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Scaling Properties of a Structure Intermediate between Quasiperiodic and Random

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We consider a one-dimensional structure obtained by stringing two types of "beads" (short and long bonds) on a line according to a quasiperiodic rule. This model exhibits a new kind of order, intermediate between quasiperiodic and random, with a singular continuous Fourier transform (i.e., neither Dirac peaks nor a smooth structure factor). By means of an exact renormalization transformation acting on the two-parameter family of circle maps that defines the model, we study in a quantitative way the local scaling properties of its Fourier spectrum. We show that it exhibits power-law singularities around a dense set of wavevectors q, with a local exponent $\gamma(q)$ varying continuously with the ratio of both bond lengths. Our construction also sheds some new light on the interplay between three characteristic properties of deterministic structures, namely: (1) a bounded fluctuation of the atomic positions with respect to their average lattice; (2) a quasiperiodic Fourier transform, i.e., made of Dirac peaks; and (3) for sequences generated by a substitution, the number-theoretic properties of the eigenvalue spectrum of the substitution.

KEY WORDS: Quasiperiodicity; inflation rules; circle maps; self-similarity.

1. INTRODUCTION

The aim of this paper is to analyze in detail the scaling properties of a one-dimensional geometrical structure, already considered in a recent work.[1] This structure is obtained by stringing two types of "beads" (short and long bonds) on a line, according to a quasiperiodic rule. We argued, using numerical evidence, that the diffraction spectrum of this structure is

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singular continuous. This means that its Fourier amplitude is neither discrete (Dirac peaks), as for periodic or quasiperiodic structures, nor absolutely continuous (smooth), as for the averaged structure factor of random structures. This type of order is therefore intermediate between quasiperiodic and random.

The possible existence of structures with such an intermediate kind of order already has been investigated.[2-6] In particular, Aubry[2] introduced the concept of "weak periodicity," a general property of classical ground states of translationally invariant short-range Hamiltonians. This concept describes a kind of deterministic order, which does not necessarily imply periodicity or quasiperiodicity. Hence, it includes a rich collection of looser and looser "ordered" structures. Number theory seems to play an important role in this field.

The present study concerns only geometrical characteristics of the model introduced in ref. 1, with emphasis on its scaling properties and their consequences for its Fourier spectrum. In Section 2, we recall the geometrical construction of the structure, as well as some of its basic properties. In Section 3, we introduce an exact renormalization transform acting on the two parameters ζ and Δ of the circle map involved in the model. This procedure leads to inflation rules on the binary sequence of short and long bonds defining the structure. These rules are best described by a substitution acting on three "letters." A similar approach was already introduced in ref. 6 for a particular case ($\Delta = 1/2$), where another type of renormalization transform was defined. The transform considered hereafter uses the approximation of Δ by multiples of ζ modulo 1, which is described in Appendix A. In Section 4, this transform is used to find the local (i.e., for fixed wavevector q) scaling behavior of the Fourier amplitude of the structure. The computation is performed in detail for a specific example, already considered in refs. 1 and 6, corresponding to the fixed point ($\zeta = \tau^{-2}, \Delta = 1/2$) of the renormalization transform. Here and in the following,

$$\tau = (\sqrt{5} + 1)/2 \tag{1.1}$$

denotes the golden mean. Our approach is akin to that of Bombieri and Taylor.[7] According to the classification of these authors, the present case is marginal, since the modulus of the second largest eigenvalue of the substitution matrix is 1. We give the analytical expression of the local scaling exponent $\gamma(q)$ of the Fourier amplitude for q belonging to some module, to be defined later. The self-similarity of the Fourier spectrum is also illustrated by a graphical representation in the complex plane. Section 5 is devoted to a discussion, where the rather technical results of the previous sections are placed in a general context.

2. THE MODEL

Let us recall briefly the construction of the model considered in ref. 1. The structure is defined by putting atoms on a line, the abscissa of the nth atom being given by

$$u_n - u_{n-1} = l_n; \qquad u_0 = 0 \tag{2.1}$$

The bond lengths l_n are chosen according to a quasiperiodic rule, namely the action of a "window" function of width Δ on the sequence ($n\zeta$ mod 1), where ζ (irrational) and Δ are given numbers between 0 and 1. The ζ was denoted l in refs. 1 and 4–6. We have

$$l_n = 1 + \xi\chi_n \tag{2.2}$$

where the binary sequence

$$\chi_n = \chi_\Delta(n\zeta) \tag{2.3}$$

is quasiperiodic, since $\chi_\Delta(x)$ is a 1-periodic function defined by

$$\chi_\Delta(x) = \mathrm{Int}(x) - \mathrm{Int}(x - \Delta) = \begin{Bmatrix} 1 & \text{if } 0 \leqslant \mathrm{Frac}(x) < \Delta \\ 0 & \text{if } \Delta \leqslant \mathrm{Frac}(x) < 1 \end{Bmatrix} \tag{2.4}$$

Here $\mathrm{Int}(x)$ and $\mathrm{Frac}(x) = x - \mathrm{Int}(x)$ denote the integer and fractional parts of x, respectively. It is easily seen that this sequence may also be generated by a circle map, as shown on Fig. 1. The third dimensionless parameter $\xi > -1$ is the difference between the lengths, 1 and $1 + \xi$, of both types of bonds. The interatomic mean distance (inverse density) of the model is

$$a = \lim_{n \to \infty} \frac{u_n}{n} = 1 + \xi\Delta \tag{2.5}$$

The "fluctuation"

$$\delta_n = u_n - na \tag{2.6}$$

of the atomic abscissas with respect to their average lattice (na) remains bounded with increasing n if, and only if, the window width Δ is a multiple of the rotation angle ζ mod 1, i.e.,

$$\Delta = \Delta_r = \mathrm{Frac}(r\zeta), \tag{2.7}$$

for some integer r.[8,9] This condition is hereafter called the "Kesten condition." This result of number theory implies the absence of an average lattice when Δ does not fulfill the Kesten condition.

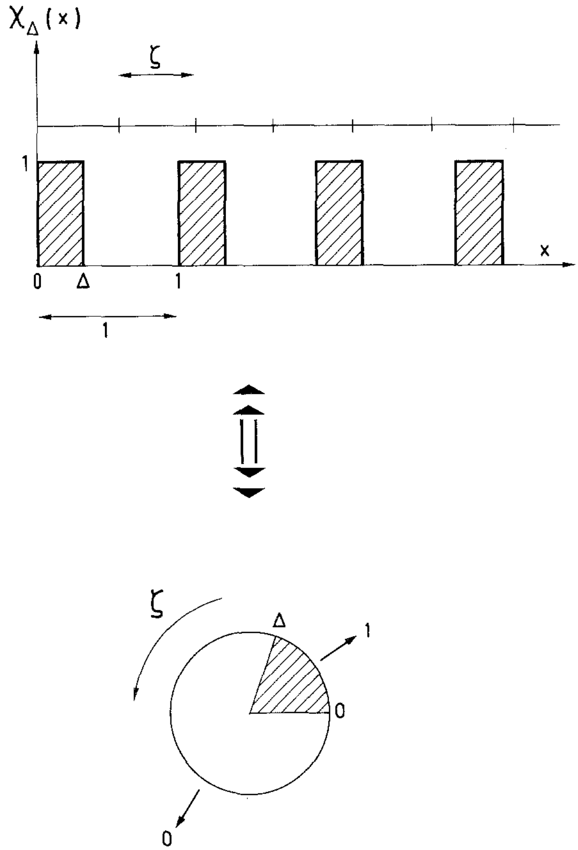

Fig. 1. The binary sequence (χ_n) can be generated by a circle map.

As noted in the introduction, we already studied, mainly by numerical means, the implications of these considerations for the Fourier spectrum of the structure. We will come back to this question in Section 3, where we derive the analytical expression of the above-mentioned local scaling index $\gamma(q)$, which had only been found numerically in ref. 1. Before doing so, we first describe a renormalization procedure that enables us to generate the binary sequence (χ_n) by a substitution acting on three letters.

3. A RENORMALIZATION TRANSFORM OF THE BINARY SEQUENCE GENERATED BY A CIRCLE MAP

Let us consider again the binary sequence $(\chi_n)_{n \geqslant 1}$ defined by Eq. (2.3). The purpose of this section is to show that this sequence can also be generated by iterating a set of renormalization operations that are determined both by the continued fraction expansion of ζ and the ζ expansion of Δ, to be defined below. In order to do so, we first need to recall some elementary results of number theory.

The continued fraction expansion of any number ζ $(0<\zeta<1)$ is defined by the expression

$$\zeta = \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\cdots}}} = [a_1, a_2, \ldots] \tag{3.1}$$

where the integer coefficients (quotients) a_n are determined by the recursion formula

$$a_{n+1} = \mathrm{Int}(1/\zeta_n) \tag{3.2}$$

The remainders ζ_n are given by

$$\zeta_{n+1} = \mathrm{Frac}(1/\zeta_n) \tag{3.3}$$

with the initial condition

$$\zeta_0 = \zeta \tag{3.4}$$

These definitions imply in particular

$$\zeta_n = \frac{1}{a_{n+1} + \zeta_{n+1}} = [a_{n+1}, \ldots] \tag{3.5}$$

The sequence of best rational approximations r_n/s_n to ζ is obtained by the vanishing of the remainders ζ_n in the continued fraction expansion. The recursion relations for the integers r_n and s_n are (for $n>1$)

$$r_n = a_n r_{n-1} + r_{n-2}; \qquad s_n = a_n s_{n-1} + s_{n-2} \tag{3.6}$$

with the initial conditions

$$r_0 = 0, \qquad s_0 = 1, \qquad r_1 = 1, \qquad s_1 = a_1 \tag{3.7}$$

We then have the useful relations

$$\zeta = \frac{r_n + r_{n-1}\zeta_n}{s_n + s_{n-1}\zeta_n}; \qquad \zeta_n = -\frac{s_n\zeta - r_n}{s_{n-1}\zeta - r_{n-1}} \tag{3.8}$$

We now define the best approximations of a given number Δ by integer multiples of ζ mod 1. A number $D = n\zeta - m$ is a best approximation to Δ if there exists $\varepsilon > 0$ such that (n, m) is the integer pair with the smallest positive n fulfilling the inequality

$$|\Delta - (n\zeta - m)| = |\Delta - D| < \varepsilon \tag{3.9}$$

When ε decreases to zero monotonically this condition determines a sequence of numbers D_i that converges to Δ.

1. When $\Delta = 0$, the sequence of best approximations of 0 by integer multiples of ζ mod 1 [fulfilling Eq. (3.9) with $\Delta = 0$] is wellknown.[10] It is given by

$$\delta_n = s_n\zeta - r_n = \frac{(-1)^n}{s_n + s_{n-1}\zeta_n} \tag{3.10}$$

The sign of δ_n alternates and its absolute value decreases monotonically to 0.

2. When $\Delta \neq 0$, we show in Appendix A that the sequence of best approximations of Δ is related to the following expansion of Δ in terms of the δ_n:

$$\Delta = \sum_{n=0}^{\infty} p_n \delta_n \tag{3.11}$$

The integers p_n and the remainders R_n are defined recursively by the relations

$$p_n = \mathrm{Min}\left[1 + \mathrm{Int}\left(\frac{R_n}{\delta_n}\right), a_{n+1}\right]; \qquad R_{n+1} = R_n - p_n\delta_n \tag{3.12}$$

with the initial condition

$$R_0 = \Delta < 1 \tag{3.13}$$

We are now able to derive an exact decimation procedure acting on the binary sequence (χ_n). This transform will involve three "letters" A, B, and C (although at the initial step there are only two symbols 0 and 1). We associate a sequence of letters W_n to the sequence of numbers $(\alpha_n = n\zeta)_{n \geqslant 1}$ by the rule

$$W_n \begin{cases} = A & \text{if} \quad 0 \leqslant \alpha_n < \mathrm{Inf}(\Delta, \zeta) \\ = B & \text{if} \quad \mathrm{Inf}(\Delta, \zeta) \leqslant \alpha_n < \mathrm{Sup}(\Delta, \zeta) \\ = C & \text{if} \quad \mathrm{Sup}(\Delta, \zeta) \leqslant \alpha_n < 1 \end{cases} \tag{3.14}$$

By choosing

$$\begin{aligned} &A \equiv 1 \\ &B \equiv 0 \quad \text{if} \quad \Delta < \zeta; \qquad B \equiv 1 \quad \text{if} \quad \zeta < \Delta \\ &C \equiv 0 \end{aligned} \tag{3.15}$$

the sequence (χ_n) of Eq. (2.3) is identical to (W_n). The set of return maps defined in Appendix A will now be used to construct a set of renormalization operations. These operations are products of four elementary transformations S, T_1, T_2, and T_3 that change both the values of ζ and Δ and the letters A, B, and C, but generate the same infinite sequence of letters (W_n). At each step, the elementary transformation is chosen according to the current values of ζ and Δ. The action of the renormalization transforms is also expressed in terms of the quotients a_n of the continued fraction expansion of ζ and of the coefficients p_n of the ζ expansion of Δ, defined above.

