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On the inflation, deflation and self-similarity of binary sequences. Application: a one-dimensional diatomic quasicrystal

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Abstract. A p sequence is an infinite sequence of 0 and 1 generated by the production rule $p(\alpha, \omega, j) = [(j+1)/\alpha + \omega] - [j/\alpha + \omega]$, $j \in \mathbb{N}$, depending upon two parameters: α, ω . The properties of quasiperiodic p sequences (α irrational) under deflation and inflation transformations are investigated. For this purpose, a set of so-called simple replacement rules (SRR) is defined, and it is shown that a p sequence is always transformed into a p sequence by repeated application of SRR. The parameters of the transformed sequence are calculated explicitly and the conditions are given under which a p sequence transforms into itself (self-similarity). The theory is applied to the construction of a one-dimensional diatomic quasicrystal, whose diffraction spectrum is calculated.

1. Introduction

The following theorem has appeared in the literature in many more or less equivalent forms and various degrees of generality. The form presented here is closest to that found in de Bruijn (1981), and will be given without proof, with slight changes in notation. The symbol $[x]$ represents the greatest integer not exceeding x .

Theorem T. Let $\alpha > 1$, and ω be real numbers, and $\alpha \neq 2$. The sequence

$$p(\alpha, \omega, j) = [(j+1)/\alpha + \omega] - [j/\alpha + \omega] \quad j \in \mathbb{N} \quad (1)$$

is an infinite sequence of 0 and 1. Let β be related to α by

$$1/\alpha + 1/\beta = 1. \quad (2)$$

Then $p(\alpha, \omega, j)$ takes its 1 and 0 on the sets

$$C_1: \{j | j = [(k - \omega)\alpha], \quad k \in \mathbb{N}\} \quad (3)$$

$$C_0: \{j | j = [(l + \omega)\beta], \quad l \in \mathbb{N}\} \quad (4)$$

respectively. The sets C_1, C_0 satisfy: $C_1 \cap C_0 = \emptyset$, and $C_1 \cup C_0 = \mathbb{N}$.

The class of binary sequences generated by (1) is an interesting object which has attracted considerable interest in the past. For a very incomplete list of relevant references see Aviram (1986). This paper is largely devoted to the study of properties of these sequences under inflation and deflation transformations to be defined below.

A sequence of 0 and 1 defined by (1) will be subsequently called a p sequence. It is periodic with an integer period J (i.e. $p(\alpha, \omega, j+J) = p(\alpha, \omega, j)$, $j \in \mathbb{N}$), if and only if $\alpha = q/r$ is a rational number with $J \bmod q = 0$. Unless otherwise specified, α will be assumed irrational throughout this paper.

Definition. A finite sequence of 0 and 1 is called a 'tile'. (This term together with 'deflation' and 'inflation' are borrowed from the terminology connected with the fascinating subject of Penrose tiles (Gardner 1977). The relationship with this paper is that both are concerned with non-periodic structures.)

In the same paper de Bruijn investigated the construction of new sequences from a given one by replacing every 0 and 1 of the original sequence by pre-assigned tiles: $0 \rightarrow t'$, $1 \rightarrow t''$. This process is called 'deflation', while the reverse action, to be called 'inflation' ($t' \rightarrow 0$, $t'' \rightarrow 1$), is possible only if the original sequence can be partitioned into tiles t' , t'' . De Bruijn called the deflated sequence the 'successor' of the old one, while the old sequence is the 'predecessor' of the new one. He focused his attention on the particular replacement rule (RR) $t' = 10$, $t'' = 100$, and investigated the conditions under which a given sequence has predecessors of all orders.

Definition. An infinite sequence of 0 and 1 is said to be 'self-similar' under a particular replacement rule $0 \rightarrow t'$, $1 \rightarrow t''$ if this deflation process transforms the sequence into itself.

An immediate consequence of this definition is that if an infinite sequence is self-similar, then the process of inflation by the reverse RR ($t' \rightarrow 0$, $t'' \rightarrow 1$) will also reproduce the original sequence. Moreover, both inflation and deflation may be repeated indefinitely, resulting in the same sequence at all stages.

