Quasiperiodicity and types of order; a study in one dimension

1987 J. Phys. A: Math. Gen. 20 4483

(http://iopscience.iop.org/0305-4470/20/13/047)

J. Phys. A: Math. Gen. **20** (1987) 4483-4499. Printed in the UK

Quasiperiodicity and types of order: a study in one dimension

C Godrèche†, J M Luck‡ and F Vallet§‖

† Service de Physique du Solide et de Résonance Magnétique, CEN-Saclay, 91191 Gif sur Yvette Cedex, France

‡ Service de Physique Théorique, CEN-Saclay, 91191 Gif sur Yvette Cedex, France

§ Laboratoire Léon Brillouin, CEN-Saclay, 91191 Gif sur Yvette Cedex, France

Received 5 January 1987

Abstract. In order to characterise the interplay between quasiperiodicity and order in one dimension, we consider sequences of 0 and 1 generated by a circle map. These sequences, which generalise the Fibonacci sequence, describe the quasiperiodic ordering of atoms and vacancies on a line. We study in a quantitative way the unbounded fluctuation of the atomic positions WRT the average lattice. For some quadratic algebraic values of the rotation number, the sequences can be generated by inflation rules, which proves their self-similarity. These rules, obtained by a renormalisation of the circle map generating the sequences, permit us, e.g., to explain the logarithmic divergence of the fluctuation. For some exceptional rotation numbers, the fluctuation diverges as N^{α}, N being the system size. Whenever $\alpha > \frac{1}{2}$, the quasiperiodic chain is therefore less 'rigid' than a random one.

1. Introduction

The discovery of quasicrystals has stressed the importance of quasiperiodic structures in condensed matter physics, already met in incommensurate materials [1]. It is thus of interest to analyse in detail the relevance of quasiperiodicity to structural models, and in particular to understand the links between types of order and quasiperiodicity. This paper, following previous works [2, 3], is concerned with the study of this question in one dimension.

Let us illustrate our purpose in a more precise way. Take a periodic linear chain with lattice spacing l. A lattice site may or may not be occupied by an atom. In the latter case, it is called a vacancy. Thus, for a finite system of size Nl, the numbers of atoms N_a and of vacancies N_v are related by $N_a + N_v = N$. We assume that the mean density of atoms defined by

$$\rho = \lim_{N \to \infty} N_a / Nl \tag{1.1}$$

exists. For any finite size Nl of the system, the number of atoms N_a fluctuates around its mean value:

$$N_a = \rho Nl + \delta(N). \tag{1.2}$$

When the distribution of atoms is periodic, the fluctuation $\delta(N)$ is periodic as well, and hence remains bounded when increasing N. If, on the other hand, this distribution

‖ Present address: Thomson-CSF, LCR, 91401 Orsay, France.

0305-4470/87/134483+17$02.50

is random (e.g. in a fluid), the fluctuation $\delta(N)$ increases typically as $\sqrt{N}$. A third case of interest is when the distribution of atoms is quasiperiodic. We will show below that the fluctuation $\delta(N)$ may exhibit various kinds of behaviour: it may be bounded as in the periodic case, or diverge with N (usually as $\ln N$, but possibly even more rapidly than in a random system).

In previous works [2, 3], a simple structural model was studied, which shows such a behaviour of $\delta(N)$. More precisely, in the ground state the fluctuation of the positions of atoms around their average lattice diverges, though the Fourier spectrum of the density is discrete. In physical terms, this means that the structure is quasiperiodic, but has no average lattice. The aim of this paper is to study in a more quantitative way these unbounded density fluctuations in a particular case of the model mentioned above.

Inasmuch as the present work is a continuation of other ones [2, 3], § 2 is devoted to a short summary of the results obtained previously. In § 3 we analyse in detail a specific example, for which it is possible to deduce the logarithmic divergence of the fluctuation from inflation rules obtained from an exact renormalisation procedure. In § 4, we present the general theory. Section 5 contains a short discussion.

2. A short summary of previous work

The model considered in [2] consists of a chain of atoms such that the distance between two consecutive atoms is constrained to be l or $2l$, l being a given number. Moreover, this chain is subjected to a periodic potential with period 1, taken to be sinusoidal for simplicity (figure 1). We denote by u_j the abscissa of the jth atom, starting from the origin ($u_0 = 0$). For a fixed fraction c of long bonds of length $2l$, the ground state of the model is obtained by minimising the potential energy of the chain:

$$\Phi(\{u_j\}) = \sum_j \cos(2\pi u_j) \tag{2.1}$$

with the constraints

$$u_{j+1} - u_j = l \text{ or } 2l. \tag{2.2}$$

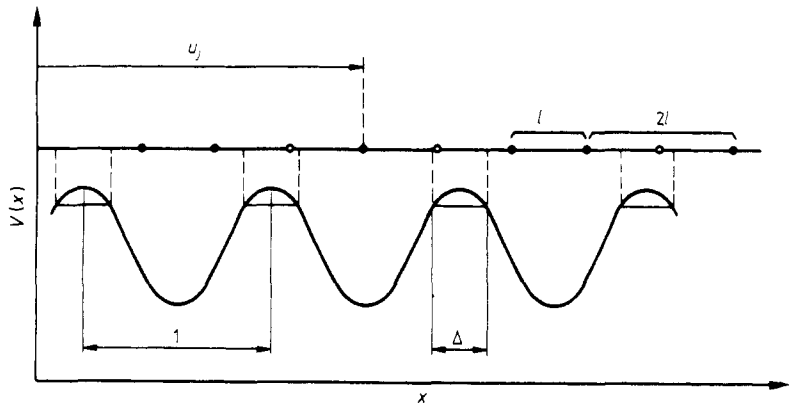

Figure 1. Definition of the model. Full circles stand for atoms, open circles for vacancies. This figure is taken from [2], where the window W was defined around 0: $W = [-\Delta/2, \Delta/2]$.

Whenever l is an irrational number, this model presents incommensurability effects between the period of the potential and the bond lengths.