3.1. $1/2 < \zeta < 1$: Transformation S (see Fig. 2a)

The simplest transformation that leaves the binary sequence (χ_n) invariant occurs when

$$1/2 < \zeta < 1 \tag{3.16}$$

which is equivalent to

$$a_1 = 1 \tag{3.17}$$

in the continued fraction expansion of ζ. The initial sequence (W_n) of letters defined in Eq. (3.14) is not changed when ζ and Δ are changed into

$$\zeta' = 1 - \zeta; \qquad \Delta' = 1 - \Delta \tag{3.18}$$

and the letters (A, B, C) are changed into $(A', B', C') = S((A, B, C))$ according to

$$A' = C, \qquad B' = B, \qquad C' = A \tag{3.19}$$

Figure 2a shows that this transformation just consists in reversing the orientation of the unit circle. The sequence of coefficients (a_n') of the continued fraction expansion of ζ' is related to the initial sequence (a_n) (with $a_1 = 1$) through

$$a_1' = a_2 + 1; \qquad a_n' = a_{n+1} \quad \text{for} \quad n > 1 \tag{3.20}$$

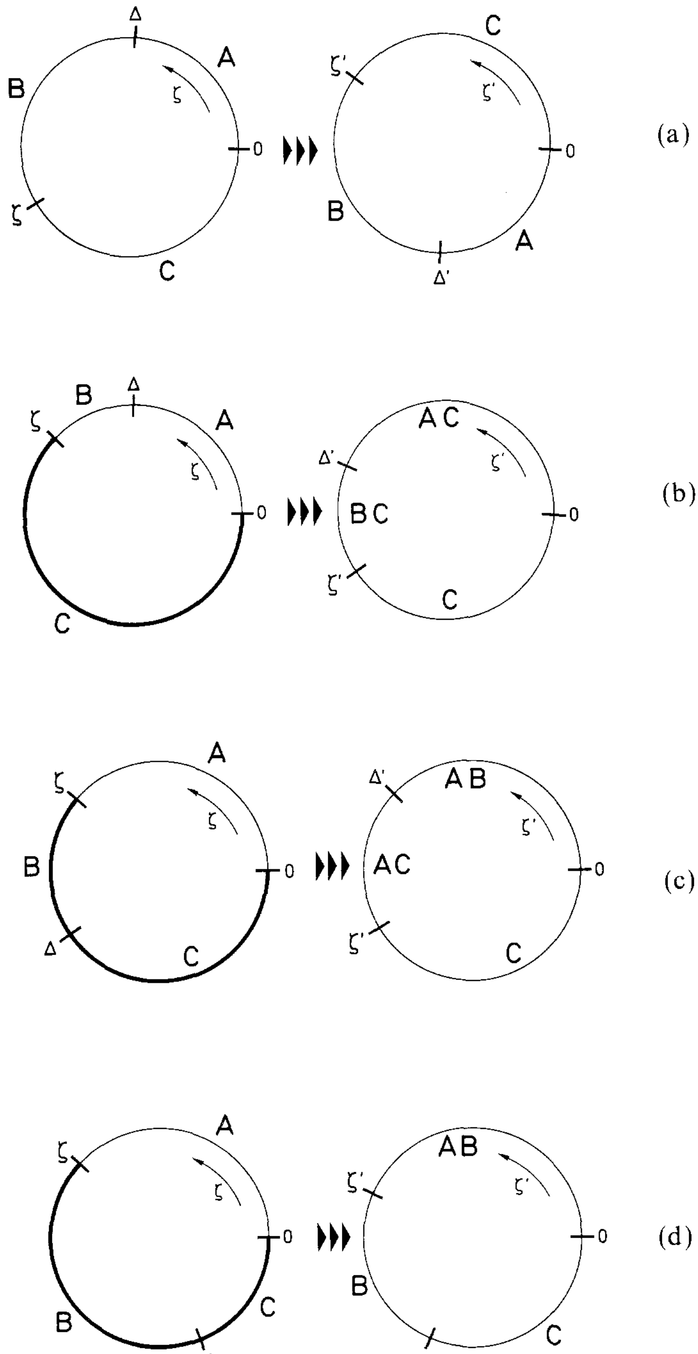

Fig. 2. Elementary renormalization transforms leaving the sequence (χ_n) invariant. (a) Transformation S, reversing the orientation of the circle, used for $1/2 < \zeta < 1$. (b) Return map on the arc shown by a heavy line, yielding the transformation T_1 $(0 < \zeta < 1/2; 0 < \Delta < \zeta)$. (c) Same as (b), for T_2 $(0 < \zeta < 1/2; \zeta < \Delta < 2\zeta)$. (d) Same as (b), for T_3 $(0 < \zeta < 1/2; 2\zeta < \Delta < 1)$.

The sequences (r'_n) and (s'_n) associated with ζ' by the recursion relation (3.6) are related to the initial sequences (r_n) and (s_n) for all $n \geqslant 0$ by

$$r'_n = s_{n+1} - r_{n+1}; \qquad s'_n = s_{n+1} \tag{3.21}$$

which yields

$$\delta'_n = s'_n \zeta' - r'_n = -s_{n+1}\zeta + r_{n+1} = -\delta_{n+1} \tag{3.22}$$

Therefore, the ζ' expansion of Δ' involves the sequence (p'_n) related to the initial sequence (p_n) (where $p_0 \neq 0$ is necessarily equal to $a_1 = 1$) by

$$p'_0 = 1 + p_1; \qquad p'_n = p_{n+1} \quad \text{for} \quad n > 1 \tag{3.23}$$

3.2. $0 < \zeta < 1/2$: Transformations T_1, T_2, T_3

The transformation S maps $\zeta > 1/2$ onto $\zeta' < 1/2$. We are thus led to study the case $0 < \zeta < 1/2$, characterized by $a_1 > 1$. The sequence of letters (W_n) can also be simply generated by the return map of the rotation with angle ζ into the interval $[\zeta, 1]$ (see Figs. 2b–2d). This return map is again a rotation with angle ζ on a circle of length $1 - \zeta$. By rescaling this circle to unity, the new rotation angle ζ' becomes

$$\zeta' = \zeta/(1 - \zeta) \tag{3.24}$$

The new sequence (a'_n) is related to the initial one (a_n) by

$$a'_1 = a_1 - 1; \qquad a'_n = a_n \quad \text{for} \quad n > 1 \tag{3.25}$$

The associated sequences (r'_n) and (s'_n) are given, for all $n \geqslant 0$, by

$$r'_n = r_n; \qquad s'_n = s_n - r_n \tag{3.26}$$

so that

$$\delta'_n = s'_n \zeta' - r'_n = \delta_n/(1 - \zeta) \tag{3.27}$$

The letters (A, B, C) that are ascribed to the different parts of this circle must be changed according to different rules, depending on the values of Δ relative to ζ and 2ζ.

$0 < \Delta < \zeta$: *Transformation* T_1 (see Fig. 2b). When

$$0 < \Delta < \zeta \tag{3.28}$$

the new value Δ' of Δ is

$$\Delta' = \Delta/(1 - \zeta) \tag{3.29}$$

and the new letters $(A', B', C') = T_1((A, B, C))$ are given by

$$A' = AC, \qquad B' = BC, \qquad C' = C \tag{3.30}$$

Since $a_1 > 1$, using Eqs. (A.7)–(A.9), one finds that Eq. (3.28) is equivalent to

$$p_0 = 1 < a_1 \tag{3.31}$$

which implies that $p_1 > 0$. Then, using Eqs. (3.26) and (3.27) one finds that for all n

$$p'_n = p_n \tag{3.32}$$

$\zeta < \Delta < 2\zeta$: *Transformation* T_2 (see Fig. 2c). The second case corresponds to

$$\zeta < \Delta < 2\zeta \tag{3.33}$$

Using the same arguments as above, it is easily seen that the new value Δ' of Δ reads

$$\Delta' = (\Delta - \zeta)/(1 - \zeta) \tag{3.34}$$

and that the new letters $(A', B', C') = T_2((A, B, C))$ are given by

$$A' = AB, \qquad B' = AC, \qquad C' = C \tag{3.35}$$

Using Eqs. (A.7)–(A.9), we find that Eq. (3.33) is satisfied if and only if both conditions

$$p_0 = 2 \qquad \text{and} \qquad p_1 > 0 \tag{3.36}$$

hold. Using Eqs. (3.26) and (3.27), one gets

$$p'_0 = 1; \qquad p'_n = p_n \quad \text{for} \quad n > 1 \tag{3.37}$$

$2\zeta < \Delta < 1$: *Transformation* T_3 (see Fig. 2d). Finally, the third case corresponds to

$$2\zeta < \Delta < 1 \tag{3.38}$$

The new value Δ' of Δ still reads

$$\Delta' = (\Delta - \zeta)/(1 - \zeta) \tag{3.39}$$

and the new letters $(A', B', C') = T_3((A, B, C))$ are given by

$$A' = AB, \qquad B' = B, \qquad C' = C \tag{3.40}$$

The condition (3.38) is fulfilled either when

$$p_0 > 2 \qquad \text{or} \qquad p_1 = 0 \qquad (\text{then } p_0 = a_1) \tag{3.41}$$

Using Eq. (3.12), one gets

$$p'_0 = p_0 - 1; \qquad p'_n = p_n \quad \text{for} \quad n > 1 \tag{3.42}$$

In Summary,

S applies when $a_1 = 1$ and is defined by Eqs. (3.19)–(3.23).

T_1 applies when $a_1 > 1$ and $p_0 = 1$ and is defined by Eqs. (3.30)–(3.32).

T_2 applies when $a_1 > 1$, $p_0 = 2$, and $p_1 > 0$ and is defined by Eqs. (3.35)–(3.37).

T_3 applies when $a_1 > 1$ and either $p_0 > 2$ or $p_1 = 0$ and is defined by Eqs. (3.40)–(3.42).

Figure 3 shows in which domain of the unit square ($0 \leqslant \zeta, \Delta \leqslant 1$) each of these transforms holds. When $a_1 = 1$, S first drops the first term of each sequence (a_n) and (p_n), then adds 1 to the first term of both remaining sequences. Thus, it cannot be applied twice consecutively, because a'_1 is always larger than 1. The operation T_1, T_2, or T_3 reduces a_1 by one unit, as well as p_0 if not equal to 1. A sequence of renormalization operations is then uniquely determined by the sequences (a_n) and (p_n).

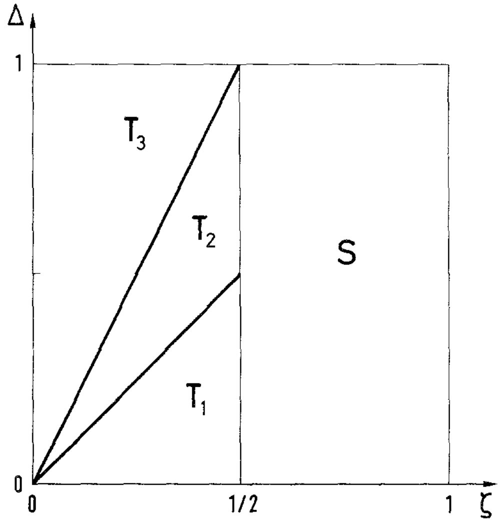

Fig. 3. Partition of the parameter space ($0 < \Delta, \zeta < 1$) into regions where the elementary transforms S, T_1, T_2, and T_3 hold.

