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1989 J. Phys.: Condens. Matter 1 5607

(http://iopscience.iop.org/0953-8984/1/33/003)

J. Phys.: Condens. Matter **1** (1989) 5607–5612. Printed in the UK

Using the Fourier spectrum to classify families of generalised extensions of the Fibonaccian lattice

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Received 17 January 1989

Abstract. The interest in non-Fibonaccian aperiodic crystals has increased during the last few years, since it appears that the physical properties of the Fibonaccian quasicrystal may in some fundamental aspects not be generic. As an example the property that all the electronic eigenstates in a tight-binding model for a Fibonaccian lattice are chaotic and correspond to a singular continuous spectrum is not shared by all aperiodic crystals. Gumbs and Ali have recently studied the trace map of the two families given by the inflational rule $A \rightarrow ABB \ldots B$, $B \rightarrow A$ with n Bs and $A \rightarrow AAA \ldots AB$, $B \rightarrow A$ with n As. They conjectured that these two families, which for n greater than one are both extensions of the Fibonaccian sequence, should have rather different physical properties. We confirm their conjecture by showing that the structure of the Fourier spectra of the two families are quite different when n is greater than one. The Fibonaccian sequence is found to be much more like the members of the second family than the first one. This classification is then related to the definition of a quasicrystal using the diffraction criterion of Bombieri and Taylor, and the member with n equal to two in the first family is shown to be a marginal case.

1. Introduction

Since the fundamental experimental discovery by Shechtman *et al* (1984) and the theoretical analysis by Levine and Steinhardt (1984) there has been considerable interest in the physical properties of quasiperiodic systems. For references, see the newly edited extensive review by Steinhardt and Ostlund (1987). Since the fabrication and study (Merlin *et al* 1985) of deterministic aperiodic superlattices of semiconducting constituents, the activity within the field of one-dimensional quasiperiodic systems has been very intense. The dominant part of the work on one-dimensional quasiperiodic systems has been focused on Fibonaccian lattices. Here we wish to argue that this can in some sense be said to be misleading, since the special properties possessed by the Fibonaccian quasicrystal are not shared by all other aperiodic crystals. The chaotic nature of all the electronic eigenstates in a Fibonaccian quasicrystal may for instance not be typical (Riklund *et al* 1987, Severin and Riklund 1989). There still seems to be interesting physics to be discovered and understood within the field of non-Fibonaccian aperiodic crystals.

The Fibonaccian sequence can be generated by the inflational rule $A \rightarrow AB$ and $B \rightarrow A$. In the well known original interpretation due to Fibonacci in 1202, the first part of the rule means that a mother rabbit A in the next generation has a baby B. The second

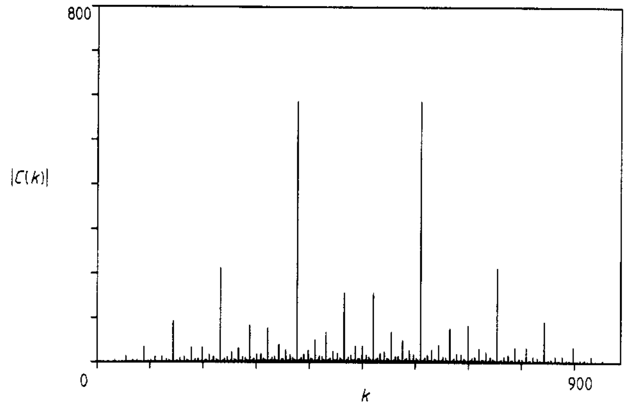

Figure 1. Fourier power spectrum for a Fibonacci sequence with $N = 987$. (Symbols are as defined in § 2.)

part of the rule then means that in the next generation the baby has grown up to be an adult mother. A very natural generalisation of that rule (Riklund and Severin 1988, Gumbs and Ali 1988) is to consider the case with birth of rabbit twins or triplets. The corresponding rules are then $A \to ABB$, $B \to A$ and $A \to ABBB$, $B \to A$, respectively. Let us denote these sequences and the corresponding aperiodic crystals with the symbols B2 and B3 and say that they belong to a family of sequences of aperiodic crystals called B. The general case $A \to ABBB \ldots B$, $B \to A$ with n Bs are similarly denoted by the symbol Bn. We will also consider the reverse sequence given by the substitutional rule $A \to AAA \ldots AB$, $B \to A$ with n As and this sequence is named the sequence An belonging to the family A. If we use this notation also for the case $n = 1$ both A1 and B1 should refer to the usual Fibonaccian sequence or quasicrystal. To avoid this double nature of the notation we will in the future when we refer to the family A or B only consider the extended cases with $n \geqslant 2$, unless otherwise stated.