There is an equivalence between the sequence $\{u_j\}$ describing the ground state and the sequence obtained by the circle map T defined as follows. The position of the ith site, occupied by an atom or a vacancy, starting from the origin, is $v_i = il$. We consider the interval $W =]0, \Delta[$, called the 'window', where Δ is simply related to the concentration of vacancies c: $\Delta = c/(c+1)$. Then the sequence $\{u_j\}$ of atomic positions in the ground state has been shown to be obtained as follows: withdraw from the sequence $\{v_i\}$ the terms which belong to W (mod 1). This choice corresponds to the fact that it costs energy for an atom to sit near the top of the periodic potential, hence it is energetically favourable to have a vacancy instead. In other words, the ith site is occupied by a vacancy if and only if $\mathrm{frac}(il) < \Delta$. Here, and in the following, $\mathrm{int}(x)$ and $\mathrm{frac}(x) = x - \mathrm{int}(x)$ denote the integer and the fractional part of x, respectively. Considering the interval W as an arc of the circle parametrised by $0 \leqslant x \leqslant 1$, the mapping $u' = T(u)$ of the circle onto itself which generates the sequence $\{u_j\}$ by iteration is defined as a piecewise uniform rotation by the following equations:

$$\begin{aligned} T(u) = u' &= u + l \qquad \text{when } u + l \text{ does not belong to } W \\ T(u) = u' &= u + 2l \qquad \text{when } u + l \text{ belongs to } W. \end{aligned} \tag{2.3}$$

In this model, no consecutive vacancies exist, which implies $\Delta < l < 1 - \Delta$. This restriction on the number of consecutive vacancies may be released, i.e. it is possible to consider the same model for arbitrary values of l and $\Delta (0 < l, \Delta < 1)$. The transformation T may also be written

$$u' = T(u) = u + (1 + \chi_\Delta(u + l))l \tag{2.4}$$

where $\chi_\Delta(x)$ is the characteristic function of W, equal to 1 when x belongs to W, and to 0 when it does not:

$$\chi_\Delta(x) = \mathrm{int}(x) - \mathrm{int}(x - \Delta). \tag{2.5}$$

A theorem in number theory due to Kesten [4] gives some information on the fluctuation $\delta(N)$ obtained from the map T. The number of vacancies from the origin until the Nth site is equal to $\Sigma_{i=1,N}\, \chi_\Delta(v_i)$, and hence the position u_n of the nth atom is $v_n = Nl$, where N satisfies the condition

$$n = N - \sum_{i=1,N} \chi_\Delta(v_i). \tag{2.6}$$

Since the sequence $\{v_i (\mathrm{mod}\ 1)\}$ is uniformly distributed on the circle, the mean value of the characteristic function is

$$\lim_{N \to \infty} (1/N) \sum_{i=1,N} \chi_\Delta(v_i) = \Delta \tag{2.7}$$

and hence the density defined in (1.1) is $\rho = (1 - \Delta)/l$. The theorem mentioned above asserts that the fluctuation

$$\delta(N) = \sum_{i=1,N} \chi_\Delta(v_i) - N\Delta \tag{2.8}$$

of the number of vacancies with respect to its mean value $N\Delta$ is bounded in N if and only if the width Δ of W is a multiple (mod 1) of the rotation angle l, i.e. $\Delta = rl + s$ for some integers r and s. If Δ does not satisfy this condition, $\delta(N)$ is expected to diverge logarithmically with N for typical values of l, in analogy with results known in the part of number theory called discrepancy theory [5].

Though the ground state of the present model is described by an incommensurate modulation of the vacancy density, it is very different from the standard 'displacive' incommensurate structures, where the 'modulation' of the atomic positions WRT their average lattice is given by

$$u_n = u_0 + na + g(qn) \tag{2.9}$$

where $a = \rho^{-1} = \langle u_{n+1} - u_n \rangle$ is the interatomic mean distance, which determines the average lattice $u_0 + na$, $g(x)$ is a one-periodic function and q is the wavevector of this modulation. In these standard incommensurate structures, the function $g(x)$ is bounded and square summable. It may be very smooth (analytic) or as irregular as a Cantor function. In the present model $a = l/(1-\Delta)$, and the difference $Nl - na = a\,\delta(N)$ formally plays the role of $g(qn)$, where $\delta(N)$ is the fluctuation considered above. When $\Delta \neq rl \pmod 1$, $\delta(N)$, and hence the displacements of the atoms WRT their average position, are not bounded. The Fourier spectrum of the atomic density is nevertheless discrete. Indeed, this density

$$\begin{aligned} \rho(r) &= \sum_j \delta(r - u_j) = \sum_i \delta(r - v_i)[1 - \chi_\Delta(v_i)] \\ &= [1 - \chi_\Delta(r)] \sum_i \delta(r - il) \end{aligned} \tag{2.10}$$

is the product of two periodic generalised functions with incommensurate periods 1 and l, respectively. Consequently, $\rho(r)$ is a quasiperiodic distribution. More precisely, its Fourier transform is

$$G(q) = \int e^{iqr} \rho(r)\, dr = \sum_{m,n} C_m(\Delta)\, \delta((ql/2\pi) - ml - n)$$

with

$$\begin{aligned} &C_m(\Delta) = [\exp(-2\pi i m\Delta) - 1]/(2\pi i m) \qquad \text{for } m \neq 0 \\ &C_0(\Delta) = 1 - \Delta = l\rho. \end{aligned} \tag{2.11}$$

To conclude this section, let us note that the central mathematical object of this study is the sequence $\{\chi_\Delta(v_i)\}$. From the knowledge of this sequence, one may construct different models.

(i) The above-mentioned model, which is a distribution of atoms and vacancies on a linear lattice.

(ii) A different model, which is defined as a distribution of links $l(i) = u_{i+1} - u_i$, given by the rule:

$$\begin{aligned} &l(i) = l_1 \qquad \text{if } v_i \notin W \\ &l(i) = l_2 \qquad \text{if } v_i \in W \end{aligned} \tag{2.12}$$

where $v_i = il$, and l_1, l_2 are two arbitrary lengths. Equivalently,

$$l(i) = l_1(1 - \chi_\Delta(v_i)) + l_2 \chi_\Delta(v_i) \tag{2.13}$$

where χ_Δ is the characteristic function of W. Then the abscissae of the atoms are $u_n = \Sigma_{i=1,n}\, l(i)$. This model is far more difficult to study than model (i). Nevertheless, when Δ is equal to l, it leads [2] to the tiling of the standard projection method [6] in one dimension. In this case the fluctuation is bounded [2, 4].

Hereafter, we will only focus our attention on the sequence $\{\chi_\Delta(il)\}$, and on the related fluctuation $\delta(N)$ defined in equation (2.8), ignoring the condition $\Delta < l < 1 - \Delta$ which was introduced in [2].

3. Study of a specific example

3.1. Preliminaries

In the following, we will study the sequence $\{\chi_\Delta(il)\}$, restricting ourselves, for technical reasons, to the more symmetric case where the window covers half the circle ($\Delta = \frac{1}{2}$). In this section, we make the choice of a particular rotation angle $l = 2 - \tau = \tau^{-2}$, where $\tau = (\sqrt{5}+1)/2$ is the golden mean. In § 4, we show how the inflation rules derived in § 3 can be generalised to arbitrary values of the rotation angle and we give some consequences on the growth of the density fluctuation. For the sake of convenience, since $\Delta = \frac{1}{2}$ we introduce the sequence

$$\varepsilon_i = 2\chi_{1/2}(il) - 1 \tag{3.1}$$

which, in this particular case, has the alternative expression

$$\varepsilon_i = \mathrm{sgn}(\sin(2\pi i l)). \tag{3.2}$$

Thus $\varepsilon_i = 1$(resp -1) if $\mathrm{frac}(il) < \frac{1}{2}$ (resp $\mathrm{frac}(il) > \frac{1}{2}$). The mean value of ε_i is 0 and the fluctuation $\delta(N)$ is

$$\delta(N) = \tfrac{1}{2}S(N) \qquad \text{with} \qquad S(N) = \sum_{i=1,N} \varepsilon_i. \tag{3.3}$$

In order to characterise the growth of $S(N)$, let us introduce its upper and lower 'hulls':

$$S(N)_{\max} = \max_{1 \leqslant n \leqslant N} S(n) \qquad S(N)_{\min} = \min_{1 \leqslant n \leqslant N} S(n). \tag{3.4}$$

These quantities have simple kinds of asymptotic behaviour, as will be shown below.