The case where both of these sequences are periodic (or at least become periodic after some order) is of special interest. In this case, there exists a unique renormalization operation on the letters A, B, and C. It is the product of transforms S and T_i corresponding to the common period of these sequences. Such values of (ζ, Δ) will be said to be renormalizable. Let us describe explicitly a simple example. The simplest irrational number with a periodic continued fraction expansion is the inverse golden mean $\zeta = \tau^{-1} = (\sqrt{5}-1)/2$, characterized by $a_i = 1$ for all i. Then, $s_{n-1} = r_n = F_n$, where F_n denote the Fibonacci numbers defined by the recursion relation

$$F_n = F_{n-1} + F_{n-2}(F_0 = 0; F_1 = 1) \tag{3.43}$$

and we have

$$\delta_n = F_{n+1}\zeta - F_n = (-1)^n/\tau^{n+1} \tag{3.44}$$

If the ζ expansion of Δ has period 1, $p_i = 1$ for all i and $\Delta = \tau^{-2} = 1 - \tau^{-1}$ fulfills the Kesten condition introduced in Section 2. If the ζ expansion of Δ has period 2, e.g., $p_{2i} = 1$ and $p_{2i+1} = 0$ for all i, $\Delta = 1$ yields a trivial model. Hence 3 is the smallest periodicity of the ζ expansion of Δ yielding a nontrivial case that does not fulfill the Kesten condition. Then

$$p_{3i+1} = p_1, \quad p_{3i+2} = p_2, \quad p_{3i+3} = p_3 \quad \text{for all} \quad i \geqslant 0 \quad (\text{with } p_0 = 1) \tag{3.45}$$

There are three possible values of Δ, namely

$$\begin{aligned} &p_1 = p_2 = 1 \quad \text{and} \quad p_3 = 0; && \Delta = 1/2 \\ &p_2 = 0 \quad \text{and} \quad p_1 = p_3 = 1; && \Delta = 1 - \tfrac{1}{2}\tau^{-1} \\ &p_1 = 0 \quad \text{and} \quad p_2 = p_3 = 1; && \Delta = \tfrac{1}{2}\tau^{-2} \end{aligned} \tag{3.46}$$

The first case $(\zeta = \tau^{-1}, \Delta = 1/2)$ is the image by S of the case $(\zeta = \tau^{-2}, \Delta = 1/2)$, already studied in refs. 1 and 6. For the sake of notational consistency, we will still use this parametrization in the following:

$$\zeta = \tau^{-2}, \qquad \Delta = 1/2 \tag{3.47}$$

According to the results of this section, the associated sequence of renormalization operations is periodic, and its period consists of T_2, S, T_3, S, T_1, S applied successively. The renormalization operation on the letters corresponding to the product

$$T = ST_1ST_3ST_2 \tag{3.48}$$

is defined by $T((A, B, C)) = (A', B', C')$ with

$$A' = CAC, \qquad B' = ACCAC, \qquad C' = ABCAC \tag{3.49}$$

The parameters ζ and Δ are invariant under the application of this renormalization operation. This case provides the simplest example for which the scaling properties of the Fourier transform of the structure associated with the sequence (χ_n) will clearly appear.

More generally, we can consider a larger class of quasiperiodic sequences of letters. They are also defined by a rotation of angle ζ on the unit circle. Consider the points 0, ζ, and p arbitrary other points Δ_i $(1 \leqslant i \leqslant p)$ on the circle, defining $(p+1)$ intervals. By ascribing to each of these intervals a different letter A, B, C, D,..., a quasiperiodic sequence of letters is then defined. The return map method, used to build the renormalization operations described above, can also be applied, but the number of possible elementary transformations T_i becomes much larger.

We end this section by noting that a similar renormalization scheme has been used in another context in ref. 11.

4. SCALING PROPERTIES OF THE FOURIER SPECTRUM

In this section, we show how the renormalization transform introduced in Section 3 can be used to study the structure factor (Fourier transform) of the model, at least for some values of the rotation number ζ and the window width Δ. Of special interest are the renormalizable values of the couple (ζ, Δ), i.e., those values that are left unchanged by some product of elementary transforms S and T_i defined above. For sake of definiteness and simplicity, we focus our attention on the example $(\zeta = \tau^{-2}; \Delta = 1/2)$, already considered in refs. 1 and 6, and quoted above.

Before we proceed to an actual derivation of the local properties of the Fourier transform of our model, let us recall some basic definitions and properties of Fourier spectra.

For any finite number N of atoms, consider the partial Fourier sums

$$G_N(q) = \sum_{k=1}^{N} \exp(iqx_k) \tag{4.1}$$

where the x_k are the atomic abscissas of the model, given by Eqs. (2.1)–(2.3). Define the associated static structure factor

$$S_N(q) = \frac{1}{N} |G_N(q)|^2 \tag{4.2}$$

and the intensity measure $dH_N(q) = S_N(q)\,dq$. In the thermodynamic limit, $dH_N(q)$ converges toward a positive measure $dH(q)$, known as the spectral (intensity) measure of the structure. In other words, it turns out that only the quantity

$$H(q) = \lim_{N \to \infty} \int_0^q S_N(q')\,dq' \tag{4.3}$$

is a well-defined nondecreasing function, called the distribution function, or integrated density, of the intensity measure. The structure factor of the infinite structure has the formal definition

$$dH(q) = S(q)\,dq \tag{4.4}$$

which does not lead to a function $S(q)$ in general, but rather to a generalized function (distribution). Such a notational prudence is needed when dealing with singular measures, which is precisely the purpose of this paper.

In a periodic or quasiperiodic structure, there are values q_0 of q such that $G(q_0) \approx C(q_0)N$, $C(q_0)$ being some complex amplitude. $H(q)$ then has a discontinuity of strength $|C(q_0)|^2$ at $q = q_0$, and the structure factor $S(q)$ contains a Dirac peak: $|C(q_0)|^2\,\delta(q - q_0)$. These values q_0 form a reciprocal lattice in the periodic case and a dense module in the quasiperiodic case. In amorphous systems, the averaged structure factor $S(q)$ is usually a smooth function: $G_N(q)$ grows typically as $N^{1/2}$.

In the present case, it will be shown in the following that there is a dense set of values q_0 of q for which $G_N(q_0)$ grows as $N^{\gamma(q_0)}$, with $1/2 < \gamma(q_0) < 1$. In particular, for the values q_0 of the form (4.23), $\gamma(q_0)$ will be given by Eq. (4.36). It should now be clear that this result implies, as far as the local properties of the Fourier spectrum are concerned, an intermediate kind of behavior between quasiperiodic and random. More precisely, let q_0 be a value of q of the form (4.23) such that $1/2 < \gamma < 1$. We then have $S_N(q_0) \approx N^{2\gamma - 1}$. Moreover, for q close enough to q_0, S_N can only depend on q through the scaling form

$$S_N(q) \approx N^{2\gamma - 1}\mathbb{S}[N(q - q_0)] \tag{4.5}$$

This argument was introduced in ref. 1, where it was confirmed by numerical computations. An integration then yields

$$H_N(q) - H_N(q_0) \approx N^{2\gamma - 2}\mathbb{H}[N(q - q_0)] \tag{4.6}$$

Since the rhs of this expression is necessarily finite in the $N \to \infty$ limit [see

Eq. (4.3)], powers of N have to cancel out, and the result of ref. 1 is recovered as

$$|H(q) - H(q_0)| \approx |q - q_0|^{\alpha} \tag{4.7}$$

with

$$\alpha = 2(1 - \gamma) \tag{4.8}$$

If $1/2 < \gamma < 1$, then $0 < \alpha < 1$, and the intensity (structure factor) $S(q_0)$, which is formally equal to the derivative of $H(q)$ at q_0, is divergent (infinite), but "less infinite" than in the presence of a Dirac peak, which corresponds to $\gamma = 1$ ($\alpha = 0$). More precisely, experimental scattering data obtained with a finite resolution Δq will show a maximal intensity $S_{\max} \approx (\Delta q)^{\alpha - 1}$ in a region of width Δq centered around q_0, such that the peak area $\mathbb{A} \approx (\Delta q)^{\alpha}$ vanishes in the limit of high resolution ($\Delta q \to 0$). Of course, this area approaches $\mathbb{A}_0 = |C(q_0)|^2$, a nonzero limit, in the case of a Dirac peak. Let us now proceed to the quantitative study of these properties in the example under consideration.

The action of the renormalization transform T of Eq. (3.48) on the letters A, B, and C, corresponding to the intervals $[0; \tau^{-2}]$, $[\tau^{-2}; 1/2]$, and $[1/2; 1]$, respectively, has already been given in Eq. (3.49),

$$T: \begin{cases} A \to CAC \\ B \to ACCAC \\ C \to ABCAC \end{cases} \tag{4.9}$$

This substitution is the central object of the present study. Let us first introduce the matrix M associated with T. By definition, M relates the numbers n_A, n_B, n_C of letters of each type in any finite word W and the numbers n'_A, n'_B, n'_C of letters in the transformed word $T(W)$:

$$\begin{pmatrix} n'_A \\ n'_B \\ n'_C \end{pmatrix} = M \begin{pmatrix} n_A \\ n_B \\ n_C \end{pmatrix}, \quad \text{with} \quad M = \begin{pmatrix} 1 & 2 & 2 \\ 0 & 0 & 1 \\ 2 & 3 & 2 \end{pmatrix} \tag{4.10}$$

The characteristic polynomial of M is $P(x) = \det(x\mathbb{1} - M) = (x+1)(x^2 - 4x - 1)$, and hence the eigenvalues of M are τ^3, -1, and $-\tau^{-3}$. The (right) eigenvector associated with the leading eigenvalue τ^3 reads $(\tau^{-2}; \tau^{-3}/2; 1/2)$. These components are the lengths of the corresponding intervals of the circle, as they should be. Indeed, these components give the relative frequencies at which the different letters occur in any infinite word of the form $\lim_{n \to \infty} T^n(W_0)$ for an arbitrary initial W_0.

In ref. 6, we introduced a different renormalization transform T_4, valid only for $\Delta = 1/2$, acting on four symbols, denoted by a, b, c, d. The T_4 also admits ($\zeta = \tau^{-2}$; $\Delta = 1/2$) as a fixed point. The associated matrix is

$$M_4 = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 2 & 1 & 2 & 2 \\ 2 & 2 & 1 & 2 \\ 1 & 0 & 1 & 0 \end{pmatrix} \tag{4.11}$$

Its eigenvalues read τ^3, -1, -1, and $-\tau^{-3}$. Hence M_4 has an extra eigenvalue (-1) with respect to M. Clearly, both mappings T and T_4 have to describe the same object. It can indeed be checked that the action of M is equivalent to that of M_4 in the three-dimensional subspace defined by $x_1 = x_4$, if $x_1 \cdots x_4$ are the coordinates in the linear space where M_4 acts.

The easiest way to deal with Fourier transforms is to leave the initial conditions unspecified and to consider the three infinite sequences of words $(n \geqslant 0)$

$$U_n = T^n(A); \qquad V_n = T^n(B); \qquad W_n = T^n(C) \tag{4.12}$$

Let ν_n^u, ν_n^v, ν_n^w denote the total numbers of letters (atoms) in these words. These quantities obey the recursion relation

$$\begin{pmatrix} \nu_{n+1}^u \\ \nu_{n+1}^v \\ \nu_{n+1}^w \end{pmatrix} = M^t \begin{pmatrix} \nu_n^u \\ \nu_n^v \\ \nu_n^w \end{pmatrix} \tag{4.13}$$

where M^t is the transposed matrix of M, and hence

$$\begin{pmatrix} \nu_n^u \\ \nu_n^v \\ \nu_n^w \end{pmatrix} = (M^t)^n \begin{pmatrix} \nu_0^u \\ \nu_0^v \\ \nu_0^w \end{pmatrix} \tag{4.14}$$

A simple recursive calculation yields

$$(M^t)^n = \begin{pmatrix} F_{3n-1} & \frac{1}{2}[F_{3n-2} + (-)^n] & \frac{1}{2}[F_{3n+1} - (-)^n] \\ F_{3n} & \frac{1}{2}[F_{3n-1} + (-)^n] & \frac{1}{2}[F_{3n+2} - (-)^n] \\ F_{3n} & \frac{1}{2}[F_{3n-1} - (-)^n] & \frac{1}{2}[F_{3n+2} + (-)^n] \end{pmatrix} \tag{4.15}$$

The obvious initial condition $\nu_0^u = \nu_0^v = \nu_0^w = 1$ gives

$$\nu_n^u = F_{3n+1}; \qquad \nu_n^v = \nu_n^w = F_{3n+2} \tag{4.16}$$

Let now l_n^u, l_n^v, and l_n^w denote the lengths of the words U_n, V_n, and W_n, respectively. These quantities also obey Eq. (4.13). The initial condition $l_0^u = l_0^v = 1 + \xi$, $l_0^w = 1$, combined with Eq. (2.5) giving the value of the mean interatomic distance a, yields

$$\begin{aligned} l_n^u &= aF_{3n+1} + (a-1)(-)^n \\ l_n^v &= aF_{3n+2} + (a-1)(-)^n \\ l_n^w &= aF_{3n+2} - (a-1)(-)^n \end{aligned} \tag{4.17}$$

The first terms on the rhs of these equations are the expected leading terms, equal to the product of a by the numbers of atoms. The second terms are related to the fluctuation δ_n, which has been shown in refs. 4 and 5 to destroy the average lattice of the structure. It will turn out that these oscillatory terms are also responsible for the absence of Dirac peaks in the Fourier spectrum. The presence of such correction terms in Eq. (4.17), which do not vanish in the $n \to \infty$ limit, obviously originates in the eigenvalue (-1) of M lying on the unit circle. The interplay between subleading eigenvalues of substitutions and Fourier transforms has already been considered in ref. 7. We will comment some more on these general aspects in the discussion. Let us just recall here that the present situation (one eigenvalue on the unit circle) has been discarded in ref. 7 as being a marginal case.