In the following three sections we investigate the conditions under which a p sequence will be self-similar. Guided by analysis of the structural properties of a p sequence (§ 2), we introduce a finite class of so-called simple replacement rules (SRR), and show that a SRR always transforms a p sequence into another p sequence of the same class (1), or possibly into itself (§ 3). The main result of this section is a set of formulae relating the parameters α' , β' , ω' of the transformed sequence to α , β , ω of the original one. The roots of the equations $\alpha = \alpha'$, $\beta = \beta'$, $\omega = \omega'$ give the values $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\omega}$, which make the corresponding p sequence self-similar under a particular SRR. It will be sometimes useful to distinguish between 'generic self-similarity' when the transformed sequence has the same α and β as the original one, but not ω , and 'complete self-similarity', when the ω are equal, too. If not specified otherwise, self-similarity throughout this paper means complete.

Composite replacement rules (CRR) can be constructed by successive application of various SRR (§ 4). The main result of this section states that if $p(\alpha, \omega, j)$ is (generically) self-similar under some CRR then α is a quadratic irrational number. Conversely, if $\alpha > 1$ is any quadratic irrational number, then a replacement rule (simple or composite) exists under which the corresponding $p(\alpha, \omega, j)$ is self-similar.

In an earlier paper (Aviram 1986) the theory of binary p sequences was used in order to construct a one-dimensional quasicrystal of pointlike identical 'atoms' separated by one of two line segments of lengths a and b , whose succession was isomorphic to that of the 1 and 0 of a given p sequence with irrational α . We then calculated the diffraction spectrum of that quasicrystal. The results of the inflation theory of p sequences are used in § 5 in order to calculate the diffraction spectrum of a one-dimensional diatomic quasicrystal. Again, a sequence of line segments a and b is

constructed isomorphically to a given p sequence. The atoms of one species occupy all sites of this quasicrystal with the exception of those sites which survive an inflation transformation performed on the original sequence of segments. The remaining subset of sites are occupied by the second species. It is shown that the locations of the spectral lines are the same as if all sites of the quasicrystal were occupied by a single species. The intensities, however, are understandably different.

The main reasons for considering one-dimensional quasicrystals isomorphic to the class of p sequences (1) are: (a) they can be built with as little as two characteristic atomic separation distances; (b) due to the property of class invariance of these sequences under inflation and deflation transformations, diatomic one-dimensional quasicrystals may be constructed whose Fourier transform is easily calculated. More general one-dimensional quasicrystals (see Bombieri and Taylor 1986) may not necessarily possess these features.

2. Structural properties of $p(\alpha, \omega, j)$ partitions

Equations (3) and (4) can be easily inverted to give k and l as functions of j :

$$k = [(j+1)/\alpha + \omega] \quad j \in N \tag{5}$$

$$l = [(j+1)/\beta - \omega] \quad j \in N \tag{6}$$

where k and l are the numbers of 1 and 0, respectively, in the first j positions of the sequence. They are staircase functions of j , increasing by unity every time a 1 or 0 is encountered along the sequence.

The following result will be needed subsequently.

Lemma L. Let σ, τ be irrational numbers, θ_1 and θ_2 , real numbers, and $k \in N$. The equality

$$[k\sigma + \theta_1] = [k\tau + \theta_2] \quad k \in N \tag{7}$$

is satisfied for all k if and only if $\sigma = \tau$, and $\theta_1 = \theta_2$.