3.2. Numerical observations

Before giving an analytical derivation of the scaling behaviour of $S(N)$, we first present, for pedagogical reasons, some numerical results concerning the example above. Table 1 gives the values of N, denoted N_n and N_{-n}, for which $S(N)$ takes for the first

Table 1. Values of N for which $S(N)_{\max}$ is increased or $S(N)_{\min}$ is decreased.

N_n	$n = S(N_n)_{\max}$	$N_n - N_{n-1}$
0	0	—
1	1	$1 = F_2$
22	2	$21 = F_8$
399	3	$377 = F_{14}$
7 164	4	$6\,765 = F_{20}$
128 557	5	$121\,393 = F_{26}$
N_{-n}	$-n = S(N_{-n})_{\min}$	$N_{-n} - N_{-n+1}$
0	0	—
5	−1	$5 = F_5$
94	−2	$89 = F_{11}$
1 691	−3	$1\,597 = F_{17}$
30 348	−4	$28\,657 = F_{23}$
544 577	−5	$514\,229 = F_{29}$

time its maxima or minima: $S(N)_{\max} = 1, 2, \ldots, n, \ldots,$ or $S(N) = S(N)_{\min} = -1, -2, \ldots, -n, \ldots$. Defining the Fibonacci numbers by

$$F_n = F_{n-1} + F_{n-2} \qquad F_0 = 0,\ F_1 = 1 \tag{3.5}$$

we note that, for all values of n, the difference $N_n - N_{n-1}$ is equal to F_{6n-4}. Similarly, the difference $N_{-n} - N_{-n+1}$ is equal to F_{6n-1}. Figure 2 shows a plot of $S(N)_{\max}$ and $S(N)_{\min}$ against $\ln N$. Since, for large p, F_p behaves as $\tau^p/\sqrt{5}$, these quantities have the following simple behaviour:

$$S(N)_{\max} \approx -S(N)_{\min} \approx \ln N / 6 \ln \tau. \tag{3.6}$$

These data exhibit some periodic structure around the average slopes $\pm 1/6 \ln \tau$, shown in figure 2 by broken lines. We shall now describe those results analytically.

3.3. Renormalisation and inflation rules

The sequence $il \pmod 1$ may be generated by a rotation on the circle parametrised by $0 \leqslant x \leqslant 1$, with the rotation angle $l = 2 - \tau$. Let us recall that when $\mathrm{frac}(il) < \frac{1}{2}$, ε_i takes the value $+1$, and when $\mathrm{frac}(il) > \frac{1}{2}$, ε_i takes the value -1. One may associate the symbols $(+)$ or $(-)$ to those two regions. The rotation generates an infinite sequence S of symbols $(+)$ or $(-)$.

In this section, we will show that this sequence is self-similar. More precisely, S can be generated by a substitution, giving inflation rules, hereafter denoted by $\mathcal{T}$, acting on four types of 'letters': a, b, c, d. These letters are symbols for the spaces between any two successive ε_i in the sequence S, according to the following correspondence:

$$++ = a \qquad +- = b \qquad -+ = c \qquad -- = d. \tag{3.7}$$

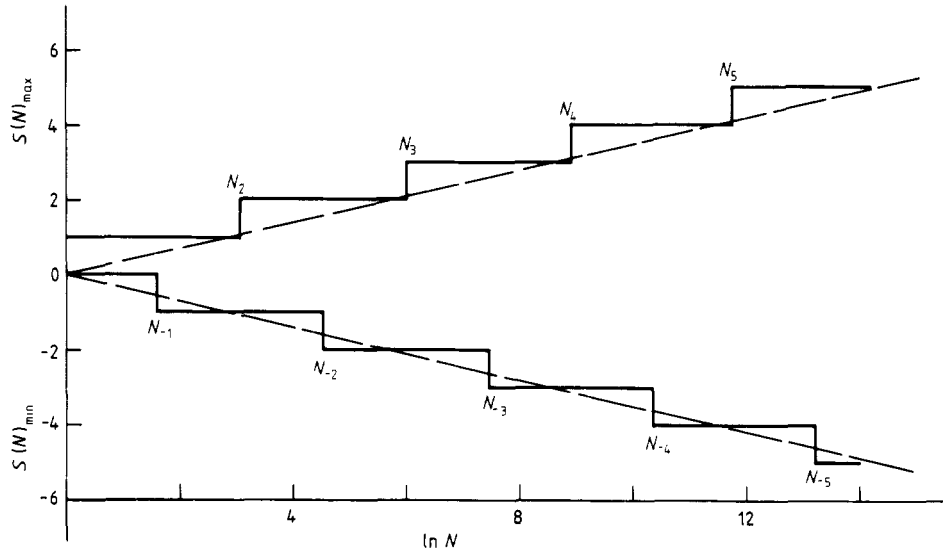

Figure 2. Plot of $S(N)_{\max}$ and $S(N)_{\min}$ against $\ln N$ for the case $\Delta = \frac{1}{2}$, $l = 2 - \tau$. The values of N for which these quantities vary are listed in table 1. The broken lines show the linear law (3.6).

These inflation rules are

$$\begin{aligned} a &\to c\,b\,c\,b\,d \\ b &\to c\,b\,c \\ c &\to a\,b\,c\,b\,d \\ d &\to a\,b\,c\,b\,c \end{aligned} \tag{3.8}$$

or, in terms of the ε_i (remembering that the substitution acts on the spaces between the ε_i),

$$\begin{aligned} &++ \to -**- \\ &+- \to -*+ \\ &-+ \to +**- \\ &-- \to +**+ \end{aligned} \tag{3.9}$$

where the star stands for the symbol $(+-)$. To be complete, a last rule should be added concerning the origin. Since the initial point $v_0 = 0$ stands at the right border between $(+)$ and $(-)$ on the circle, ε_0 is not defined. The beginning of the sequence, hereafter denoted $(0+)$ (for $l < \frac{1}{2}$), is understood as being the limit between $(++)$ and $(-+)$. The inflation rule for $(0+)$ is $0+ \to 0**-$.

The rest of this section is devoted to a proof of this assertion. The demonstration proceeds by steps.