We define the Fourier amplitudes of the words U_n, V_n, and W_n as

$$\begin{aligned} g_n^u &= \sum_{k=0}^{F_{3n+1}} \exp(iqx_k^u) \\ g_n^v &= \sum_{k=0}^{F_{3n+2}} \exp(iqx_k^v) \\ g_n^w &= \sum_{k=0}^{F_{3n+2}} \exp(iqx_k^w) \end{aligned} \tag{4.18}$$

where $x_0^u = 0$, and $x_k^u - x_{k-1}^u = (1+\xi)$ (resp. 1) if the kth letter of U_n is A or B (resp. C). The same construction holds for V_n and W_n. It follows from their definition (4.12) that these words satisfy

$$U_{n+1} = W_n U_n W_n; \qquad V_{n+1} = U_n W_n U_{n+1}; \qquad W_{n+1} = U_n V_n U_{n+1} \tag{4.19}$$

Their Fourier amplitudes therefore obey the recursions

$$\begin{aligned} g_{n+1}^u &= g_n^w + \exp(iql_n^w)\, g_n^u + \exp[iq(l_n^u + l_n^w)]\, g_n^w \\ g_{n+1}^v &= g_n^u + \exp(iql_n^u)\, g_n^w + \exp[iq(l_n^u + l_n^w)]\, g_{n+1}^u \\ g_{n+1}^w &= g_n^u + \exp(iql_n^u)\, g_n^v + \exp[iq(l_n^u + l_n^v)]\, g_{n+1}^u \end{aligned} \tag{4.20}$$

with the initial conditions

$$g_0^u = g_0^v = \exp[iq(1+\xi)]; \qquad g_0^w = \exp(iq) \tag{4.21}$$

For generic values of the wavevector q, the phases such as $\exp(iql_n^u)$ form complicated aperiodic sequences, and hence the behavior of the Fourier amplitudes as functions of the word sizes seems very difficult to predict in general. Their asymptotic growth as $n \to \infty$ can, however, be extracted from Eq. (4.20), for those values of q for which all the phases entering this equation have a simple limit behavior, such as, e.g., a limit cycle. Hence, this study will only give local information on the spectrum at a dense but countable set of values of q. The oscillatory character of the correction terms $(a-1)(-)^n$ in Eq. (4.17) leads us to treat even and odd values of n separately, and hence to consider the sequences of numbers

$$X_n^{(p)} = qaF_{6n+p} (\mathrm{mod}\ 2\pi) \tag{4.22}$$

for fixed p between 0 and 5. The simplest possible behavior for these sequences is convergence to some limits $\theta_p = \lim_{n\to\infty} X_n^{(p)}$. It is proved in Appendix B that this convergence occurs if and only if q has the form

$$qa/2\pi = \tfrac{1}{4}(j + k\tau) \tag{4.23}$$

where j, k are (positive or negative) integers. The limits are readily obtained from the values of $F_p (\mathrm{mod}\ 4)$:

$$\begin{aligned} &\theta_0 = \frac{\pi}{2} k; && \theta_1 = \frac{\pi}{2}(j+k); && \theta_2 = \frac{\pi}{2}(j+2k) \\ &\theta_3 = \frac{\pi}{2}(2j-k); && \theta_4 = \frac{\pi}{2}(k-j); && \theta_5 = \frac{\pi}{2} j \end{aligned} \tag{4.24}$$

We now define an angle φ through

$$\varphi = q(a-1) = \frac{\pi}{2}\frac{\xi}{2+\xi}(j+k\tau) \tag{4.25}$$

in terms of which all the required phases have simple limits, namely

$$\begin{aligned} &ql_{2n}^u \to \theta_1 + \varphi; && ql_{2n}^v \to \theta_2 + \varphi; && ql_{2n}^w \to \theta_2 - \varphi \\ &ql_{2n+1}^u \to \theta_4 - \varphi; && ql_{2n+1}^v \to \theta_5 - \varphi; && ql_{2n+1}^w \to \theta_5 + \varphi \end{aligned} \tag{4.26}$$

(mod 2π) as $n \to \infty$. These limits are reached exponentially rapidly (with τ^{-6n} corrections). Equation (4.26) allows us to write the asymptotic form of the recursion relations (4.20) as follows:

$$\begin{pmatrix} g^u_{2n+1} \\ g^v_{2n+1} \\ g^w_{2n+1} \end{pmatrix} = M_1(q) \begin{pmatrix} g^u_{2n} \\ g^v_{2n} \\ g^w_{2n} \end{pmatrix}; \qquad \begin{pmatrix} g^u_{2n+2} \\ g^v_{2n+2} \\ g^w_{2n+2} \end{pmatrix} = M_2(q) \begin{pmatrix} g^u_{2n+1} \\ g^v_{2n+1} \\ g^w_{2n+1} \end{pmatrix} \tag{4.27}$$

where $M_1(q)$ and $M_2(q)$ are now two constant complex matrices:

$$M_1(q) = \begin{pmatrix} e^{i(\theta_2 - \varphi)} & 0 & 1 + e^{i\theta_3} \\ 1 + e^{i(\theta_4 - \varphi)} & 0 & e^{i(\theta_1 + \varphi)} + e^{i\theta_3} + e^{2i\theta_0} \\ 1 + e^{i(\theta_4 + \varphi)} & e^{i(\theta_1 + \varphi)} & e^{i(\theta_3 + 2\varphi)} + e^{2i(\theta_0 + \varphi)} \end{pmatrix}$$

$$M_2(q) = \begin{pmatrix} e^{i(\theta_5 + \varphi)} & 0 & 1 + e^{i\theta_0} \\ 1 + e^{i(\theta_1 + \varphi)} & 0 & e^{i(\theta_4 - \varphi)} + e^{i\theta_0} + e^{2i\theta_3} \\ 1 + e^{i(\theta_1 - \varphi)} & e^{i(\theta_4 - \varphi)} & e^{i(\theta_0 - 2\varphi)} + e^{2i(\theta_0 - \varphi)} \end{pmatrix} \tag{4.28}$$

These matrices depend on q, i.e., on the integers j and k, through both the θ_p and φ. They also depend on the parameter ξ in a continuous way through φ. For $q=0$, Eq. (4.13) is recovered, as it should be, since $M_1(0) = M_2(0) = M^t$.

The asymptotic behavior of the Fourier amplitudes for q given by Eq. (4.23) is now very simple to obtain. If Λ denotes the (possibly complex) largest eigenvalue of the matrix product $M_1(q)\, M_2(q)$, then we have

$$|g^u_n| \approx |g^v_n| \approx |g^w_n| \approx |\Lambda|^{n/2} \tag{4.29}$$

Since the word lengths (numbers of atoms) grow as τ^{3n} [see Eq. (4.16)], the above result implies the following power-law relation between the size N of a finite sample of the structure and its Fourier amplitude G_N:

$$G_N \approx N^\gamma \qquad \text{with} \quad \gamma = (\ln |\Lambda|)/(6 \ln \tau) \tag{4.30}$$

The general considerations of the beginning of this section show that the local scaling exponent γ has to obey the inequalities $0 \leqslant \gamma \leqslant 1$.

Let us now give the value of the exponent γ for any wavevector q of the form (4.23). We have shown that this exponent is related by Eq. (4.30) to the largest eigenvalue of the matrix product $M_1(q)\, M_2(q)$; these matrices are themselves explicitly given in Eq. (4.28). A standard but tedious calculation of the matrix product and of its characteristic polynomial

$$P(x) = \det[x\mathbb{1} - M_1(q)\, M_2(q)] \tag{4.31}$$

yields

$$P(x) = (x-1)[x^2 - \sigma x + (-)^k] \tag{4.32}$$

with

$$\sigma = 2 + 2(-)^k + (-)^j + (-)^{j+k} + [(-)^j + 1]\chi_k + \{\chi_j\chi_k + [(-)^k + 1]\chi_j\} \cos\varphi + \{\omega_j\omega_k + [(-)^k - 1]\chi_j\} \sin\varphi \tag{4.33}$$

and where $\chi_n = i^n + i^{-n}$ and $\omega_n = -i(i^n - i^{-n})$. These quantities are functions of n (mod. 4) only, and

$$\begin{array}{llll} \chi_0 = 2; & \chi_1 = 0; & \chi_2 = -2; & \chi_3 = 0 \\ \omega_0 = 0; & \omega_1 = 2; & \omega_2 = 0; & \omega_3 = -2 \end{array} \tag{4.34}$$

The eigenvalues are therefore given by

$$\begin{array}{lll} k \text{ even:} & x = e^{\mu}, 1, e^{-\mu} & \text{with } 2\cosh\mu = \sigma \\ k \text{ odd:} & x = e^{\mu}, 1, -e^{-\mu} & \text{with } 2\sinh\mu = \sigma \end{array} \tag{4.35}$$

The largest eigenvalue Λ, yielding the scaling exponents γ and α through Eqs. (4.30) and (4.8), is such that $|\Lambda| = \exp|\mu|$ in both cases, and hence

$$\gamma = |\mu|/(6 \ln \tau) \tag{4.36}$$

According to the values of the integers j and k (mod 4), Eqs. (4.33)–(4.35) yield different analytical forms for the "dispersion relation" giving μ (i.e., the scaling exponents) as a continuous function of φ (i.e., the parameter ξ and the wavevector q). The 16 possible values of (j, k) (mod 4) lead to three different kinds of behavior, described just below. Figure 4 summarizes the discussion.

(I) No singularity at all, i.e., $\mu = 0$, $\gamma = 0$, and $\alpha = 1$, for all values of the angle φ. This occurs for six values of the couple (j, k) (mod 4), namely $k = 2$ (any j) and $k = 0$ (and $j = 1$ or 3).

(II) Nondivergent singularity: γ varies in a continuous way between 0 and $\gamma_{\max} = 1/2$ as a function of the angle φ. This occurs for eight values of the couple (j, k) (mod 4), namely $k = 1$ or 3 (any j). The dispersion relation then reads

$$\begin{array}{l} k = 1 \text{ (mod 4)} \Rightarrow \sigma/2 = \sinh\mu = (\omega_j - \chi_j)\sin\varphi \\ k = 3 \text{ (mod 4)} \Rightarrow \sigma/2 = \sinh\mu = -(\omega_j + \chi_j)\sin\varphi \end{array} \tag{4.37}$$

$\gamma_{\max} = 1/2$ occurs when $\sin\varphi = \pm 1$ in both cases.

(III) Possibly divergent singularity: γ varies in a continuous way between 0 and $\gamma_{\max} = 1$ as a function of the angle φ. This occurs for the

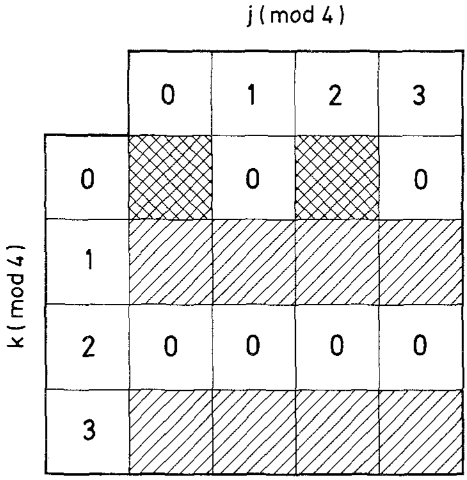

Fig. 4. Behavior of the local scaling exponent γ as a function of j and k (mod 4): Class I (no singularity at all) is denoted by 0. Class II (nondivergent singularity) corresponds to shaded areas. Class III, (possibly divergent singularity) corresponds to cross-hatched areas.

remaining two 2 values of the couple (j, k) (mod 4), namely $k=0$ and $j=0$ or 2. The dispersion relation then reads

$$\left| \begin{array}{l} j=0 \text{ (mod 4)} \Rightarrow \sigma/2=\cosh\mu=5+4\cos\varphi \\ j=2 \text{ (mod 4)} \Rightarrow \sigma/2=\cosh\mu=5-4\cos\varphi \end{array} \right. \tag{4.38}$$

A divergent structure factor $S(q)$ (a peak) is observed if and only if $H(q)$ is not differentiable, i.e., for $\alpha<1$ or $\gamma>1/2$, as mentioned below Eq. (3.8). This occurs whenever the angle φ obeys the inequality

$$(-)^{j/2}\cos\varphi>(\sqrt{5}-5)/4= -0.690983 \tag{4.39}$$

For a given structure, i.e., a given value of the parameter ξ, the "peak condition" (4.39) will be satisfied for some of the wavevectors of class (III).

