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LETTER TO THE EDITOR

Intermittency in Fibonacci chains

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Abstract. The devil's staircase spectrum of a Fibonacci chain is obtained using a simple non-linear map. This map exhibits intermittency for all Fibonacci number iterates of the function whenever the frequency lies in a gap of the spectrum. The self-similar nature of the eigenfunctions is shown to be a consequence of the intermittency behaviour. Certain simple patterns that emerge in the gap-labelling theorem are discussed.

The spectrum of a tight-binding electron Hamiltonian on a quasiperiodic chain is the same as that of a Schrödinger equation with an almost periodic potential in one dimension (Kohmoto et al 1987). Both problems have been widely studied in recent years (Simon 1982, Kohmoto et al 1983, 1987, Ostlund et al 1983a, b, Kohmoto and Oono 1984, Ostlund and Pandit 1984, Kohmoto and Banavar 1986, Luck and Petritis 1986, Lu et al 1986, Niu and Nori 1986, Nori and Rodriguez 1986, Tang and Kohmoto 1986, Evangelou 1987). The harmonic vibrations of masses or the diffusion of a particle are mathematically equivalent to the electron tight-binding Hamiltonian in one dimension. On a Fibonacci chain, the electronic spectrum is a Cantor set; in lattice dynamics or diffusion the integrated density of states (IDS) of phonons, or the eigenvalues of the diffusion equation, is a devil's staircase. Though the major features of the spectra in the electron and phonon case are complementary to each other (bands in the electronic spectrum correspond to gaps in the phonon case), there are certain essential differences (Kohmoto and Banavar 1986). The long time behaviour is the only aspect that has been studied so far in diffusion (Kohmoto and Banavar 1986, Khantha and Stinchcombe 1987). In this regime the behaviour is similar to the low-frequency phonon dynamics.

The technique commonly used for studying the spectrum of a Fibonacci chain (in the electron, phonon or diffusion case) is based on a renormalisation group equation which is a two-dimensional dynamical system (see, for example, Kohmoto *et al* 1987). This was first deduced for the almost periodic Schrödinger equation (Kohmoto *et al* 1983). Since the recursion relation for the transfer matrices of the Fibonacci chain gives rise to the same trace mapping as the almost periodic Schrödinger operator, the two problems have identical spectra.

In this letter, a simple transformation is used to deduce an effective one-dimensional map from which all features of the spectrum are easily obtained. A different interpretation is proposed for the self-similar structure of the eigenfunctions in the bands (or

[†] Address from 1 September 1987: Department of Materials Science, University of Pennsylvania, Philadelphia, PA 19104-6272, USA. the gaps in the phonon case) of the spectrum of a Fibonacci chain. This is shown to be a consequence of the intermittency exhibited by the non-linear map for all Fibonacci number iterates of the function whenever the frequency lies in a gap. A main advantage of the present method is in speeding up the numerical computation of the spectrum. It is therefore possible to do calculations on very long chains of the order of 10^5 . This enables greater accuracy in determining the widths of the bands (or gaps). Schneider *et al* (1986a, b) have used a similar map in studying the motion of a quantum particle in a random medium. A theoretical analysis of the spectrum of a Fibonacci chain has been carried out recently (Stinchcombe 1987) based on a perturbation approach. The locations and widths of all the gaps are predicted by this technique for small values of the perturbation parameter. The numerical results obtained using the method outlined here agree well with the theoretical predictions (Stinchcombe 1987).

A 'gap-labelling' theorem (Simon 1982) which identifies every gap in the spectrum uniquely is known to be valid for the Fibonacci spectrum. It is shown here that the ordering of the gaps follows systematically by choosing adjacent pairs of integers of various Fibonacci sequences. This ordering is similar to that found by Ostlund *et al* (1983a, b) for the self-similar peaks in the spectrum of a two-parameter quasiperiodic map.

