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VIBRATIONAL MODES IN A ONE DIMENSIONAL "QUASI-ALLOY" : THE MORSE CASE

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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

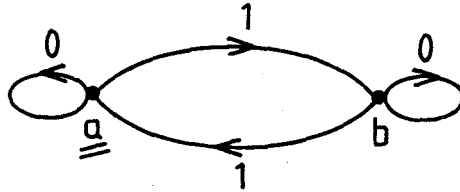
$$\begin{aligned}\sigma(a) &= ab \\ \sigma(b) &= abb\end{aligned}$$

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

$$\begin{aligned}\sigma(a) &= ab \\ \sigma(b) &= ba \quad \text{and for instance} \\ \sigma^4(a) &= abbabaabbaababba\end{aligned}$$

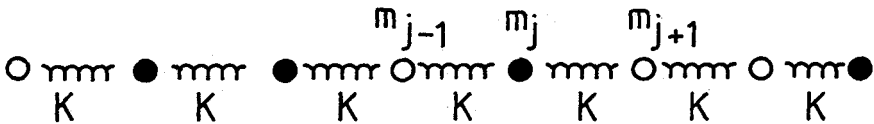
is not quasi-periodic and called automatic because it can also be generated by travelling on the following 2-automaton starting from a : the fifth term of the sequence, (which has a zeroth term) is obtained using the decomposition in base 2 of 5 : 101. (The result is a). All these sequences are completely 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_0 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

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

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

Let $m_j = \rho_j m$, $\omega_0^2 = \frac{K}{m}$, $x = \frac{\omega^2}{\omega_0^2}$, $\rho_0 = 1$, $\rho_1 < 1$, then one has

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

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

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

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

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

$$(5) \quad \begin{pmatrix} u_{p+1} \\ u_p \end{pmatrix} = T_p \begin{pmatrix} u_p \\ u_{p-1} \end{pmatrix} = T_p T_{p-1} T_{p-2} \cdots T_3 T_2 T_1 \begin{pmatrix} u_1 \\ u_0 \end{pmatrix} \\ = M_p(x) \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}$$

When M_p has eigenvalues of modulus 1, propagation may occur

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

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

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

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

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 $|\text{Tr } M_p| < 2$, in the second $|\text{Tr } M_p| > 2$

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_{2n} 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 $\phi : \mathbb{R}^5 \rightarrow \mathbb{R}^5$ with integer coeffi-

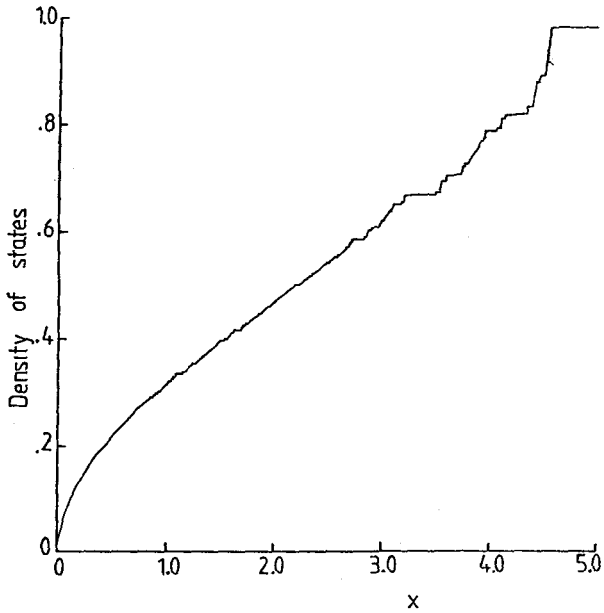


Fig. 1 : The integrated density of states $\beta(\omega^2)$ for a Morse elastic chain of $2^9 = 512$ masses m_0 and m_1 , $\frac{m_1}{m_0} = 0.8$

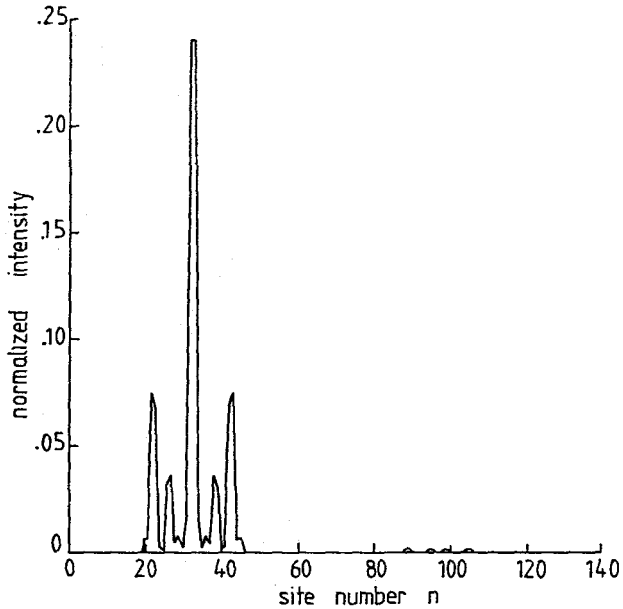


Fig. 2 : Normalized mode for $x = 6.487$ in a Morse elastic chain of $2^7 = 128$ sites with $\frac{m_1}{m_0} = 0.5$

cients such that if A and B are 2×2 matrices and one considers the matrix product M_{2n} obtained by replacing a by A and b by B in $\sigma^n(a)$ then : $\text{Tr } M_{2n} = 1\text{st component } \{\phi^n(\text{Tr}A, \text{Tr}B, \text{Tr}AB, \det A, \det B)\}$
 ϕ can be explicitly constructed. See /10/ for the proof.

For the Morse sequence, the trace mapping with $t_n = \frac{1}{2} \text{Tr } M_{2n}(\omega^2)$ is

$$(9) \quad t_{n+1} = 4t_n t_{n-1}^2 - 4t_{n-1}^2 + 1 \quad n > 2$$

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

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

with the quantity

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

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 - MODES

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

$$(12) \quad u_0 = u_{2n+1} = 0$$

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/.

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