Let us give an example of these analytical results by considering the case studied in ref. 1: $q=3\pi/a$ (i.e., $j=6$, $k=0$) and $\xi=2$. Equations (4.25) and (4.38) then yield $\varphi=3\pi/2$, and $\cosh\,\mu=5$. We have therefore $\Lambda=e^{\mu}=5+2\sqrt{6}$ and $\gamma=\mu/(6\ln\tau)=0.793979>1/2$. The scaling index λ introduced in ref. 1 is just $\lambda=\Lambda/\tau^6$. Hence we have $\lambda=(5+2\sqrt{6})/\tau^6=0.551651$, in excellent agreement with the numerical value $\lambda\approx0.552$ of ref. 1, extracted from a numerical scaling analysis, based on a different approach, namely the approximation of $\Delta=1/2$ by a sequence of values Δ_r fulfilling Eq. (2.7).

We now aim to exhibit which values of q and ξ lead to a maximal scaling exponent $\gamma = 1$, since this particular value corresponds formally to a Dirac peak. Any wavevector q belonging to class (III) can be written as

$$\frac{qa}{2\pi} = \frac{J}{2} + K\tau \tag{4.40}$$

with the notation $j = 2J$ and $k = 4K$, where J and K are now arbitrary integers. According to Eqs. (4.36) and (4.38), $\gamma = 1$ occurs whenever cosh $\mu = 9$, i.e., $(-)^J \cos \varphi = 1$, and hence $\varphi = (2M + J)\pi$, for some integer M. This condition determines uniquely q and ξ as follows:

$$q = 2\pi(K\tau - M); \qquad \xi = \frac{2M + J}{K\tau - M} \tag{4.41}$$

For any values of the rotation number ζ and the window width Δ that do not obey the Kesten condition (2.7), the only possible Dirac peaks are expected to be trivial Dirac peaks, for q multiple of $2\pi y$, if the parameter $\xi = x/y$ is rational. We hope to give a general proof of this assertion in a further publication. These peaks are recovered by taking $K = 0$ in Eq. (4.41). What occurs for $K \neq 0$ is more subtle: when ξ tends toward a value given by (4.41), the exponent γ of the structure factor at the corresponding value of q indeed goes to unity in a continuous way, but the associated amplitude of the singularity (4.30) vanishes in such a way that there is no Dirac peak in the limit structure. The occurrence of this striking discontinuous kind of behavior has been checked by a numerical iteration of Eq. (4.20).

We have been led to study values of q of the form (4.23) by an argument of simplicity: these are the values of the wavevector for which the asymptotic behavior of the sequences $X_n^{(p)}$ of Eq. (4.22) is the simplest, namely convergence to limit values θ_p. More general values of q, corresponding to limit cycles for the sequences $X_n^{(p)}$, are also tractable along the very same lines as we did previously. A general method for finding these values of q is given in Appendix B. For instance, the values of q

$$\frac{qa}{2\pi} = \frac{1}{40}\,[J(2 + \tau) + K(3 - \tau)] \tag{4.42}$$

where J and K are two integers, yield a limit two-cycle, namely $X_{2n}^{(p)} \to \theta'_p$ and $X_{2n+1}^{(p)} \to \theta''_p$. For any value of q such that the $X_n^{(p)}$ of Eq. (4.22) admit a (p-dependent) limit m-cycle ($m \geqslant 1$), the asymptotic form of Eq. (4.20) involves $2m$ constant matrices $M_1(q),\ldots, M_{2m}(q)$, and the entries of those matrices depend on $6m$ limit angles. The associated Fourier amplitude still grows according to a power law, namely

$$g_N \approx N^{\gamma} \qquad \text{with} \quad \gamma = (\ln |A|)/(6m \ln \tau) \tag{4.43}$$

where A is now the largest eigenvalue of the ordered matrix product $M_1(q) \cdots M_{2m}(q)$. The complexity of the calculation hence increases drastically with the length m of the limit cycles.

We end this section by two numerical illustrations of our results. Figure 5 shows plots of numerical values of the structure factor $S_N(q)$ defined in Eq. (4.2) corresponding to the values (a) $\xi = \sqrt{2}$ and (b) $\xi = \sqrt{3}$, as a function of $qa/2\pi$. We have chosen a rather small sample size ($N = 200$), in order to improve the readability of the plot. A large number of peaks are clearly visible. All the bigger ones have been labeled by couples of integers (J, K), according to Eq. (4.40). The above analysis of the wavevectors of the form (4.23), corresponding to convergence of the sequences (4.22), therefore describes correctly the most clearly visible singularities of the spectrum.

Another way to visualize the scaling properties of the Fourier amplitude G_N defined in Eq. (4.1) is to plot, in the complex plane, the points $G_0 = 0$, $G_1,..., G_N,...$, successively, and to join G_N to G_{N+1} ($N = 0, 1, 2,...$). Such complex plottings have been extensively used to study other arithmetical sequences (see, e.g., ref. 12). In particular, the curve thus obtained is self-similar for the values of q given by Eq. (4.23). Indeed, the modulus of G_N behaves as

$$R_N = |G_N| \approx N^{\gamma(q_0)} \tag{4.44}$$

It is therefore clear that the fractal dimension of this curve is

$$D = 1/\gamma(q_0) \tag{4.45}$$

Let us take, for example, the values $q_0 = 3\pi/2$, $\xi = 2$ considered above, for which $\gamma = \ln(5 + 2\sqrt{6})/(6 \ln \tau) = 0.793979$. Hence the fractal dimension of this curve is $D = 1.259480$. Figure 6 shows two parts of this curve at two different scales. The numbers of points of these plots are $\rho_4 = 305$ and $\rho_6 = 5473$ for Figs. 6a and 6b, respectively. Here ρ_n are the integers, denoted by r_n in ref. 1, defined through

$$\rho_n = \rho_{n-1} + F_{3n+1}; \qquad \rho_0 = 1 \tag{4.46}$$

Hence ρ_n are asymptotically proportional to the lengths of the words defined in (4.12):

$$\rho_n : v_n^u : v_n^v : v_n^w \approx \tfrac{1}{2}\tau^2 : \tau : 1 : 1 \tag{4.47}$$

(a)

(b)

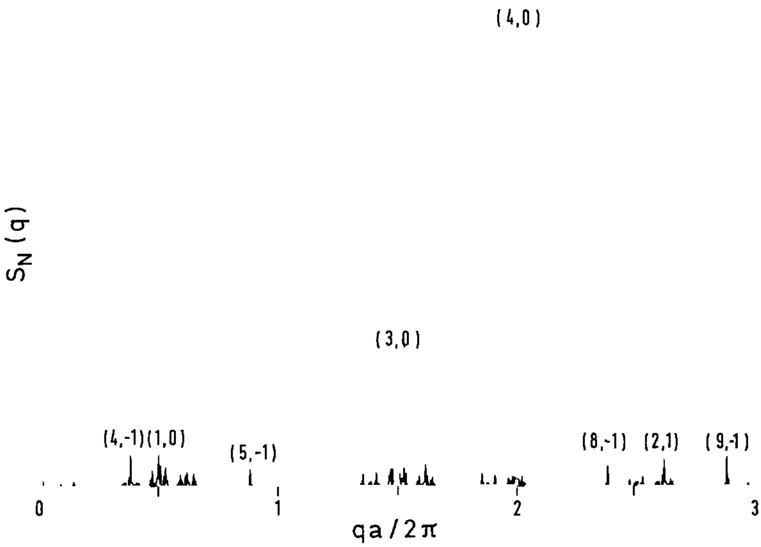

Fig. 5. Plot of the structure factor $S_N(q)$ of Eq. (4.2) of a finite sample with $N = 200$ atoms as a function of $qa/2\pi$ for (a) $\xi = \sqrt{2}$ and (b) $\xi = \sqrt{3}$. The largest peaks are labeled by integers (J, K) according to Eq. (4.40).

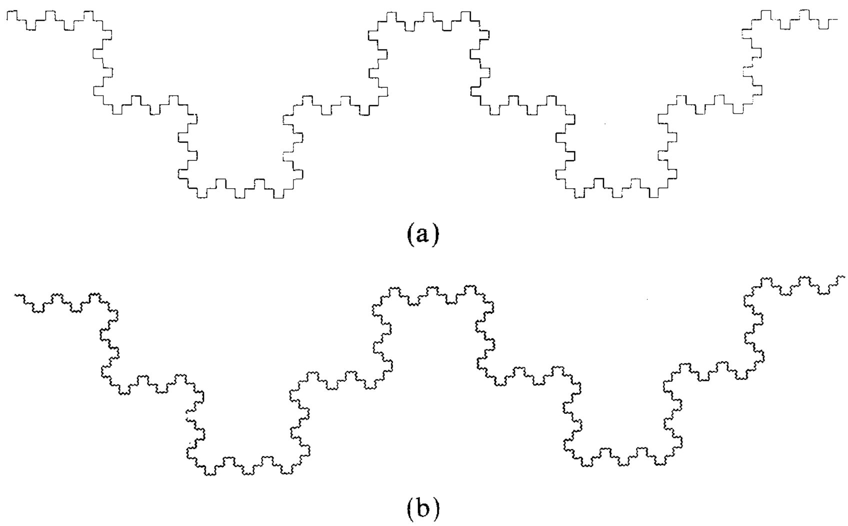

Fig. 6. Complex plot of the sequence of Fourier amplitudes $G_N(q_0)$ for $q_0 = 3\pi/2$ and $\xi = 2$: (a) $\rho_4 = 305$ points, (b) $\rho_6 = 5473$ points. The fractal nature of this curve is discussed in the text.

It turns out that stopping the plots after ρ_n steps ($n = 2, 4, 6,...$) makes them especially symmetric and aesthetically appealing. The associated amplitudes G_N are real, and read $G_{\rho_4} = 88$ and $G_{\rho_6} = 880$, respectively. Hence, these parts of the curve yield the approximate value

$$\frac{\ln(880/88)}{\ln(5473/305)} \approx 0.7971$$

of γ. More generally, self-similar curves may be drawn for the values of q corresponding to limit m-cycles described above. Figure 7 shows plots of ρ_6 points in two examples with a value of q of the form (3.42), yielding a limit 2-cycle behavior, namely (a) $qa/2\pi = 13/8$, $\xi = 2.1$ ($\gamma = 0.53632$), and (b) $qa/2\pi = 7/8$, $\xi = 0.9$ ($\gamma = 0.58540$). These values of γ have been obtained by a numerical iteration of Eq. (4.20).

5. CONCLUSION

In the present work, we have considered geometrical properties of a model of a nonrandom structure beyond quasiperiodicity. More precisely, we analyzed the self-similarity (inflation rules) of the structure and the scaling properties of its Fourier transform. It is remarkable that, although the binary sequence generating the structure is quasiperiodic, the structure

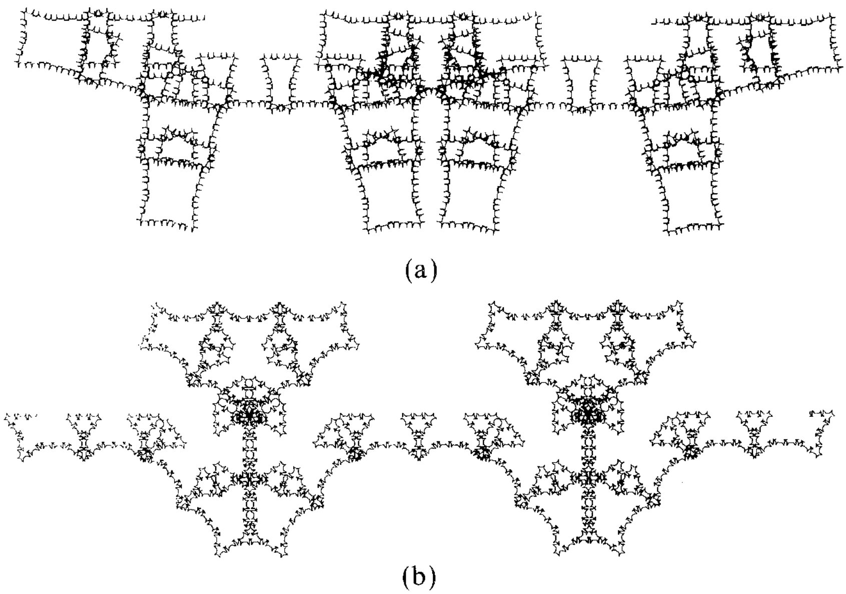

Fig. 7. Same as Fig. 6, for two values of q_0 corresponding to a limit 2-cycle of the sequence (4.22): (a) $qa/2\pi = 13/8$, $\xi = 2.1$. (b) $qa/2\pi = 7/8$, $\xi = 0.9$. Each plot contains $\rho_6 = 5473$ points.

itself is not. This transition from quasiperiodic to "somewhere beyond" is a subtle effect, since it involves number-theoretic considerations.