2. Fourier transform

Consider a specific generation of length N and let in general the sequence considered be denoted by $c(j)$ where j goes from 0 to $N - 1$. The discrete Fourier transform is then given by (Schroeder 1986)

$$C(k) = \sum_{j=0}^{N-1} c(j) \exp(-2\pi i jk/N) \qquad k = 1, 2, \ldots, N.$$

To agree with the calculations in the above-mentioned book (Schroeder 1986), we will choose $c(j)$ equal to $+1$ if it corresponds to an A and -1 if it corresponds to a B. Other choices of the two possible values of $c(j)$ could be physically motivated, but since this does not influence our discussion, we will use this simple choice. The result will be represented by graphs showing the Fourier power spectrum, which is the absolute value $|C(k)|$ as a function of k for the different sequences studied.

3. Results and comparisons

As a reference we first show in figure 1 the Fourier power spectrum for the Fibonaccian case with $N = 987$. The corresponding Fourier spectrum for the family B (corresponding to several babies) is shown in figure 2(*a*)–(*d*) for $n = 2, 3, 4$, and 5 with $N = 1365, 1159, 1165$ and 781, respectively. The variation in N is due to the fact that we have always chosen whole generations for all sequences, although this is not necessary. The gross features of the structure, at least for larger values of n, is seen to be n humps separated by $(n - 1)$ empty regions. Inside these humps there is a blurred structure built up of very densely packed delta-spikes. The analogous result for the family A (with several As) is given in figure 3(*a*)–(*d*) for $n = 2$, 3, 4 and 5 with $N = 1393$, 1549, 1597 and 836, respectively. Here we see a very clear distinction between the two families. In the A case the dominant peaks are much more isolated and larger. Although harder, it is still possible to recognise the gross features with n humps as discussed above for the B family. It seems reasonable that it should be possible to detect the demonstrated difference in peaks by high resolution x-ray diffraction experiments. The natural question then arises as to whether there is a logical explanation for this remarkable discrepancy. Both the families considered can be generated by a matrix multiplication scheme (Lu *et al* 1986, Bombieri and Taylor 1986, 1987). The matrices $\mathbf{M}_{\mathrm{A}n}$ and $\mathbf{M}_{\mathrm{B}n}$ corresponding to generating the sequences An and Bn are respectively

$$\mathbf{M}_{\mathrm{A}n} = \begin{bmatrix} n & 1 \\ 1 & 0 \end{bmatrix} \qquad \mathbf{M}_{\mathrm{B}n} = \begin{bmatrix} 1 & n \\ 1 & 0 \end{bmatrix}.$$

The eigenvalues $A(n)_\pm$ and $B(n)_\pm$ are easily found to be

$$A(n)_\pm = \tfrac{1}{2}n \pm \sqrt{\tfrac{1}{4}n^2 + 1} \qquad B(n)_\pm = \tfrac{1}{2} \pm \sqrt{\tfrac{1}{4} + n}.$$

We show in table 1 the numerical values given by these formulae for n up to 10 for both families. To facilitate a comparison we have in both cases included the value for the Fibonacci sequence in the top row ($n = 1$). Note the monotonic variation with n in all the four columns. In the family A all the members with $n \geqslant 2$ have one eigenvalue greater than one and one with absolute value less than one. In the family B all the members with $n \geqslant 3$ have two eigenvalues with absolute value greater than one. It is to be noted that the Fibonaccian sequence in this sense belongs to the same class as the members in family A. Since the sequence B2 has one eigenvalue with absolute value greater than one and one eigenvalue with absolute value exactly equal to one, it can be said to be a marginal case. According to the definition given by Bombieri and Taylor (1986, 1987), the characteristic equation of the generating matrix should have exactly one eigenvalue greater than one to define quasicrystals as aperiodic crystals that diffract. Thus our findings are in agreement with the definition according to Bombieri and Taylor (1986, 1987), although our definition of the Fourier transform is not exactly the same. They consider a quasilattice with only one weight and instead vary the distances between the points, but this does not seem to be of importance for the global type of analysis of the structure of the Fourier transform we perform here.

4. Summary and outlook

We have confirmed the conjecture recently raised by Gumbs and Ali (1988) concerning the different physical properties of the two families of extensions of the Fibonaccian quasicrystal. The most natural extension called family B (letting the rabbit have multiplets) is shown to give an extension that is not in the same category as the original Fibonaccian quasicrystal. Referring to the definition due to Bombieri and Taylor (1986,