(*i*) *Cutting and rescaling on the circle.* Since $l = 2 - \tau < \frac{1}{2}$, at least one symbol $(+)$ is met whenever a complete revolution is done on the circle (figure 3(*a*)). One thus

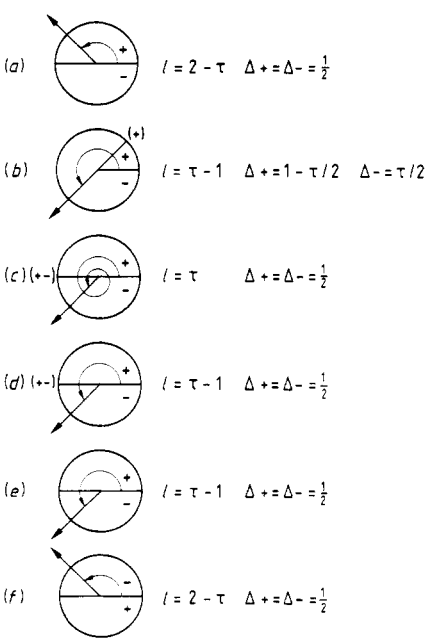

Figure 3. Different steps in the renormalisation procedure for the case $\Delta = \frac{1}{2}$, $l = 2 - \tau$, with the corresponding values of the rotation angle l, and of the widths Δ_+ and Δ_- of regions $(+)$ and $(-)$, respectively.

obtains the same sequence S by cutting a sector of angle l out of the region $(+)$ of the circle, and replacing it by a symbol $(+)$ on the border between the new regions $(+)$ and $(-)$. The new region $(+)$ has size $\frac{1}{2}-l$, and the whole circle has size $1-l$. Rescaling the circle to unity, the new region $(+)$ has size $(\frac{1}{2}-l)/(1-l)=1-\tau/2$, the new region $(-)$ has size $\tau/2$, and the new rotation angle is $l/(1-l)=\tau-1$ (figure 3(b)). Repeating this process of cutting a sector and rescaling for region $(-)$, one recovers two regions of equal size $\frac{1}{2}$ and the rotation angle is equal to τ. The two sectors that have been cut out are replaced by a symbol $(*)=(+-)$ located at the left border between the regions $(+)$ and $(-)$ (see figure 3(c)). Thus every passage through this border generates a $(*)=(+-)$ in the sequence built by the rotation on the circle.

(ii) *Changing the angle of rotation.* Instead of taking τ as rotation angle, let us take its fractional part $\tau-1$. The new sequence S' associated with this new angle allows us to reconstruct S in the following way: insert once the symbol $(*)=(+-)$ before every $(+)$ or $(-)$ (except those contained in the symbols $(*)=(+-)$ coming from the border) (figure 3(d)).

(iii) *Inflation.* Let us consider the sequence S'' obtained by the previous rotation ($\Delta=\frac{1}{2}$, $l=\tau-1$), forgetting the symbols $(+-)$ on the border (figure 3(e)). The sequence S' is recovered from S'' by the substitution

$$\begin{aligned}
&0+\to 0\,(*)+\\
&++\to +(*)+\\
&+-\to +(*)-\\
&-+\to -+\\
&--\to -(*)-.
\end{aligned}\tag{3.10}$$

These are indeed the only ways of crossing the borders.

(iv) *Going back to S.* The sequence S'' may also be generated by taking the rotation angle $1-(\tau-1)\equiv 2-\tau$ and exchanging the roles of regions $(+)$ and $(-)$ (see figure 3(f)). One then remarks that S'' is identical to $(-S)$, i.e. S'' is the sequence of $(-\varepsilon_i)$ while S is the sequence of (ε_i).

Starting from S and reversing the order of steps (i)-(iv) gives the announced result (equations (3.8) and (3.9)). Indeed, let us start from the initial word 0+, and transform it by the successive steps (iv)-(i):

$$0+\to 0-\to 0*-\to 0**-=0+-+--.\tag{3.11}$$

We have thus obtained the beginning of the sequence S. Let us inflate this finite part of the sequence once more:

$$\begin{aligned}
(S)\quad &:0\quad +\quad -\quad +\quad -\quad -\\
(S''=-S)&:0\quad -\quad +\quad -\quad +\quad +\\
(S')\quad &:0\ *\ -\quad +\ *\quad -\quad +\ *\ +\\
(S)\quad &:0\ *\ *\ -\ *\ +\ *\ *\ -\ *\ +\ *\ *\ +.
\end{aligned}\tag{3.12}$$

This process shows the self-similar character of the sequence S, and proves equations (3.8) and (3.9). Moreover, in the notation of the letters $a, b, \ldots$, equations (3.11) and (3.12) become

$$0\to 0\,b\,c\,b\,d\to 0\,b\,c\,b\,d\,c\,b\,c\,a\,b\,c\,b\,d\,c\,b\,c\,a\,b\,c\,b\,c\tag{3.13}$$

(see figure 4(*b*)). We note that the successive sizes of the words are $1 = F_2$, $5 = F_5$, $21 = F_8$, where the F_n are the Fibonacci numbers defined in equation (3.5).

3.4. Consequences of the inflation rules

Let us now analyse the consequences of the substitution $\mathcal{T}$ given by equations (3.8) and (3.9). These inflation rules contain, in principle, all the desired information on the sequence S. In particular, they permit us to understand the observations made in § 3.2. Nevertheless, instead of giving detailed and lengthy proofs of these properties, we will capture their gross features by noting the most important consequences of the inflation rules given by equations (3.8) and (3.9).

To do so, we first introduce the matrix M associated with this transformation. By definition, M transforms the numbers n_a, n_b, n_c, n_d of letters a, b, c, d in any finite part of the sequence S into the corresponding numbers n'_a, n'_b, n'_c, n'_d in the inflated sequence:

$$\begin{bmatrix} n'_a \\ n'_b \\ n'_c \\ n'_d \end{bmatrix} = M \begin{bmatrix} n_a \\ n_b \\ n_c \\ n_d \end{bmatrix} \qquad M = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 2 & 1 & 2 & 2 \\ 2 & 2 & 1 & 2 \\ 1 & 0 & 1 & 0 \end{bmatrix}. \tag{3.14}$$

The characteristic polynomial of the matrix M is

$$P(\lambda) = \det(\lambda \mathbb{1} - M) = (\lambda + 1)^2(\lambda^2 - 4\lambda - 1) \tag{3.15}$$

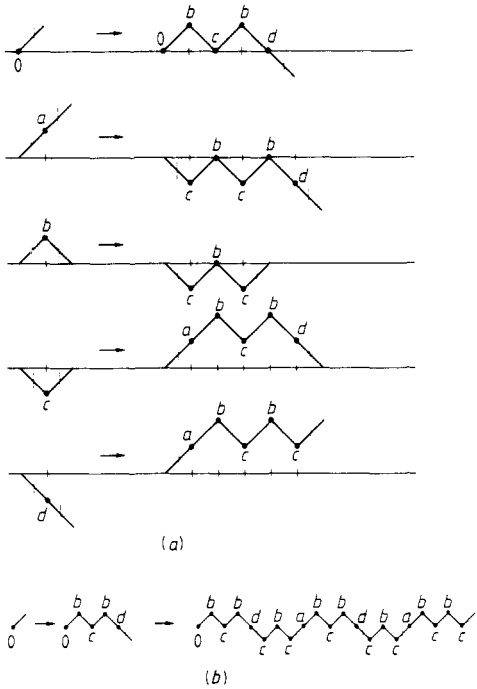

Figure 4. (*a*) Representation of the inflation rules for the case $\Delta = \frac{1}{2}$, $l = 2 - \tau$. An ascending segment corresponds to $\varepsilon_i = +$, a descending one to $\varepsilon_i = -$. (*b*) Two steps of inflation generating the beginning of the sequence S.

