac{\omega^2}{\omega_o^2}$, $\rho_o = 1$, $\rho_1 < 1$, then one has

(3) $u_{j+1} + u_{j-1} - (2 - \rho_j x)\, u_j = 0$

The relationship to a tight-binding model for electrons will be analysed elsewhere /7/.

We can write, using a transfer matrix formalism /8, 17/

(4) $$\begin{pmatrix} u_{j+1} \\ u_j \end{pmatrix} = T_j(x) \begin{pmatrix} u_j \\ u_{j-1} \end{pmatrix} = \begin{pmatrix} 2-\rho_j x & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_j \\ u_{j-1} \end{pmatrix}$$

with det $(T_j(x)) = 1$; then

(5) $$\begin{pmatrix} u_{p+1} \\ u_p \end{pmatrix} = T_p \; T_{p-1} \; T_{p-2} \cdots T_3 \; T_2 \; T_1 \begin{pmatrix} u_1 \\ u_o \end{pmatrix} = M_p(x) \begin{pmatrix} u_1 \\ u_o \end{pmatrix}$$

When M_p has eigenvalues of modulus 1, propagation may occur

(6) $$M_p \sim \begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} \quad \text{and}$$

(7) $$\cos \beta = \frac{1}{2} \operatorname{Tr} M_p(\omega^2)$$

where $M_p(\omega^2)$ is a polynomial of degree p in ω^2 (or x) and β characterizes the rotation of the wave function phase and plays the rôle of the wave number in the periodic case. One then obtains the analytic dispersion relation

(8) $$\beta(\omega^2) = \operatorname{Arc\,cos} \left(\frac{1}{2} \operatorname{Tr} M_p(\omega^2) \right)$$

In one dimension, β, conveniently normalized, is also the integrated density of states (IDS) /9/.

When M_p has real eigenvalues, the phase is blocked (gap), the Ljapounov exponent γ is non zero. In the first case $|\operatorname{Tr} M_p| < 2$, in the second $|\operatorname{Tr} M_p| > 2$

III - THE TRACE MAPPING THEOREM AND ITS APPLICATIONS

The fundamental rôle of the trace of the mapping, which controls the behaviour of the phase β, the gaps, the Ljapounov exponent and the escape properties /11/, has prompted two of us to investigate more generally the properties of the trace of such a matrix product M_{2^n} for a class of substitutions σ ./10/

Theorem : Let σ be a substitution on a two letter alphabet (a,b). Then there exists a polynomial map $\phi : R^5 \to R^5$ with integer coeffi-

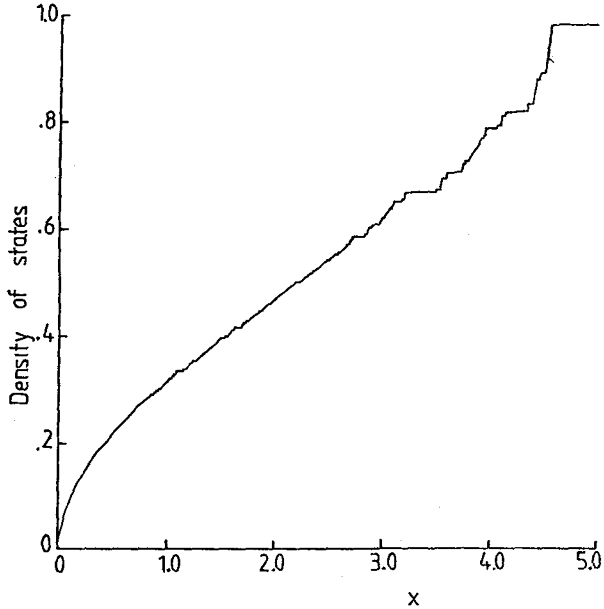


Fig. 1 : The integrated density of states $\beta(\omega^2)$ for a Morse elastic chain of $2^9 = 512$ masses m_o and m_1 , $\frac{m_1}{m_o} = 0.8$

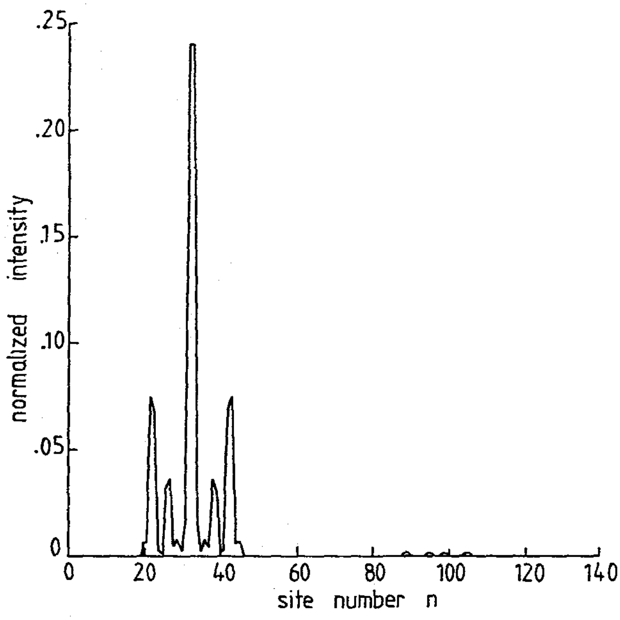


Fig. 2 : Normalized mode for x = 6.487 in a Morse elastic chain of $2^7 = 128$ sites with $\frac{m_1}{m_o} = 0.5$

cients <u>such that</u> if A and B are 2 × 2 matrices and one considers the matrix product M_{2^n} obtained by replacing a by A and b by B in $\sigma^n(a)$ then : Tr M_{2^n} = 1st component $\{\phi^n(\mathrm{TrA}, \mathrm{TrB}, \mathrm{TrAB}, \det A, \det B)\}$
ϕ can be explicitly constructed. See /10/ for the proof.
For the Morse sequence, the trace mapping with $t_n = \frac{1}{2}\,\mathrm{Tr}\, M_{2^n}(\omega^2)$ is

(9) $$t_{n+1} = 4t_n\, t^2_{n-1} - 4\, t^2_{n-1} + 1 \qquad n > 2$$

One sees that the use of the analytic dispersion relation (8) together with the trace mapping (9) constitutes a very powerful tool to describe the band structure (stability, total measure of gaps, behaviour of singularities...) of such chains / 7/. In particular it allows very accurate numerical calculations. Note that the theorem yields, for the Fibonacci sequence the trace mapping

(10) $$t_{n+1} = 2t_n\, t_{n-1} - t_{n-2}$$

with the quantity

(11) $$I = -1 + t_n^2 + t^2_{n-1} + t^2_{n-2} - 2t_n\, t_{n-1}\, t_{n-2}$$

independent of n. (10) and (11) have previously been found by several authors /11, 12, 13/.

The IDS for a Morse elastic chain of $2^9 = 512$ sites derived from (8) is shown on Figure 1. Observation of a succession of iterates indicates that gaps increase in number but also stabilize. The existence of a self similar structure /14/ is already obvious at this stage /7/.

IV - <u>MODES</u>

The modes of a Morse elastic chain of 2^n sites are studies using the symmetric tridiagonal dynamical matrix deduced from the 2^n equations (8) with fixed end boundary conditions :

(12) $$u_o = u_{2^n+1} = 0$$

Having derived 2^n frequencies ω_j^2 one numerically calculates the corresponding modes. Figure 2 shows an example of such a mode, localized/15/, that has a non trivial decrease from the center peak. Analogous wave functions have been described in certain quasiperiodic situations /16/.

Acknowledgements

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