Proof. The 'if' part of the lemma is trivial. As for the 'only if' part, first assume that $\sigma > \tau$. If (7) is true, then $[k\sigma + \theta_1] < k\tau + \theta_2$ for all k , from which it follows that

$$k(\sigma - \tau) < \theta_2 - \theta_1 + \{k\sigma + \theta_1\} \tag{8}$$

where $\{ \}$ denotes the fractional part of the argument. It is clear that for any given values of θ_1, θ_2 , there exist some k_1 such that for all $k > k_1$ inequality (8) is violated. Next, assume that $\tau > \sigma$. If (7) is true, then $k\tau + \theta_2 < [k\sigma + \theta_1] + 1$ for all k ; it follows that

$$k(\tau - \sigma) < 1 - (\theta_2 - \theta_1) - \{k\sigma + \theta_1\}. \tag{9}$$

Again, it is clear that for any pair θ_1, θ_2 , there exists some k_2 such that for all $k > k_2$ inequality (9) will be violated. Therefore $\sigma = \tau$. Substitute this result into (8) and (9) and combine the inequalities:

$$0 < \theta_2 - \theta_1 + \{k\sigma + \theta_1\} < 1. \tag{10}$$

Since the set $\{k\sigma + \theta_1\}, k = 1, 2, \dots$, is uniformly and densely distributed in the open interval $(0, 1)$ (Weyl 1916), the only way in which both ends of the inequality (10) can be satisfied for all k is by requiring $\theta_1 = \theta_2$.

The elementary properties of p sequences have already been discussed to some extent in the earlier paper (Aviram 1986) and will be restated here for the sake of completeness in (a)–(e) below. The inflation and deflation properties of p sequences are described in detail in (f).

(a) Let $z(M, j)$ denote the fraction of 1 in a finite segment of length M starting at position j of the infinite sequence. The fraction of 0 is $1 - z(M, j)$. Let $\epsilon > 0$ be an arbitrarily small number. We say that the density of 1 is uniform, on average, if there exists $M_0(\epsilon)$ such that for any $M > M_0(\epsilon)$ the following inequality holds independently of j_1 and j_2 :

$$|z(M, j_1) - z(M, j_2)| < \epsilon. \tag{11}$$

For the sequence $p(\alpha, \omega, j)$, the fraction $z(M, j)$ is obtained from (5): $z(M, j) = ((j+M)/\alpha + \omega) - [j/\alpha + \omega] / M$. Using the inequality $a - b - 1 < [a] - [b] < a - b + 1$, it suffices to choose $M_0(\epsilon) = 2/\epsilon$ in order to satisfy (11). The condition is also satisfied independently of the parameters α, ω , a result which follows from the fact that k and l are $O(j)$. More precisely, $k = j/\alpha + O(1)$ and $l = j/\beta + O(1)$. Uniform average density is, of course, a trivial property of periodic, and uniformly random, sequences. If, however, α is irrational, the sequence $p(\alpha, \omega, j)$ will be quasiperiodic due to property (11) which distinguishes this from other types of aperiodicity.

Example E1. $\alpha = 1.273\ 457\ 813 \dots < 2$, $\beta = 4.656\ 871\ 196 \dots > 2$, $\omega = 0$, $[\beta] = 4$. The sequence $p(\alpha, 0, j)$ is

11101111011101111011110111101111011110111101110...

Figure 1 shows the graphs of $k(j)$ and $l(j)$ for this example, upon which the lines of slope $1/\alpha$ and $1/\beta$ are superimposed. The staircase functions at any point deviate from the average slope by less than one unit of the ordinate. If α and β are irrational numbers, the deviation never vanishes at integer values of j , except for 0.

(b) In a sequence $p(\alpha, \omega, j)$, one of the binary constituents, 0 or 1, always appears isolated, while the other occurs in strings of consecutive elements. Assume that two consecutive 1 appear in positions j and $j+1$. Then, according to (3) we must have

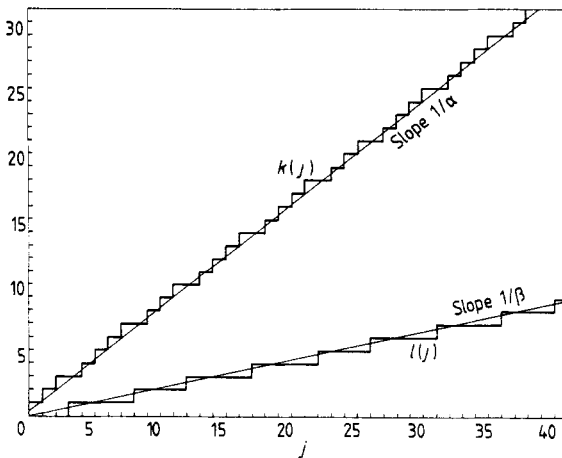


Figure 1. The functions $k(j)$ and $l(j)$.