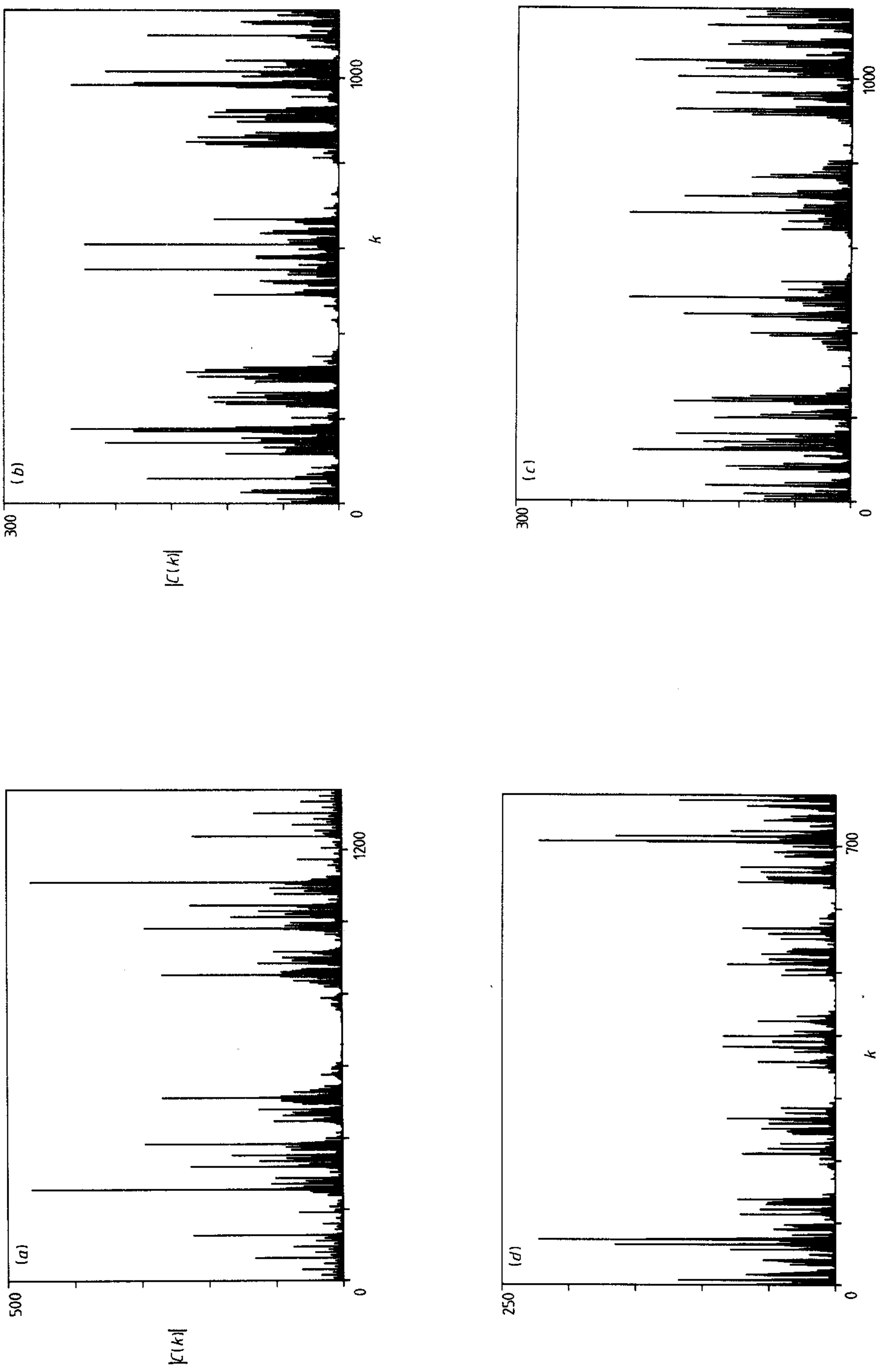

Figure 2. Fourier power spectrum for the sequences (*a*) B2, $N = 1365$; (*b*) B3, $N = 1159$; (*c*) B4, $N = 1165$; (*d*) B5, $N = 781$. (Symbols are as defined in § 2.)