Consider a Markovian master equation for the diffusion of a particle via nearestneighbour jumps on a Fibonacci chain:

$$dP_n/dt = T_{n,n+1}P_{n+1} + T_{n,n-1}P_{n-1} - (T_{n+1,n} + T_{n-1,n})P_n$$
(1)

where $P_n(t)$ is the probability of finding the particle at site *n* at time *t*, $T_{n,n'}$ is the transition rate for the particle to hop from site *n'* to *n* and $1 \le n \le N$. On a Fibonacci chain, the nearest-neighbour sites are linked either by an *A* or a *B* bond. We choose two different symmetric rates that correspond to jumps over *A* and *B* bonds. The conditional probability P(n, t | n', 0) can be expressed as a superposition of *N* eigenfunctions $\Phi_n(x)$ weighted appropriately by the eigenvalues λ_n (Schneider *et al* 1986a, b). This yields

$$P_n(t) = e^{-\omega t} (P_n^0)^{1/2} \Phi_n$$
(2)

where P_n^0 is the stationary distribution at the *n*th site. Substituting this in the master equation we obtain

$$(\omega - T_{n,n+1} - T_{n,n-1})\Phi_n + T_{n,n+1}\Phi_{n+1} + T_{n,n-1}\Phi_{n-1} = 0.$$
(3)

A tight-binding electron Hamiltonian or the harmonic vibrations on a quasiperiodic chain yields an equation similar to (3). Rewriting it as a transfer matrix equation we obtain

$$\begin{pmatrix} \Phi_{n+1} \\ \Phi_n \end{pmatrix} = \begin{pmatrix} 1 + \frac{T_{n,n-1}}{T_{n,n+1}} - \frac{\omega}{T_{n,n+1}} & -\frac{T_{n,n-1}}{T_{n,n+1}} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \Phi_n \\ \Phi_{n-1} \end{pmatrix}.$$
(4)

A similar matrix equation for the electron case has been the starting point of the two-dimensional dynamical map of Kohmoto *et al* (1983).

We consider, instead, a relation between the integrated density of states and the nature of eigenstates for one-dimensional nearest-neighbour coupling problems, first derived by Thouless (1972). Let $\Gamma(\Omega)$ be the characteristic function

$$\Gamma(\Omega) = \int_0^\infty \ln(\Omega + z)\rho(z) \, dz$$
(5)

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where $\rho(z)$ is the density of states. Let the inverse localisation length and the integrated density of states be denoted by $\gamma'(\omega)$ and $\gamma''(\omega)$ respectively. Thouless showed that $\gamma'(\omega) + i\pi\gamma''(\omega)$ is the boundary value of the analytic function $\Gamma(\omega)$:

$$\Gamma(-\omega + i0^+) = \gamma'(\omega) + i\pi\gamma''(\omega).$$
(6)

Consider the ratio U_n of eigenfunctions at two neighbouring sites

$$U_n = \Phi_n / \Phi_{n+1}. \tag{7}$$

The transfer matrix equation (4) can be expressed in terms of U_n as a one-dimensional map:

$$U_{n+1} = \left(1 + \frac{T_{n,n-1}}{T_{n,n+1}} - \frac{\omega}{T_{n,n+1}}\right) - \frac{T_{n,n-1}}{T_{n,n+1}} \frac{1}{U_n}.$$
(8)

It has been shown (Nieuwenhuizen 1982, Simon 1982) that the Lyapunov exponent of the map U_n defined by

$$\gamma(\Omega) = \lim_{N \to \infty} \sum_{n=0}^{N} \ln U_n$$
(9)

is identical to the characteristic function $\Gamma(\Omega)$ in (5). Therefore, using (6), we obtain

$$\gamma(\Omega = -\omega + i0^+) = \gamma'(\omega) + i\pi\gamma''(\omega).$$
⁽¹⁰⁾

Choosing the cut trailing the singularity of $\ln(U_n)$ to lie along the negative real axis, one finds (Schneider *et al* 1986a, b)