the roots of which are $\lambda = -1, -1, -\tau^{-3}, \tau^3$. This implies that the action of the substitution $\mathcal{T}$ on any large part of the sequence S corresponds asymptotically to a dilatation of its size by the leading eigenvalue τ^3. One may check this result. Indeed, the eigenvector corresponding to the leading eigenvalue τ^3 is $(\tau^{-3}/2, \tau^{-2}, \tau^{-2}, \tau^{-3}/2)$, the components of which are the relative frequencies of latters a, b, c and d, respectively. Since, by inflation, these letters give words of sizes 5, 3, 5, 5, respectively (see figure 4(a)), any finite part of the sequence S will be dilated by the factor

$$5\tau^{-3}/2 + 3\tau^{-2} + 5\tau^{-2} + 5\tau^{-3}/2 = \tau^3. \tag{3.16}$$

The value of this scaling factor is in agreement with the increase of the sizes of words through inflation, noted above. Furthermore, it is also related to the observations made in § 3.2 on the behaviour of $S(N)_{\max}$ and $S(N)_{\min}$.

A second feature observed in § 3.2 was the 'oscillating' behaviour of $S(N)$ (see table 1). This is related to the fact that each letter is 'reversed' by inflation (see figure 4(a)), which would not happen if step (iv) was absent (see § 4).

A last remark is in order. We notice that in figure 4(a) the relation $-+ = c \to a\,b\,c\,b\,d$ plays a special role. Indeed, let us compare the successive sums of the ε_i contained in a letter $a, b, \ldots$, and in the word obtained by inflation. To do so, consider figure 4(a) as representing mountains and valleys. For instance, the maximum height of a is 2 and the maximum depth of the word obtained after inflation is -2. For b, these numbers are 1 and -1, respectively. Similarly, the maximum depth of d is -2 and the maximum height of the word obtained after inflation is 2. The crucial point comes from the fact that for c these numbers are -1 and 2, respectively. This difference is at the origin of the divergence of the fluctuation considered in this paper.

These considerations taken together thus provide a quantitative explanation of the logarithmic divergence of $S(N)$ observed in § 3.2. In § 4, the study of the general case will complete this description.

4. Generalisation to an arbitrary rotation angle

The purpose of this section is to show how the exact renormalisation transformation $\mathcal{T}$ described in § 3.3 in the particular example $l = \tau^{-2}$ can be easily generalised to arbitrary irrational values of the rotation angle $l < \frac{1}{2}$. We define $\omega = 2l$ for further convenience.

4.1. On continued fraction expansions

Since the construction which follows will make an extensive use of the continued fraction expansion (CFE) of the number $\omega = 2l$, we must first recall some basic notation. Any irrational number $0 < \omega < 1$ can be written in a unique way as

$$\omega = \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ldots}} = [a_1, a_2, \ldots] \tag{4.1}$$

where the integers a_k are called the quotients of the CFE. If we truncate this expansion, we obtain a sequence of rational approximants

$$\Omega_k = \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ldots + (1/a_k)}} = \frac{p_k}{q_k} \tag{4.2}$$

called the principal convergents of the CFE. Their numerators and denominators both obey linear recursion relations:

$$\begin{aligned} p_k &= a_k p_{k-1} + p_{k-2} \qquad p_{-1} = 1 \qquad p_0 = 0 \\ q_k &= a_k q_{k-1} + q_{k-2} \qquad q_{-1} = 0 \qquad q_0 = 1. \end{aligned} \tag{4.3}$$

In the following, we will also make use of the quantities

$$\omega_1 = [a_2, a_3, a_4, \dots] \qquad \omega = \frac{1}{a_1 + \omega_1}$$

$$\omega_2 = [a_3, a_4, a_5, \dots] \qquad \omega = \frac{1}{a_1 + \dfrac{1}{a_2 + \omega_2}}. \tag{4.4}$$

4.2. The renormalisation transformation $\mathcal{T}$

The renormalisation procedure described in § 3.3 in the particular case $l = \tau^{-2}$ can easily be generalised to an arbitrary rotation angle. We will now derive this transformation $\mathcal{T}$ explicitly, following closely the set-up of § 3.3. We consider the sequence $\{\varepsilon_n = 2\chi_{1/2}(nl) - 1 = \operatorname{sgn}\sin(2\pi nl)\}$, where $\omega = 2l$, and perform the following operations.

Step (i). The sequence $\{\varepsilon_n\}$ remains invariant if we cut out of each region (+) or (−) of the circle a given number of successive sectors with angle l. It is clear from equation (4.1) that the maximal number of sectors we can cut out is $a_1 = \operatorname{int}(\omega)$. We add a symbol $* \equiv (+^{a_1} -^{a_1})$ at the left border between the new (+) and (−) regions. Both now have a size $\frac{1}{2}(1 - a_1\omega)$. If we rescale these regions to their initial size $\frac{1}{2}$, we obtain a new rotation angle which is $\omega/2(1 - a_1\omega)$, or equivalently $1/2\omega_1$, by virtue of (4.4).

Steps (ii) and (iii). These consist in replacing the rotation angle $1/2\omega_1$ by its fractional part, after keeping track of a given integer number ν of revolutions. Since equation (4.4) implies $1/2\omega_1 = \frac{1}{2}(a_2 + \omega_2)$, two cases have to be considered separately, according to the parity of a_2. If a_2 is even, then we choose $\nu = \frac{1}{2}a_2$, and the remaining fractional part is $\frac{1}{2}\omega_2 < \frac{1}{2}$. We have therefore achieved our goal: the sequence $\{\varepsilon_n(\omega)\}$ is indeed related to another sequence $\{\varepsilon_n(\omega')\}$ through an unambiguous transformation $\mathcal{T}$, and the renormalised rotation angle is such that $\omega' = \omega_2$, where ω_2 defined in (4.4) is closely related to the CFE of ω. If a_2 is odd, then we choose $\nu = \frac{1}{2}(a_2 - 1)$, and the remaining fractional part is $\frac{1}{2}(1 + \omega_2) > \frac{1}{2}$. We therefore need a last operation to achieve the renormalisation procedure.

Step (iv). This step, which we perform if a_2 is odd, consists in reversing the signs of the ε_n and replacing the rotation angle $\frac{1}{2}(1 + \omega_2)$ by its complement $1 - \frac{1}{2}(1 + \omega_2) = \frac{1}{2}(1 - \omega_2)$. The renormalised angle is therefore defined by $\omega' = 1 - \omega_2$.