More generally, we now comment on a general framework, introduced in ref. 2, able to describe structures with such an intermediate order. Any translationally invariant classical Hamiltonian (with sufficiently decreasing long-range interactions) always has "weakly periodic" ground states. Weak periodicity implies local order at all scales, but, as already mentioned in the introduction, does not imply periodicity or quasiperiodicity. Reciprocally, it is not proven that any weakly periodic structure is always the ground state of some translationally invariant Hamiltonian. Concerning the model studied here, it will be proven in a forthcoming publication that it is a weakly periodic structure, and that there exists a translationally invariant Hamiltonian for which the set of ground states uniquely consists of this configuration, all the translated structures, and all their possible limits. In spite of this degeneracy, the ground-state entropy will be shown to remain zero, as for standard incommensurate structures.

The present study also has the virtue of revealing, on a particular example, the interplay among three kinds of properties:

1. Existence of an underlying average lattice. In one dimension, this problem just amounts to considering the fluctuation δ_n defined in Eq. (2.6).

In the present case, since δ_n diverges whenever the Kesten condition [Eq. (2.7)] is not fulfilled, the structure is said to have no average lattice.

2. Quasiperiodicity (or more generally almost-periodicity), i.e., a Fourier transform composed of Dirac peaks.

3. In the case of sequences generated by a substitution (inflation rules), Bombieri and Taylor[7] have stressed the importance of a characteristic of the eigenvalue spectrum of the substitution referred to as the Pisot–Vijayaraghavan (PV) property. A substitution is said to have this property if all the eigenvalues of the associated matrix lie inside the unit circle, except the leading one (which is always real and larger than 1).

First, it is intuitive that properties (1) and (3) should be related, since an unbounded fluctuation is expected to destroy (in general) diffraction peaks. Furthermore, Bombieri and Taylor[7] have shown that properties (2) and (3) generally come together. Let us illustrate these points by the example of the Fibonacci sequence. A Fibonacci sequence of short and long bonds is easily generated by the well-known projection method.[13–15] Thus, it has a quasiperiodic spectrum. It can also be generated by a substitution acting on two letters:

$$0 \to 1, \qquad 1 \to 10 \tag{5.1}$$

The associated eigenvalue spectrum is $(\tau, -\tau^{-1})$, which satisfies the PV property. Let us also note that this sequence corresponds to the case $\Delta = \zeta = \tau^{-2}$, which obeys the Kesten condition (2.7). Hence, the fluctuation δ_n is a simple bounded function of n.

Before coming back to our model, let us mention the example of the Thue–Morse sequence, generated by the substitution

$$0 \to 01, \qquad 1 \to 10 \tag{5.2}$$

It is known in the mathematical literature[16] that the Fourier transform (with respect to n) of that binary sequence σ_n is singular continuous. It is easy to realize that the geometrical Fourier transform of the short and long bonds model generated by this sequence has the same nature. Since the eigenvalue spectrum of the substitution (5.2) is (0, 2), this substitution has the PV property. Hence the Thue–Morse sequence is an exception to the Bombieri and Taylor rule. This paradox is easily solved by realizing that a simple prefactor vanishes in the Fourier amplitude for the values of the wavevector where a Dirac peak would be expected.

The example studied in this paper is also special, since it corresponds to the marginal case where the second leading eigenvalue has unit modulus. Let us note that there exist substitutions that belong to this marginal class and nevertheless lead to quasiperiodic structures. A very simple example of such an occurrence is given by the case ($\zeta = \tau^{-2}, \Delta = \tau^{-1} = 1 - \zeta$) of our model, which fulfills the Kesten condition (2.7).

We will describe in a forthcoming publication the applications of some of the ideas contained in this paper to the case of aperiodic tilings of the plane. The physical properties of such structures are also of interest. We hope to come back to this subject in the future.

To be complete, we mention that the consequences of the violation of the Kesten condition (2.7) have been considered in the study of a particular diffusion model in two dimensions.[17]

The methods used in this paper are adequate to study the local properties of the Fourier transform, but do not bring any further information on its global properties, such as those studied numerically in ref. 1. In particular, the absence of an absolutely continuous part in the Fourier spectrum, as well as its multifractal properties, have not received an analytical proof. Indeed, such statistical properties gather information through the whole spectrum, and hence give weight to generic values of the wavevector where no simple behavior is expected. This will be all the more true when considering physical properties of these structures.

APPENDIX A. BEST APPROXIMATIONS OF A GIVEN NUMBER BY THE INTEGER MULTIPLES OF AN IRRATIONAL NUMBER MODULO 1

The problem is to find the sequence of best approximations to a given number Δ by integer multiples modulo 1 of an irrational number ζ. For convenience, we assume in the following that $0 < \zeta < 1$ and $0 < \Delta < 1$.

Definition 1. A number $D \doteq n\zeta - m$ is a best approximation to Δ if there exists $\varepsilon > 0$ such that (n, m) is the integer pair with the smallest positive integer n satisfying the inequality

$$|\Delta - (n\zeta - m)| = |\Delta - D| < \varepsilon \tag{A.1}$$

When ε decreases to zero monotonically, this condition determines a sequence of numbers D_i that converges to Δ. It is also useful to define the best approximations to Δ by lower and upper values

Definition 2. A number $D^+ = n\zeta - m$ (resp. D^-) is a best approximation to Δ by upper values (resp. by lower values) if there exists $\varepsilon > 0$ such that (n, m) is the integer pair with the smallest positive integer n satisfying the inequality

$$0 < (n\zeta - m) - \Delta = D^+ - \Delta < \varepsilon \tag{A.2}$$

[resp. the inequality

$$0 < \Delta - (n\zeta - m) = \Delta - D^{-} < \varepsilon] \tag{A.3}$$

When $\Delta = 0$, the solution to this problem is well known (see, e.g., ref. 10). When $\Delta \neq 0$, the sequences of best approximations can be obtained from an expansion of Δ on the basis of the known best approximations to zero by integer multiples of ζ mod 1.

A1. Expansion of Δ on the Basis (δ_n)

We define recursively a sequence of integers p_n and of remainders R_n by the relations

$$p_n = \mathrm{Min}[1 + \mathrm{Int}(R_n/\delta_n), a_{n+1}] \tag{A.4}$$

and

$$R_{n+1} = R_n - p_n \delta_n \tag{A.5}$$

with the initial condition

$$R_0 = \Delta < 1 \tag{A.6}$$

For all n, we have the inequality

$$-1 < R_n/\delta_n < -\delta_{n-1}/\delta_n = 1/\zeta_n \tag{A.7}$$

or equivalently

$$-\delta_n < R_n < -\delta_{n-1} \qquad \text{for } n \text{ even} \tag{A.8}$$

and

$$-\delta_{n-1} < R_n < -\delta_n \qquad \text{for } n \text{ odd} \tag{A.9}$$

which is proven recursively. This property is checked for $n = 0$. Assuming that (A.7)–(A.9) are fulfilled at order n, the inequalities are proven at order $n+1$ by using (3.8) and (A.3)–(A.6). The cases $R_n/\delta_n < a_{n+1}$ and $a_{n+1} < R_n/\delta_n$ have to be studied separately and yield that $0 < R_{n+1}/\delta_{n+1} < 1/\zeta_{n+1}$ or $-1 < R_{n+1}/\delta_{n+1} < 0$, respectively. One checks that if $p_{n+1} = 0$, then $R_{n+1}/\delta_{n+1} < 0$, which implies $a_{n+1} < R_n/\delta_n$ and $p_n = a_{n+1}$. Note that (A.4) implies, for $0 < \Delta < 1$, that $p_0 \neq 0$. Because of (A.7)–(A.9), the remainder $|R_n|$ is smaller than $|\delta_{n-1}|$ and goes to zero as n goes to infinity. Therefore, Δ can be expanded as a convergent series:

$$\Delta = \sum_{n=0}^{\infty} p_n \delta_n \tag{A.10}$$

Conversely, a given sequence (p_n) fulfilling the conditions that

$$\begin{gathered} 0 \leqslant p_n \leqslant a_{n+1} \\ p_{n-1} = a_n \qquad \text{if} \quad p_n = 0 \\ p_0 \neq 0 \end{gathered} \tag{A.11}$$

determines by (A.10) some number $0 < \Delta < 1$. Note that this condition implies that for any n, p_n and p_{n+1} cannot be both zero. If conditions (A.11) are fulfilled, by using the fact that the sequence of signs of δ_n is alternate and that $a_{n+1} = \mathrm{Int}(-\delta_{n-1}/\delta_n)$, the remainders

$$R_n = \sum_{i=n}^{\infty} p_i \delta_i \tag{A.12}$$

fulfill the inequalities (A.7)–(A.9) and more precisely $-1 < R_n/\delta_n < 0$ if $p_{n+1} \neq 0$ and $0 < R_n/\delta_n < -\delta_{n-1}/\delta_n$ if $p_{n+1} = 0$. Then, it is readily shown that the recursion relations (A.4)–(A.6) are fulfilled for all n by these sequences of integers p_n and of remainders R_n.

As a result, a number Δ is characterized by any arbitrary sequence of integers p_n fulfilling conditions (A.11).

Now, we define the truncations of the series (A.10) as

$$D_{n,p} = p\delta_n + \sum_{i=0}^{n-1} p_i \delta_i \tag{A.13}$$

for $0 \leqslant p \leqslant p_n$ (p integer). Note that we have $D_{n,p_n} = D_{n+1,0}$. Because of definition (3.10), we have

$$D_{n,p} = S_{n,p}\zeta - R_{n,p} \tag{A.14}$$

where $R_{n,p}$ and $S_{n,p}$ are positive integers

$$R_{n,p} = pr_n + \sum_{i=0}^{n-1} p_i r_i \tag{A.15}$$

$$S_{n,p} = ps_n + \sum_{i=0}^{n-1} p_i s_i \tag{A.16}$$

Both these sequences are increasing as n and (or) p grows. With these definitions, we have the following theorem.

Theorem 1. The sequence of best approximations by lower values to Δ by the integer multiples of ζ modulo 1 (cf. Definition 2) is the sequence $D_{n,p}$ defined by (A.13) for all even indices $n = 2q$ and for $0 \leqslant p < p_n$. The sequence of best approximations by upper values to Δ by the integer multiples of ζ modulo 1 is the sequence $D_{n,p}$ defined by (A.13) for all odd indices $n=2q+1$ and for $0 \leqslant p < p_n$.

In order to prove this theorem, we first describe a recursive procedure giving both the best approximations to Δ upper and lower values. We define a series of return maps of the rotation with angle ζ on the unit circle in intervals where the lower edge (resp. upper edge) is a best approximation to Δ by lower values (resp. upper values).

A2. Recursion Procedure

The integer multiples modulo 1 of ζ are generated by the rotation R_0 with angle $\theta_0=\zeta$ on the circle with length $L_0=1$. Let us start from the simplest best approximations to Δ by upper values $D_0^+=1$ [obtained for $\varepsilon=1$, $n=0$, $m=-1$ in (A.2)] and by lower values $D_0^-=0$ ($\varepsilon=1$, $n=0$, $m=0$ in (A.3)].

The next multiple of ζ with the lowest n that appears in the interval $]D_0^-, D_0^+[$ is $D=\theta_0+D_0^-=R_0(D_0^-)$. If $D<\Delta$, $D=D_1^-$ is the approximation to Δ by lower values next to D_0^-. Then, we set $D_1^+=D_0^+$. If $\Delta<D$, $D=D_1^+$ is the best approximation to Δ by upper values next to D_0^+ and we set $D_1^-=D_0^-$.

All the next best approximations to Δ by upper and lower values belong to the new interval $]D_1^-, D_1^+[$. They are generated by the return map R_1 of the rotation R_0 into the interval $]D_1^-, D_1^+[$.

The return map $\mathbb{R}(R, \mathscr{I})$ of a rotation R into the interval $\mathscr{I}$ is defined in general as follows: for x a point of $\mathscr{I}$,

$$\mathbb{R}(R, \mathscr{I})(x)=R^n(x) \tag{A.17}$$

where n is the smallest integer such that $R^n(x)$ belongs to $\mathscr{I}$ (n depends on the point x).

Because the images by the return map R_1 of the two edges D_1^- and D_1^+ of this interval are obviously the same, this return map is continuous on the circle obtained by topological identification of the two edges of $]D_1^-, D_1^+[$ and therefore is also a rotation with a new angle θ_1 on a circle with length $L_1=D_1^+-D_1^-$. According to whether $D<\Delta$ or $\Delta<D$, different recursion formulas are obtained.