Re
$$\gamma(\omega) = \gamma'(\omega) = \lim_{N \to \infty} \left(\frac{1}{N}\right) \sum_{n=0}^{\infty} \ln|U_n|$$

Im $\gamma(\omega) = \pi \gamma''(\omega) = \pi \lim_{N \to \infty} \left(\frac{1}{N}\right) \sum_{n=0}^{\infty} A_n$
(11)

where

$$A_n = \begin{cases} 1 & U_n < 0 \\ 0 & \text{otherwise.} \end{cases}$$

Thus the IDS is proportional to the number of times the function U_n changes sign. Fixing ω and iterating (8), the successive values of *n* representing the sites along the Fibonacci chain, and choosing appropriate values for T_n depending on the local environment at site *n*, we see that (11) yields easily the inverse localisation length and the integrated density of states. Equation (8) is a one-dimensional map in the variable U_n . It should, however, be noted that the T_n are defined via the recurrence relation generating the Fibonacci chain (Levine and Steinhardt 1984). At any site *n*, the ratio $T_{n,n-1}/T_{n,n+1}$ takes one of the three values: 1, $T_A/T_B \equiv r$ or $T_B/T_A \equiv 1/r$. The *T* are not constant parameters of the map.

Figure 1 shows the IDS $\gamma''(\omega) = N(\omega)$ for a chain of length $N = 10\,946$ and r = 0.5 with periodic boundary conditions. A similar devil's staircase spectrum is obtained for every value of the ratio r in the range 0 < r < 1. As the main interest in this paper is to point out special features of the map U_n , results are shown for a representative chain of length 10^4 . It is, however, possible to extend the calculations to chains ten or a hundred times longer than the one presently chosen.



Figure 1. The IDS $N(\omega)$ plotted against ω for $T_A/T_B \equiv r = 0.5$. The results were obtained by iterating (8) on a chain of length N = 10946.

The low-frequency behaviour of the IDS is well known. $\gamma''(\omega)$ behaves as $\omega^{1/2}$ as $\omega \to 0$. The same is true for the pure chain. This feature becomes evident by considering the intermittency property of the map U_n as $\omega \to 0$ (Schneider *et al* 1986a, b). Let

$$x_n = 1 - U_n. \tag{12}$$

Then (8) can be expressed as

$$x_{n+1} = \frac{\omega}{T_{n,n+1}} + \frac{T_{n,n-1}}{T_{n,n+1}} \frac{x_n}{1 - x_n}.$$
(13)

A map of this type is known to exhibit intermittency as $\omega \to 0$ (Hirsch *et al* 1982) for all values of *r* in the range $0 \le r \le 1$. This behaviour is independent of the ordering of the T_n . Due to the hyperbolic nature of the map U_n , Schneider *et al* (1986a, b) point out that the IDS is inversely proportional to the length of the laminar region in intermittency. The latter scales as $\omega^{-1/2}$ and, hence, $\gamma''(\omega) \simeq \omega^{1/2}$ as $\omega \to 0$.

The devil's staircase spectrum which is markedly different from that of a pure chain at finite values of ω arises due to the interesting and generic behaviour of the map for a Fibonacci sequence $(\ldots ABAABABAABAAB...)$ of T_n . The map U_n (or x_n) exhibits intermittency for every value of ω that lies in the gap of the spectrum for any given rsuch that 0 < r < 1. Further, the intermittency is exhibited in all iterates x_{n+F_m} where F_m are the Fibonacci numbers (1, 1, 2, 3, 5, 8, 13, ...). This is clearly seen for large values of F_m , typically greater than 80. Figures 2 and 3 show $|U_q|$ plotted against qwhere $q = j \times 89$ and $q = j \times 144$, j = 1, 2, 3, 4, ..., respectively. Thus the values of n at which $|U_n|$ has the same value are found all along the chain at intervals of multiples of Fibonacci numbers (1, 1, 2, 3, 5, 8, 13, 21, ...). This yields self-similar eigenfunctions Φ_n when ω is in a gap as shown in figure 4 of Kohmoto *et al* (1987). No particular structure is discernible in the iterates x_{n+F_m} for a value of ω that does not lie in a gap.