Hence the main result of this section is as follows: the sequence $\{\varepsilon_n(\omega)\}$ is related to another sequence $\{\varepsilon_n(\omega')\}$ by an explicit renormalisation procedure $\mathcal{T}$ (inflation rules). We summarise below the definition of ω', together with the inflation rules acting on the sequence $\{\varepsilon_n\}$. We recall that ω_2 is defined in (4.4), and that the star stands for the symbol $(+^{a_1} -^{a_1})$.

a_2 even	a_2 odd
$\mathcal{T}(\omega)=\omega'=\omega_2$	$\mathcal{T}(\omega)=\omega'=1-\omega_2$
$\nu=\frac{1}{2}a_2$	$\nu=\frac{1}{2}(a_2-1)$

(4.5)

$++\to+*^{\nu}+$	$++\to-*^{\nu+1}-$
$+-\to+*^{\nu+1}-$	$+-\to-*^{\nu}+$
$-+\to-*^{\nu}+$	$-+\to+*^{\nu+1}-$
$--\to-*^{\nu}-$	$--\to+*^{\nu+1}+.$

(4.6)

These rules generalise to arbitrary values of $\omega=2l$ the main result (3.9) of § 3.3. In the first case (a_2 even), the renormalisation of ω just amounts to a shift of the index k of its quotients a_k by two units. In the second case (a_2 odd), the CFE of $\omega'=1-\omega_2$ has a slightly more intricate expression:

$$\omega=[a_1,a_2,a_3,\dots]\Rightarrow\begin{vmatrix}a_3=1\colon\ \omega'=[a_4+1,a_5,a_6,\dots]\\ a_3\neq 1\colon\ \omega'=[1,a_3-1,a_4,a_5,\dots].\end{vmatrix}\tag{4.7}$$

The transformation $\mathcal{T}\colon\omega\to\omega'$ defined in equation (4.5) maps the interval $[0;1]$ onto itself. As ω varies from $\omega=0$ to $\omega=1$, $\mathcal{T}(\omega)=\omega'$ oscillates infinitely many times between 0 and 1. The function $\mathcal{T}$ is everywhere continuous, except at the points $\omega=1/N$ ($N\geqslant 2$) and $\omega=0$.

4.3. Self-similar sequences as fixed points of the transformation $\mathcal{T}$

Consider a value of the rotation angle l for which $\omega=2l$ is a fixed point of the renormalisation map $\mathcal{T}$, i.e. $\mathcal{T}(\omega)=\omega'=\omega$. Then equation (4.6) expresses the invariance of the sequence $\{\varepsilon_n\}$ through an inflation procedure or, in other words, its self-similarity. The particular case $l=\tau^{-2}$ considered in § 3 is an example of such a fixed point. The purpose of the present subsection is to study analytically all the fixed points of the map $\mathcal{T}$. They correspond to quadratic algebraic values of ω, in one-to-one correspondence with couples (a_1,a_2) of positive integers. Just as in the previous subsection, even and odd values of a_2 have to be considered separately.

If a_2 is even, then the fixed point ω obeys $\omega=\omega_2$, i.e. $a_1\omega^2+a_1a_2\omega-a_2=0$. The positive solution is

$$\omega=\frac{1}{2a_1}\{-a_1a_2+[a_1a_2(a_1a_2+4)]^{1/2}\}.\tag{4.8}$$

The inflation rules (4.6) of the sequence $\{\varepsilon_n\}$ can be rewritten as a substitution acting on a four-letter alphabet (see § 3.3). The matrix form of this transformation is given by (using the same notation as in § 3)

$$M=\begin{bmatrix}(a_1-1)\nu+1 & (a_1-1)\nu+a_1 & (a_1-1)\nu & (a_1-1)\nu\\ \nu & \nu+1 & \nu & \nu\\ \nu & \nu & \nu+1 & \nu\\ (a_1-1)\nu & (a_1-1)\nu+a_1 & (a_1-1)\nu & (a_1-1)\nu+1\end{bmatrix}\tag{4.9}$$

where $\nu=\frac{1}{2}a_2$. The characteristic polynomial of the substitution is

$$P(\lambda)=\det(\lambda\mathbb{1}-M)=(\lambda-1)^2[\lambda^2-(a_1a_2+2)\lambda+1].\tag{4.10a}$$

The non-trivial zeros of $P(\lambda)$ are x and x^{-1}, where $x>1$ is simply related to ω through

$$x = a_1(a_2+\omega)+1. \tag{4.10b}$$

Before discussing the implications of these results, let us first derive the analogous formulae which hold in the other case.

If a_2 is odd, then the fixed point ω obeys $\omega = 1-\omega_2$, i.e. $a_1\omega^2-(a_1a_2+a_1+2)\omega+a_2+1=0$. The admissible solution $(0<\omega<1)$ is

$$\omega = \frac{1}{2a_1}\{a_1(a_2+1)+2-[a_1^2(a_2+1)^2+4]^{1/2}\}. \tag{4.11}$$

The matrix of the associated substitution is given by

$$M = \begin{bmatrix} (a_1-1)(\nu+1) & (a_1-1)\nu & (a_1-1)\nu+a_1 & (a_1-1)\nu+a_1 \\ \nu+1 & \nu & \nu+1 & \nu+1 \\ \nu+1 & \nu+1 & \nu & \nu+1 \\ (a_1-1)\nu+a_1 & (a_1-1)\nu & (a_1-1)\nu+a_1 & (a_1-1)(\nu+1) \end{bmatrix} \tag{4.12}$$

where $\nu=\frac{1}{2}(a_2-1)$. The characteristic polynomial of the substitution is

$$P(\lambda) = \det(\lambda\mathbb{1}-M) = (\lambda+1)^2[\lambda^2-a_1(a_2+1)\lambda-1]. \tag{4.13a}$$

The non-trivial zeros of $P(\lambda)$ are x and $(-x^{-1})$, where $x>1$ is simply related to ω through

$$x = a_1(a_2+1-\omega)+1. \tag{4.13b}$$

The results of § 3.3 are easily recovered: $l=\tau^{-2}$ corresponds to $(a_1=1, a_2=3)$, equations (4.11) and (4.13) yield $\omega = 3-\sqrt{5} = 2\tau^{-2}$, and $x = 2+\sqrt{5} = \tau^3$, as they should. The first eight fixed points (according to increasing values of x) are listed in table 2. Some degeneracies can be seen: different values of a_1 and a_2 (and hence different self-similar sequences) may have the same scaling index x; we will see below that the details of their properties are nevertheless different.

The scaling index x has the meaning that the action of the transformation (4.6) on any large but finite part of the sequence $\{\varepsilon_n\}$ dilates its length by a factor of x. Therefore any geometrical quantity that characterises the sequence $\{\varepsilon_n\}$ can be expected to exhibit in some sense periodicity in the variable $\ln n$, with period $\ln x$. It can be shown explicitly that the quantities $S(N)_{\max}$ and $S(N)_{\min}$, defined in equation (3.4), indeed obey such a scaling behaviour.