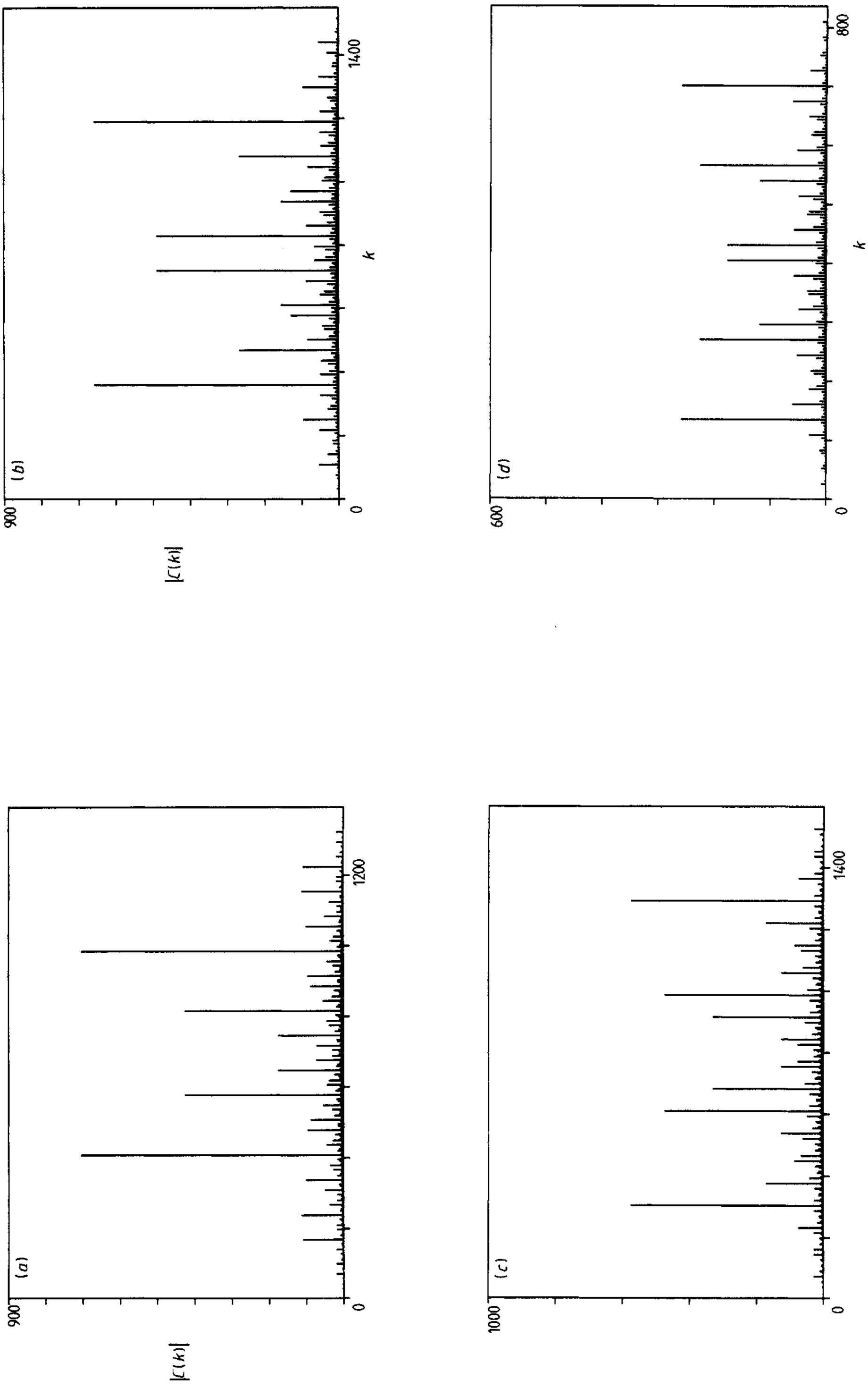

Figure 3. Fourier power spectrum for the sequences of family A. (*a*) A2, $N = 1393$; (*b*) A3, $N = 1549$, (*c*) A4, $N = 1597$ and (*d*) A5, $N = 836$. (Symbols are as defined in § 2.)

Table 1. The eigenvalues $A(n)_{\pm}$ and $B(n)_{\pm}$ of the generating matrices for the sequences An and Bn of the families A and B. The parameter n goes from 1 to 10. Note that the Fibonaccian case has also been included in the first row ($n = 1$).

n	$A(n)_+$	$A(n)_-$	$B(n)_+$	$B(n)_-$
1	1.6180340	−0.6180340	1.6180340	−0.6180340
2	2.4142136	−0.4142136	2.0000000	−1.0000000
3	3.3027756	−0.3027756	2.3027756	−1.3027756
4	4.2360680	−0.2360680	2.5615528	−1.5615528
5	5.1925824	−0.1925824	2.7911278	−1.7912878
6	6.1622777	−0.1622777	3.0000000	−2.0000000
7	7.1400549	−0.1400549	3.1925824	−2.1925824
8	8.1231056	−0.1231056	3.3722813	−2.3722813
9	9.1097722	−0.1097722	3.5413813	−2.5413813
10	10.0990195	−0.0990195	3.7015621	−2.7015621

1987) the B family should really be called an aperiodic crystal and not a quasicrystal because of the non-atomic diffraction properties. The reverse family A, however, diffracts very well as does the Fibonaccian quasicrystal.

In a further study we plan to relate these findings to the correlation functions of the different sequences. It should also be of great interest to see the consequences of these discrepancies between the two families considered for the structure of the electronic spectrum and the localisation character of the electronic eigenstates in a tight-binding model. The optical transmission through multilayers arranged according to sequences belonging to the two families studied above should also be different in character.

Acknowledgments

Financial support from the Swedish Natural Science Research Council is gratefully acknowledged.

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