A2.1. First Kind Recursion (see Fig. 8a). When $D<\Delta$, we set

$$D_1^-=D, \qquad D_1^+=D_0^+ \tag{A.18}$$

The length of the circle $[D_1^-, D_1^+]$ with origin $D_1^-=D_1^+$ is

$$L_1=L_0-\theta_0 \tag{A.19}$$

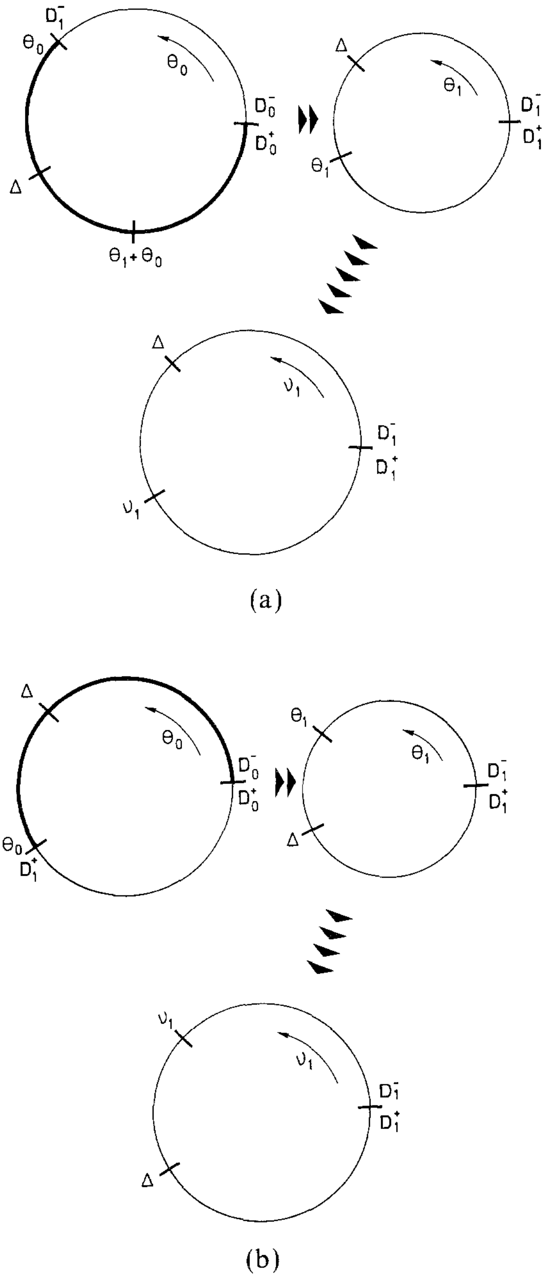

Fig. 8. Scheme of the return map of the rotation on the circle $[D_0^-, D_0^+]$, with angle θ_0, in the interval $[D_1^-, D_1^+]$: (a) $D_1^- = D < \Delta$. (b) $\Delta < D_1^+ = D$.

With ν_0 the rotation number $\theta_0/L_0 = \zeta$ of R_0, the rotation angle θ_1 of R_1 is readily found to be

$$\theta_1 = \theta_0 \text{ modulo } L_1 \tag{A.20}$$

and the rotation number $\nu_1 = \theta_1/L_1$ is

$$\nu_1 = \mathrm{Frac}\left(\frac{\nu_0}{1-\nu_0}\right) = \mathrm{Frac}\left(\frac{1}{1-\nu_0}\right) \tag{A.21}$$

A2.2. Second Kind Recursion (see Fig. 8b). When $\Delta < D$, we set

$$D_1^- = D_0^+, \qquad D_1^+ = D \tag{A.22}$$

The length of this interval $[D_1^-, D_1^+]$ defining the return map R_1 is now

$$L_1 = \theta_0 \tag{A.23}$$

The rotation angle of R_1 is simply equal to the image of the origin modûlo L_0 by the return map in the interval $[D_1^-, D_1^+] = [D_0^-, D_0^- + \theta_0]$

$$\theta_1 = \theta_0[\mathrm{Int}(1/\nu_0) + 1] - L_0 = \theta_0[1 - \mathrm{Frac}(1/\nu_0)] \tag{A.24}$$

and the rotation number is

$$\nu_1 = 1 - \mathrm{Frac}(1/\nu_0) \tag{A.25}$$

These recursion formulas are also easily obtained from the first-kind recursion formula by considering the symmetric problem where θ_0 is changed into $1-\theta_0$ and Δ is changed into $1-\Delta$. One can check that formulas (A.21) and (A.25) are interchanged by changing ν_0 into $1-\nu_0$ and ν_1 into $1-\nu_1$.

The same recursion procedure applied to the return map R_1 yields the return map R_2, and so on. An infinite sequence of return maps R_i is thus generated. They are rotations with angles θ_i on the intervals $[D_i^-, D_i^+]$ with topologically identified edges. Because of its definition, the sequence D_i^- is monotonically increasing, but may contain consecutive equal terms. The new sequence obtained from D_i^- by withdrawing all D_i^- such that $D_i^- = D_{i-1}^-$ is the sequence of best approximations to Δ by lower values by the integer multiples of ζ. The sequence (D_i^+) yields similarly the sequence of best approximations to Δ by upper values by the integer multiples of ζ. In order to find the sequences (D_i^-), (D_i^+), and (θ_i), we need to define a subsequence (D_n) of $(D_{n,p})$ [defined by (A.13)]

$$D_{n+1} = D_{n,p_n-1} \qquad \text{if} \quad p_n \neq 0 \tag{A.26}$$

or recursively

$$D_{n+1} = D_{n-1} \qquad \text{if} \quad p_n = 0 \tag{A.27}$$

and we set as initial conditions $D_0 = 1$ and $D_{-1} = 0$. This sequence has the useful property that

$$\begin{aligned} D_n &> D_{m,p} && \text{for } n \text{ even and for all } m \geqslant n \text{ and } p \leqslant p_m \\ D_n &< D_{m,p} && \text{for } n \text{ odd and for all } m \geqslant n \text{ and } p \leqslant p_m \end{aligned} \tag{A.28}$$

In order to prove this result, it is convenient to use the identity

$$\delta_{n-1} = -\sum_{i=0}^{\infty} a_{n+2i+1}\,\delta_{n+2i} \tag{A.29}$$

which is easily proven by using (3.6)–(3.10). Since we have $p_i \leqslant a_{i+1}$ and $p \leqslant p_m \leqslant a_{m+1}$, the sum

$$D_{m,p} - D_n = \delta_{n-1} + \sum_{i=0}^{m-n-1} p_{n+i}\delta_{n+i} + p\delta_m \tag{A.30}$$

can be written as a series where all terms have the sign of δ_{n-1} or are zero. Consequently $D_{m,p} - D_n$ has the sign of $(-1)^n$, which proves (A.28). When taking the limit $m \to \infty$, these inequalities also imply

$$\begin{aligned} \Delta < D_n &< D_{n-1,p} && \text{for } n \text{ even and } p < p_{n-1} \\ D_{n-1,p} < D_n &< \Delta && \text{for } n \text{ odd and } p < p_{n-1} \end{aligned} \tag{A.31}$$

It is also convenient to consider the sequence $D_{n,p}$ as a sequence D_{n_i,q_i} with a single index i. Then (n_i, q_i) is the ith term of the set of (n, q) fulfilling the condition $0 \leqslant q < p_n$, ordered with the "lexicographic" definition

$$i = (n, q) < i' = (n', q') \qquad \text{if} \quad n < n' \text{ or if } n = n' \text{ and } q < q' \tag{A.32}$$

Then we can prove the following result, which implies Theorem 1:

The sequence of intervals $[D_i^-, D_i^+]$ is the sequence $[D_{n_i,q_i}, D_{n_i}]$ for n_i odd and $[D_{n_i}, D_{n_i,q_i}]$ for n_i even. In addition, the rotation angle of the return map R_i in $[D_i^-, D_i^+]$ is

$$\theta_i = \theta_{n_i,q_i} = \delta_{n_i} \tag{A.33}$$

and the rotation number is

$$\nu_i = \frac{(-1)^{n_i}\zeta_{n_i}}{1 - q_i\zeta_{n_i}} \tag{A.34}$$

First it is useful to check that (A.33) implies (A.34). According to the definition of D_n, there exists an integer m positive or zero such that $p_{n-2i-1}=0$ for $0 \leqslant i < m$ and $p_{n-2m-1} \neq 0$; then $p_{n-2i-2}=a_{n-2i-1}$ for $0 \leqslant i < m-1$. The length of the interval of definition for the return map R_i is then

$$\begin{aligned} L_i &= (-1)^n (D_{n,p} - D_n) \\ &= (-1)^n \left(\delta_{n-2m-1} + p\delta_n + \sum_{i=0}^{m-1} a_{n-2i-1} \delta_{n-2i-2} \right) \end{aligned} \tag{A.35}$$

Using the identity $a_{i+1}\delta_i = \delta_{i+1} - \delta_{i-1}$, we find

$$L_i = (-1)^{n_i - 1} (\delta_{n_i - 1} + p_i \delta_{n_i}) \tag{A.36}$$

which yields (A.34) for $v_i = \theta_i / L_i$ by using (3.8) and (3.10).

We now prove recursively the main result. For $i=0$, $n=p=0$, this assertion is exact. R_0 is the initial rotation on the unit circle. We have $D_{0,0}=0$, $D_0=1$, and $\theta_{0,0}=\zeta=\delta_0$.

Let us assume now that at order i the return map R_i is defined on an interval $[D_{n_i,p_i}, D_{n_i}]$ and is a rotation with angle $\theta_i = \delta_{n_i}$. We prove that the next return map, which is defined by the recursion procedure described above, is indeed a rotation on the next interval defined by $[D_{n_{i+1},q_{i+1}}, D_{n_i}]$ with the expected angle $\theta_{n_{i+1}}$.

For sake of simplicity, we omit the index i of n_i. We also assume that n is even, but the same proofs hold by symmetry for n odd. We consider separately three possible cases: (1) $p < p_n - 1$, (2) $p = p_n - 1$ and $p_{n+1} \neq 0$, and (3) $p = p_n - 1$ and $p_{n+1} = 0$.

Case 1. $p < p_n - 1$. Since $\theta_n = \delta_n$, the image of both interval edges is $D_{n,p} + \delta_n = D_{n,p+1}$. Considering that n is even, the condition $p+1 < p_n$ implies (A.31),

$$D_{n,p} < D_{n,p} + \theta_n = D_{n,p+1} < \Delta < D_n \tag{A.37}$$

Therefore, the return map R_{i+1} on the interval $[D_{n,p+1}, D_n]$ that contains Δ is defined by a first-kind recursion transformation. Since $p+2 \leqslant p_n$, we also have

$$D_{n,p} < D_{n,p+2} = D_{n,p} + 2\theta_n < D_n \tag{A.38}$$

which implies that the rotation number of the return map R_i is smaller than 1/2. Therefore, the rotation angle of R_{i+1} given by (A.21) is the same $\theta_{i+1} = \theta_i = \delta_n$. The recursion condition for the return map R_{i+1} is then proven.

Case 2. $p = p_n - 1$ and $p_{n+1} \neq 0$. The image of both interval edges by the return map R_i is $D_{n,p} + \delta_n = D_{n+1,0}$. Then (A.31) implies

$$D_{n+1} = D_{n,p} < \Delta < D_{n,p} + \theta_n = D_{n+1,0} < D_n \tag{A.39}$$

The new return map is now defined on the interval $[D_{n+1}, D_{n+1,0}]$ next in the sequence to the interval $[D_{n,p}, D_n]$ and is a rotation. The rotation number of the return map R_{i+1} is given by the second-kind recursion transformation (A.25) and is

$$v_{i+1} = 1 - \mathrm{Frac}\left(\frac{1 - p\zeta_n}{\zeta_n}\right) = 1 - \zeta_{n+1} = \mathrm{Frac}(-\zeta_{n+1}) \tag{A.40}$$

The new return map R_{i+1} fulfills the recursion condition (A.34).

Case 3. $p = p_n - 1$ and $p_{n+1} = 0$. Then we have $p = p_n - 1 = a_{n+1} - 1$ and $p_{n+2} \neq 0$. The image of both interval edges by the return map R_i is $D_{n,p} + \delta_n = D_{n+2,0}$ and (A.31) implies

$$D_{n+1} = D_{n,p} < D_{n,p} + \theta_n = D_{n+2,0} < \Delta < D_n \tag{A.41}$$

The new return map R_{i+1} is defined on the interval $[D_{n+2,0}, D_n]$ next in the sequence to the interval $[D_{n,p}, D_n]$ and is a rotation. The rotation number of the return map R_{i+1} is given by the first-kind recursion transformation (A.21). We have

$$v_i = \frac{\zeta_n}{1 - (a_{n+1} - 1)\,\zeta_n} = \frac{1}{1 + \zeta_{n+1}} \tag{A.42}$$

and

$$v_{i+1} = \mathrm{Frac}\left(\frac{1}{1 - v_i}\right) = \zeta_{n+2} \tag{A.43}$$

Again, the new return map R_{i+1} fulfills the recursion condition (A.34).