Table 2. Values of $\omega = 2l$ and the scaling index x for the first eight fixed points of $\mathcal{T}$. The particular example of § 3 is the third one in the table.

a_1	a_2	$\omega = 2l$	x
1	1	$2-\sqrt{2} = 0.585\,79$	$1+\sqrt{2} = 2.414\,21$
1	2	$\sqrt{3}-1 = 0.732\,05$	$2+\sqrt{3} = 3.732\,05$
1	3	$3-\sqrt{5} = 0.763\,93$	$2+\sqrt{5} = 4.236\,07$
2	1	$\frac{1}{2}(3-\sqrt{5}) = 0.381\,97$	
1	4	$2(\sqrt{2}-1) = 0.828\,43$	$3+2\sqrt{2} = 5.828\,43$
2	2	$\sqrt{2}-1 = 0.414\,21$	
1	5	$4-\sqrt{10} = 0.837\,72$	$3+\sqrt{10} = 6.162\,28$
3	1	$\frac{1}{3}(4-\sqrt{10}) = 0.279\,24$	

Consider first the simpler case (a_2 even). It can be seen from equation (4.6) that $S(N)_{\min}$ vanishes identically, since the only way a new $(-)$ sign can show up in an inflation procedure is inside a star, i.e. at the right of at least one new $(+)$ sign. Analogous considerations show that $S(N)_{\max}$ is increased a_1 times by one unit in each inflation procedure. More precisely, let us start from the original word $W_0 = 0+$, and build its successive transforms $W_1 = 0*^{\nu}+$, $W_2 = 0*^{\nu}[(+*^{\nu})^{a_1}*(-*^{\nu})^{a_1}]^{\nu}+$, etc. It can be shown by recursion that the length (number of signs except the initial 0) of the word W_k is nothing else than q_{2k}, where the integers q_k have been defined in (4.3). These results imply that $S(N)_{\max}$ is increased a_1 times (by one unit) for a_1 values of N separated by a distance q_0 (the last of these values is q_1, i.e. $S(q_1)_{\max} = a_1$), then for a_1 values of N separated by a distance q_2 (the last of these values is q_3, i.e. $S(q_3)_{\max} = 2a_1$), and so on. Since q_{2k} grows asymptotically as x^k, where x is precisely the scaling index defined in (4.10*b*), these exact results concerning the points where $S(N)_{\max}$ increases yield the following asymptotic expression:

$$a_2 \text{ even} \qquad S(N)_{\max} \approx a_1 \frac{\ln N}{\ln x} \qquad S(N)_{\min} \equiv 0. \tag{4.14a}$$

In the other case (a_2 odd), analogous results can be derived. Since the points where $S(N)_{\max}$ is increased, or $S(N)_{\min}$ is decreased, are not as simple as above, we will just mention their asymptotic scaling form

$$a_2 \text{ odd} \qquad S(N)_{\max} \approx -S(N)_{\min} \approx \frac{a_1}{2} \frac{\ln N}{\ln x}. \tag{4.14b}$$

Equations (4.14*a*) and (4.14*b*) generalise to all the fixed points of the map $\mathcal{T}$ the scaling result (3.6) which was derived in § 3 for the particular example $l = \tau^{-2}$.

We have shown that the sums $S(N)$ defined in (3.3) grow as $\ln N$ for some special values of N, which are more and more rare ($N \sim x^k$). Let us now present some evidence that $|S(N)|$ is also growing at a similar rate as $S(N)_{\max}$ or $|S(N)_{\min}|$ for typical values of N. For that purpose, we define the mean squared fluctuation $\Sigma(N)$ at scale N by

$$a_2 \text{ odd} \qquad \Sigma(N) = \frac{1}{N} \sum_{n=1}^{N} S(n)^2 \tag{4.15a}$$

$$a_2 \text{ even} \qquad \Sigma(N) = \frac{1}{N} \sum_{n=1}^{N} \left(S(n) - \frac{a_1}{2} \frac{\ln n}{\ln x} \right)^2. \tag{4.15b}$$

We are led from numerical evidence to argue that this quantity also has a logarithmic asymptotic behaviour:

$$\Sigma(N) \approx C \ln N + P\left(\frac{\ln N}{\ln x} \right) \tag{4.16}$$

irrespective of the parity of a_2. Both the slope C and the periodic correction P (with period $\mu = 1$ (a_2 even) or 2 (a_2 odd)) depend on a_1 and a_2. Figures 5 and 6 illustrate the behaviour (4.16) in one example for each parity of a_2. Let us remark that the analytical study of the constant C and the function P remain a difficult open question.

The above analysis of the fixed points of the renormalisation map $\mathcal{T}: \omega \to \omega'$ can be extended to the periodic points ω, such that $\mathcal{T}^k(\omega) = \omega$ for some finite integer k. These values of ω are still quadratic algebraic numbers, in one-to-one correspondence with $2k$-uplets of integers $(a_1, a_2, \ldots, a_{2k})$. The main results of this section remain

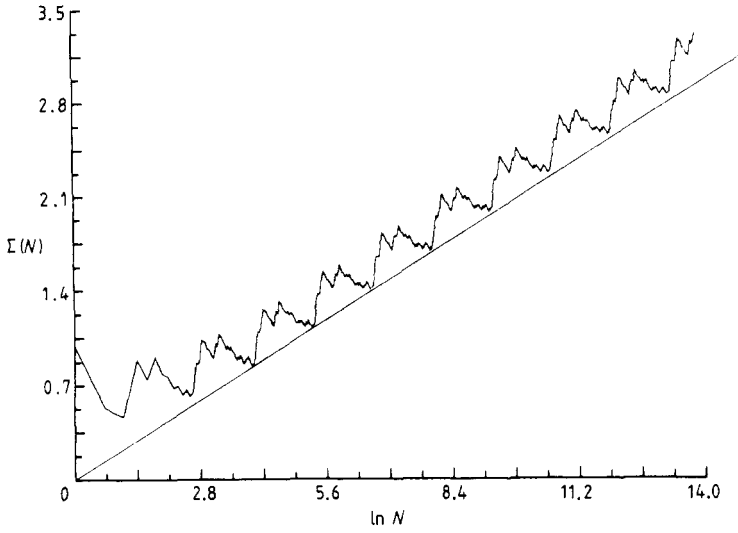

Figure 5. Plot of the mean squared fluctuation $\Sigma(N)$, defined in (4.15), against $\ln N$, for $\omega = 2l = \sqrt{3} - 1$ (second case in table 2).