Figure 2. A log-linear plot of the successive values of the iterate $|U_q|$ corresponding to the Fibonacci number q = 89 for $T_A/T_B \equiv r = 0.5$ at the principal gap. The abscissa shows $q = j \times 89$ where j = 1, 2, 3, 4, ...

A 'gap-labelling' theorem (Simon 1982) that uniquely identifies every gap is known to hold good for the spectrum of a Fibonacci chain (Luck and Petritis 1986). According to this, every value of $\gamma''(\omega)$ that corresponds to a gap in the spectrum is expressible in the form $|n - m/\tau|$, where *n* and *m* are integers and τ is the golden mean. The value of $\gamma''(\omega)$ at the biggest gap is $1/\tau$ for all 0 < r < 1 which corresponds to the pair (0, 1) for *n* and *m*. There is an interesting ordering of *n* and *m* which gives the values of γ'' that correspond to gaps of decreasing widths. The next few values of γ'' are obtained by choosing *n* and *m* to be adjacent members of Fibonacci sequences

(0, 1, 1, 2, 3, 5, 8,)	(2, 2, 4, 6, 10, 16,)	(1, 3, 4, 7, 11, 18,)
(3, 3, 6, 9, 15, 24,)	(2, 5, 7, 12, 19, 31,)	(1, 4, 5, 9, 14, 23,)

etc. Thus the pairs (1, 1), (2, 2), (1, 3), (2, 4), (3, 4), (1, 2), (6, 3), (5, 7) label the next seven gaps. Any adjacent pair that gives a value of γ'' greater than unity is prohibited. Beyond (1, 3), all subsequent pairs of the first two integers of all Fibonacci series yield $\gamma'' > 1$ and are therefore excluded. The ordering then proceeds to the next pair of adjacent numbers beginning at (2, 4) since the pair (1, 1) has already been taken into consideration. A new column always begins at the top sequence as can be seen by writing the Fibonacci sequences one below the other taking care to shift them appropriately to account for certain non-contributing pairs. As an example the numerical results obtained for the widths of the first few gaps for r = 0.5 on a chain of length $N = 10\,946$ are shown in table 1. It is curious to note that a similar ordering identifies



Figure 3. The successive values of the iterate $|U_q|$ corresponding to the Fibonacci number q = 144 for $T_A/T_B \equiv r = 0.5$ at the principal gap. The abscissa shows $q = j \times 144$ where $j = 1, 2, 3, 4, \ldots$

Table 1. The values of $\gamma''(\omega) = N(\omega)$ and the gap widths for the prominent gaps observed on a chain of length $N = 10\,946$ for the ratio $T_A/T_B \equiv r = 0.5$. The corresponding gaplabelling integers are also shown. The error in the gap width is of $O(10^{-3})$.

Range of ω	Gap width	$N(\omega)$	(n, m)
1.415-2.310	0.895	0.618 07	(0, 1)
0.670-0.900	0.230	0.382 02	(1, 1)
2.450-2.625	0.175	0.763 86	(2, 2)
2.685-2.815	0.130	0.854 11	(1, 3)
1.075-1.155	0.080	0.472 09	(2, 4)
1.250-1.315	0.065	0.527 91	(3, 4)
0.300-0.340	0.040	0.236 04	(1, 2)
2.380-2.415	0.035	0.708 23	(6,3)
2.335-2.360	0.025	0.673 70	(5,7)

the prominent peaks in the spectrum of a quasiperiodic map with the golden mean rotation number (Ostlund *et al* 1983a, b).

Finally, we note that the multifractal exponents that describe the scaling of the IDS around a gap (Kohmoto *et al* 1987) can be obtained by constructing generalised Lyapunov exponents (Paladin and Vulpiani 1987) for the non-linear map U_n . Further work is in progress.

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