Now let us discuss the possibility of finding the sequence of best approximations to Δ according to Definition 1. Clearly, it is a subsequence of the sequence $D_{n,p}$ of best approximations by upper and by lower values. Unfortunately, it is impossible to determine this sequence. We get the following negative results, which sharply contrast with the well-known case where $\Delta = 0$.

Theorem 2. Suppose that we know the coefficients of the ζ expansion (A.10) of Δ up to some finite order N. Then the minimum value of N

that allows one to decide with certainty whether a given number $D_{n,p}$ in this expansion is a best approximation to Δ or not is not bounded.

As a consequence of this theorem, it is impossible to give a recursive procedure *involving only Δ through a finite number of terms of the sequence* $D_{n,p}$ that determines unambiguously the subsequence of $D_{n,p}$ that forms the best approximations to Δ. However, there exist sufficient (but non-necessary) conditions involving finitely many terms that allow one to decide whether $D_{n,p}$ is a best approximation to Δ or not.

Proof of Theorem 2. The knowledge of the ζ expansion (A.10) of Δ up to order N determines the sequence $D_{n,p}$ for $n \leqslant N$. In order to prove this theorem, it is sufficient to show an example in which this determination is impossible. Suppose that for some n, p we have

$$|\Delta - (D_{n,p} + D_n)/2)| < \varepsilon \tag{A.44}$$

where ε is smaller than the lower bound of $|D_{n',p'} - (D_{n,p} + D_n)/2|$ for all n' and $0 \leqslant p' < p_{n'}$ with $n' \leqslant N$. Then, because of (A.7)–(A.9), for all Δ' in the interval determined by (A.44) the ζ expansion is the same as for Δ up to order N. However, for

$$0 < \Delta' - (D_{n,p} + D_n)/2 < \varepsilon \tag{A.45}$$

$D_{n,p} = S_{n,p}\zeta - R_{n,p}$ is a best approximation to Δ' because, due to (A.28), (A.31), there exists no $D_{n',p'}$ with $n' < n$, or $n = n'$ and $p < p'$, that belongs to the interval generated by D_n and $D_{n,p}$. By contrast, in the interval

$$0 < (D_{n,p} + D_n)/2 - \Delta' < \varepsilon \tag{A.46}$$

$D_{n,p}$ cannot be a best approximation to Δ' (according to Definition 1) because

$$|D_n - \Delta'| < |D_{n,p} - \Delta'| \qquad \text{with} \quad D_n = S_n\zeta - R_n \quad \text{and} \quad S_n < S_{n,p} \tag{A.47}$$

To determine whether $D_{n,p}$ is a best approximation or not, one needs to know the coefficients of the ζ expansion of Δ up to an order N' that diverges as ε goes to zero.

To be complete, we mention that an expansion similar to Eq. (A.10) was introduced in ref. 18 (see also ref. 8).

APPENDIX B. CONVERGENCE PROPERTIES OF THE SEQUENCE xF_n (mod 1)

We determine the values of the real number x such that the sequence

$$X_n = xF_n \ (\mathrm{mod}\ 1) \tag{B.1}$$

converges to a limit, or a limit-cycle, as $n \to \infty$. Here F_n denote the Fibonacci numbers, introduced in Section 2, and defined by Eq. (3.43):

$$F_n = F_{n-1} + F_{n-2} \qquad (F_0 = 0; F_1 = 1) \tag{B.2}$$

We consider first the simpler case, where the sequence X_n has a limit:

$$\lim_{n \to \infty} X_n = l \tag{B.3}$$

The recursion (B.2) then implies $l = l + l$ (mod. 1), and hence $l = 0$ (mod 1). Introduce now the decomposition

$$xF_n = a_n + \varepsilon_n \tag{B.4}$$

where a_n is the nearest integer to xF_n. Hence $|\varepsilon_n| \leqslant 1/2$, and $\lim_{n \to \infty} \varepsilon_n = 0$. The recursion (B.2) now implies

$$a_{n+2} - a_{n+1} - a_n = \varepsilon_{n+1} + \varepsilon_n - \varepsilon_{n+2} \tag{B.5}$$

The lhs of this equation is an integer, while the rhs converges to zero. Hence, both sides vanish identically for n larger than some N:

$$a_{n+2} = a_{n+1} + a_n \qquad (n \geqslant N) \tag{B.6}$$

It is then easy to show recursively that

$$a_{N+n} = F_n a_{N+1} + F_{n-1} a_N \qquad (n \geqslant 0) \tag{B.7}$$

The definition (B.4) now implies

$$xF_{N+n} = F_n a_{N+1} + F_{n-1} a_N + \varepsilon_{N+n} \tag{B.8}$$

We recall here that the F_n are related to the golden mean, defined in Eq. (1.1)

$$\tau = (\sqrt{5} + 1)/2 \tag{B.9}$$

by

$$F_n = (1/\sqrt{5})[\tau^n - (-\tau^{-1})^n] \tag{B.10}$$

Conversely,

$$\begin{aligned} \tau^n &= F_n \tau + F_{n-1} \\ \tau^{-n} &= (-)^n (F_{n+1} - \tau F_n) \end{aligned} \tag{B.11}$$

By dividing both sides of Eq. (B.8) by F_{N+n}, taking the $n \to \infty$ limit, and using Eq. (B.10), we obtain

$$x = a_{N+1}\tau^{-N} + a_N\tau^{-N-1} \tag{B.12}$$

Hence, Eq. (B.11) shows that x has the form

$$x = j + k\tau \qquad j, k \text{ integers} \tag{B.13}$$

Conversely, for x given by Eq. (B.13), Eq. (B.11) yields $X_n = k(-)^{n+1}\tau^{-n}$ (mod 1). This sequence obviously converges to zero.

We consider now the general case, where the sequence X_n has a limit-cycle of length μ. This means that the following limit exists:

$$\lim_{n\to\infty} X_{\mu n+p} = l_p \qquad (p \geqslant 0) \tag{B.14}$$

These numbers clearly obey the recursion

$$l_p = l_{p-1} + l_{p-2} \pmod 1 \tag{B.15}$$

as well as the periodicity

$$l_{p+\mu} = l_p \pmod 1 \tag{B.16}$$

Hence the l_p can be shown to obey the following equation, analogous to Eq. (B.7):

$$l_p = F_p l_1 + F_{p-1} l_0 \tag{B.17}$$

Equation (B.16), taken for $p = 0$ and $p = 1$, implies the existence of integers (M, N) such that

$$\begin{aligned} l_\mu &= F_\mu l_1 + F_{\mu-1} l_0 = l_0 + M \\ l_{\mu+1} &= F_{\mu+1} l_1 + F_\mu l_0 = l_1 + N \end{aligned} \tag{B.18}$$

In order to solve Eq. (B.18), we are led to define δ as being the greatest common divisor of F_μ and $(F_{\mu-1} - 1)$,

$$\delta = \mathrm{GCD}(F_\mu; F_{\mu-1} - 1) \tag{B.19}$$

and to introduce the integers A, B such that

$$F_\mu = A\delta; \qquad F_{\mu-1} = 1 + B\delta \tag{B.20}$$

Then Eqs. (B.18) read

$$\begin{aligned} Al_1 + Bl_0 &= M/\delta \\ (A+B)\,l_1 + Al_0 &= N/\delta \end{aligned} \tag{B.21}$$

Let now D denote the determinant of these coupled linear equations,

$$D = A^2 - AB - B^2 > 0 \tag{B.22}$$

It follows that l_0, l_1, and all the l_p are integer multiples of $1/D\delta$. Hence the sequence $Y_n = D\delta x F_n$ (mod 1) converges to zero. The first part of this Appendix implies that x has the form

$$x = \frac{j + k\tau}{D\delta} \tag{B.23}$$

It turns out that, in contrast to what occurred with the x of the form (B.13) in the case of a fixed point ($\mu = 1$), there are restrictions on the values of j and k, for some values of μ. For x given by Eq. (B.23), Eq. (B.11) yields

$$X_n = \frac{1}{D\delta}\,[jF_n + kF_{n+1} + k(-)^{n+1}\,\tau^{-n}] \quad (\text{mod } 1) \tag{B.24}$$

Hence the sequence X_n has a limit cycle of length μ if and only if the quantities Z_n defined by

$$j(F_{n+\mu} - F_n) + k(F_{n+\mu+1} - F_{n+1}) = Z_n D\delta \tag{B.25}$$

are integers for large enough n. In analogy with Eqs. (B.7), (B.17), it can be shown that

$$F_{n+\mu} = F_\mu F_{n+1} + F_{\mu-1} F_n \tag{B.26}$$

Hence, Eq. (B.25) is equivalent to

$$F_n(Bj + Ak) + F_{n+1}(Aj + (A+B)\,k) = Z_n D \tag{B.27}$$

with the notation (B.20). The Z_n therefore obey the recursion $Z_n = Z_{n-1} + Z_{n-2}$, and all of them are integers if and only if $Z_0 = J$ and $Z_1 = K$ are integers. We are left with the coupled equations

$$\begin{aligned} Aj + (A+B)k &= DJ \\ Bj + Ak &= DK \end{aligned} \tag{B.28}$$

which have for solution

$$j = JA - K(A+B), \qquad k = KA - JB \tag{B.29}$$

In summary, the sequence X_n defined in Eq. (B.1) has a limit cycle of length μ if and only if x is of the form (B.23), with j and k given by (B.29), where J and K are arbitrary integers. In other words, these values of x are the linear combinations, with integer coefficients J and K, of the numbers

$$x_1 = \frac{A - B\tau}{D\delta}, \qquad x_2 = \frac{A\tau - A - B}{D\delta} \tag{B.30}$$

This set of values of x is called the $\mathbb{Z}$-module generated by x_1 and x_2. If $D = 1$, all numbers of the form (B.23) are in this module, since Eq. (B.28) is obeyed for all j and k. If $D \geqslant 2$, then $(j = 1, k = 0)$ clearly does not obey Eq. (B.28) (otherwise A and B would have the common divisor D), and hence the $\mathbb{Z}$-module defined above is only a subset of the numbers given in Eq. (B.23).

Moreover, it is worth noticing that the above-defined numbers x_1 and x_2 obey

$$x_1 = \tau x_2, \qquad x_2 = \sum_{n \geqslant 1} \tau^{-\mu n} \tag{B.31}$$

Therefore it can be checked that any number x of the form

$$x = \sum_{n \geqslant 1} \sigma_n \tau^{-n} \qquad (\sigma_n = 0 \text{ or } 1) \tag{B.32}$$

where the σ_n are eventually periodic with period $\mu(\sigma_{n+\mu} = \sigma_n$ for $n \geqslant N)$ belongs to the $\mathbb{Z}$-module generated by x_1 and x_2. It can be shown that the converse is true. Thus, we have obtained another characterization of the module.

In Section 3, we need in particular the values of x that yield a limit cycle of length 6 or 12. If $\mu = 6$, $\delta = 4$, and $D = 1$, then x is of the form

$$\mu = 6 \Rightarrow x = (j + k\tau)/4 \tag{B.33}$$

If $\mu = 12$, $\delta = 8$, and $D = 5$, then x belongs to the module generated by

$$x_1 = (18 - 11\tau)/40, \qquad x_2 = (18\tau - 29)/40 \tag{B.34}$$

An equivalent but simpler basis reads

$$\overline{x_1} = (2 + \tau)/40, \qquad \overline{x_2} = (3 - \tau)/40 \tag{B.35}$$

It is also easy to prove the following reciprocal property. For any number x of the form

$$x = (j + k\tau)/\nu \tag{B.36}$$

the sequence X_n of Eq. (B.1) converges to a limit μ-cycle, with $\mu \leqslant \nu^2$. Indeed, for x given by Eq. (B.36), we have

$$X_n = \frac{1}{\nu} \left[jF_n + kF_{n+1} + k(-)^{n+1} \tau^{-n} \right] \pmod 1 \tag{B.37}$$

Now let λ_n be the integers defined by

$$jF_n + kF_{n+1} = \lambda_n \pmod \nu; \qquad 0 \leqslant \lambda_n \leqslant \nu - 1 \tag{B.38}$$

This sequence obeys

$$\begin{aligned} \lambda_n &= \lambda_{n-1} + \lambda_{n-2} && (\lambda_{n-1} + \lambda_{n-2} \leqslant \nu - 1) \\ &= \lambda_{n-1} + \lambda_{n-2} - \nu && (\lambda_{n-1} + \lambda_{n-2} \geqslant \nu) \end{aligned} \tag{B.39}$$

This last equation defines a map $\mathbb{F}$ of the finite set $S = \{0,..., \nu - 1\}^2$ onto itself by $(\lambda_n, \lambda_{n-1}) = \mathbb{F}(\lambda_{n-1}, \lambda_{n-2})$. Since S has ν^2 elements, every point of S is eventually periodic under $\mathbb{F}$, with a period $\mu \leqslant \nu^2$. Then Eq. (B.37) implies that X_n converges to a cycle of length μ.

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