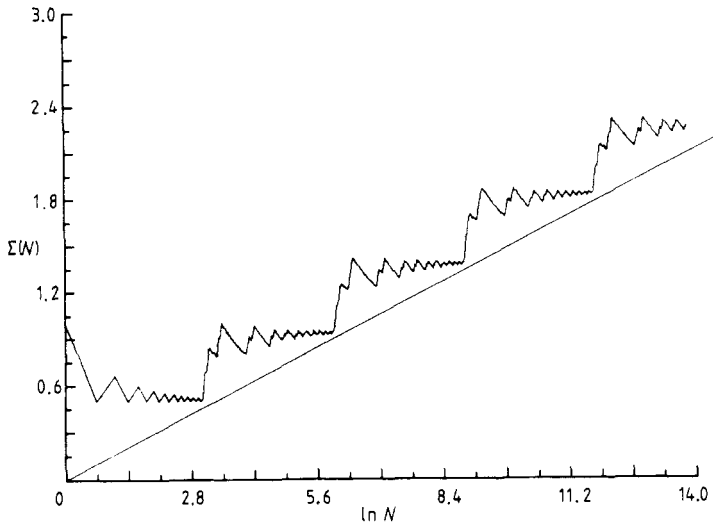

Figure 6. Same as figure 5, for $\omega = 3 - \sqrt{5}$, i.e. $l = 2 - \tau$ (third case in table 2, which was considered in § 3).

qualitatively the same for fixed points and periodic points, in particular the self-similarity of the sequence $\{\varepsilon_n\}$ and the logarithmic growth of its fluctuation $S(N)$.

4.4. Properties of some aperiodic orbits

If we consider a 'generic' irrational value, such as the transcendental numbers $e^{-\pi}$ or $1/\pi^2$, of the rotation angle l, then the CFE of $\omega = 2l$ does not present any special regularity. Hence the orbit of ω by $\mathcal{T}$, i.e. the set of its successive iterates $\omega' = \mathcal{T}(\omega)$,

$\omega'' = \mathcal{T}(\omega')$, etc, under the renormalisation map $\mathcal{T}$, defined in (4.5), is generically a complicated irregular aperiodic object.

Contrary to the case of the self-similar sequences studied in § 4.3, the sequences associated with aperiodic orbits are expected to have more intricate asymptotic properties. It is therefore hopeless to attempt to describe in detail the behaviour of quantities such as $S(N)_{\max}$ for all values of l. The purpose of this section is to show that some scaling results concerning $S(N)_{\max}$ can nevertheless be derived for some exceptional values of the rotation angle. In particular, we will show explicit examples for which $S(N)_{\max}$ grows much quicker, or much slower, than a logarithm.

We restrict ourselves in the following to values of the rotation angle such that the even quotients of the CFE of $\omega(a_2, a_4, a_6, \dots)$ are all even integers. This ensures that step (iv) of the renormalisation procedure will never take place, and that $S(N)_{\min}$ vanishes identically. Moreover, the values of N for which $S(N)_{\max}$ increases can be described in an exact fashion, along the same lines as in § 4.3, namely, starting from $S(0)_{\max} \equiv 0$, we first meet a_1 values of N, equidistant by q_0, at which $S(N)_{\max}$ is increased by one unit, and we then meet a_3 values of N, equidistant by q_2, then a_5 values of N, equidistant by q_4, etc. Finally all the values of N for which $S(N)_{\max}$ is increased (by one unit) are

$$N = q_{2l-1} + Kq_{2l} : S(N)_{\max} = \sum_{k=0}^{l-1} a_{2k+1} + K \qquad (l \geqslant 0;\ 0 \leqslant K \leqslant a_{2l+1}). \tag{4.17}$$

This general result yields interesting unexpected scaling laws in some specific examples. Consider first values of l, such that the quotients a_k grow very quickly, e.g.

$$a_k \sim A \exp(st^k) \tag{4.18}$$

where A, s, t are real parameters. It can then be derived from (4.17) that $S(N)_{\max}$ grows asymptotically like

$$S(N)_{\max} \sim N^{1-1/t} (\ln N)^{-\ln A/t \ln t}. \tag{4.19}$$

Since there exist values of the rotation angle which correspond to arbitrary values of $t > 1$, the exponent $(1-1/t)$ may assume any *a priori* given value between 0 and 1. If $t > 2$, the exponent exceeds the value $\frac{1}{2}$ which characterises typical values of $S(N)$ in a random system; there are some quasiperiodic sequences which exhibit at some locations a larger fluctuation than a typical random one.

Consider now other values of l, such that all the odd quotients $(a_1, a_3, a_5, \dots)$ assume the common value 1, while the even ones $(a_2, a_4, \dots)$ still grow like (4.18). Equation (4.17) now yields asymptotically

$$S(N)_{\max} \sim \frac{\ln \ln N}{2 \ln t} \tag{4.20}$$

For such values of l, the fluctuation grows much slower than the one of self-similar structures.

5. Conclusions

The renormalisation transform $\mathcal{T}$ described in the present paper allows a detailed description of the sequence generated by the circle map T, defined in § 2, for arbitrary

values of the rotation number l, in the particular symmetric case $\Delta=\frac{1}{2}$. The results concerning the fluctuation of atomic positions assume a simple form in the following two instances. Fixed points of $\mathcal{T}$, corresponding to some quadratic rotation numbers, yield self-similar sequences with a logarithmic fluctuation; for some exceptional rotation numbers, the fluctuation can be shown to diverge as a power of the system size, although the orbit of $\mathcal{T}$ is aperiodic. A quantitative description of the general case, where Δ has any value between 0 and 1, remains an open question.

Let us mention that it is possible to construct sequences of 0 and 1 generated by automata, which also exhibit various types of diverging fluctuation [7]. Reference [8] also deals with the relationship between self-similarity, quasiperiodicity and number theory.

To conclude, one may guess that a rich variety of types of order with discrete spectrum may exist in nature. As far as the two-lengths model mentioned at the end of § 2 is concerned, one may expect a more subtle spectrum. We will address this question in a subsequent publication [9]. A generalisation of the methods used in this paper to higher dimensions, e.g. quasiperiodic packings of two types of spheres, would also be desirable.

References

[1] Gratias D and Michel L (ed) 1986 *J. Physique Coll.* **C3** 1-503
[2] Aubry S and Godrèche C 1986 *J. Physique Coll.* **C3** 187
Aubry S, Godrèche C and Vallet F 1987 *J. Physique* **48** 327
[3] Aubry S, Fesser K and Bishop A 1985 *J. Phys. A: Math. Gen.* **18** 3157
[4] Kesten H 1966 *Acta Arith.* **12** 193
[5] Kuipers L and Niederreiter H 1974 *Uniform Distribution of Sequences* (New York: Wiley)
[6] de Bruijn N G 1981 *Neder. Akad. Wetensch. Proc.* A **43** 39
Duneau M and Katz A 1985 *Phys. Rev. Lett.* **54** 2688; 1986 *J. Physique* **47** 181
Elser V 1985 *Phys. Rev.* B **32** 4892
Kalugin P A, Kitayev A Yu and Levitov L S 1985 *J. Physique Lett.* **46** L601; 1985 *JETP Lett.* **41** 145
[7] Mendes-France M and Allouche J P 1986 private communication
[8] Bombieri E and Taylor J E 1986 *J. Physique Coll.* **C3** 19
[9] Aubry S, Godrèche C and Luck J M 1987 *Preprint* Saclay SPhT/87/72