$[(k+1-\omega)\alpha] - [(k-\omega)\alpha] = 1$. The arguments of the greatest integer functions in this equation must therefore satisfy $0 < (k+1-\omega)\alpha - (k-\omega)\alpha < 2$, or since $\alpha > 1$, one must have

$$1 < \alpha < 2. \tag{12}$$

An attempt to derive a similar condition for two consecutive 0 leads to $1 < \beta < 2$, which means, of course, $\alpha > 2$. Conclusion: consecutive 0 and 1 cannot coexist in a p sequence. The rule is

$$1 < \alpha < 2 \quad \beta > 2 \quad \text{consecutive 1 and isolated 0}$$

(this p sequence will be called 1-dominant);

$$1 < \beta < 2 \quad \alpha > 2 \quad \text{consecutive 0 and isolated 1}$$

(this p sequence will be called 0-dominant). Note that the parameter ω plays no role in establishing this property.

(c) Interchange of α and β produces the complementary sequence $p(\beta, \omega, j) = 1 - p(\alpha, \omega, j)$, i.e. 0 and 1 are interchanged. The following properties will be specifically derived for 1-dominant sequences and can be readily translated to 0-dominant ones by use of property (c).

(d) The number of consecutive 1. What must be the value of β in order to have strings of h consecutive 1 preceded and followed by isolated 0? The sites of these 0 will be $h+1$ places apart, which means that there must exist some values of l such that $[(l+1+\omega)\beta] - [(l+\omega)\beta] = h+1$. Hence

$$h < \beta < h+2. \tag{13}$$

The next question is: given β in the interval (13), are there strings of consecutive 1 of different lengths $h+g$, $g = \pm 1, \pm 2, \dots$, also present in the sequence? By the same argument there must be values of l for which $[(l+1+\omega)\beta] - [(l+\omega)\beta] = h+g+1$, from which it follows that

$$h+g < \beta < h+g+2. \tag{14}$$

Intervals (13) and (14) will partially overlap in two instances: $g = -1$ and $g = 1$. This means that, for any β in the unit interval

$$h < \beta < h+1 \tag{15}$$

the corresponding 1-dominant p sequence will contain strings of consecutive 1 of sizes $h = [\beta]$ and $h-1 = [\beta-1]$ only, separated by isolated 0 (see example E1 with $[\beta] = 4$). Note again that the parameter ω plays no role in the determination of this property either.

(e) What, then, is the role of ω ? Let us take in example E1, say, $\omega = -0.4$ instead of $\omega = 0$. The new sequence will be

$$10111101111011101111011110111101111011 \dots$$

By property (a) this sequence will have exactly the same density of 1 as the former; however the strings of four and three consecutive 1 follow each other in a different way. The role of ω therefore is to rearrange the binary elements of the sequence while preserving the string structure and the average density; it is called the 'shift parameter'.

As a matter of fact, there are as many different p sequences with the same string structure (i.e. α) as there are points ω on a line, i.e. an uncountable infinity of them. This can be proven as follows: for two different values ω and ω' construct the sets C_1 and C'_1 according to equation (3): $C_1: j = [(k - \omega)\alpha]$, $k \in N$, and $C'_1: j' = [(k - \omega')\alpha]$, $k \in N$. According to the second part of lemma L these sets will be identical if and only if $\omega = \omega'$. We conclude that two p sequences with the same α but different ω will eventually differ from each other starting from some finite position j .

The parameter β (or α) determines the global structure of a p sequence. By looking at some finite segment in the middle of an infinite sequence, there is no way one can tell what is the value of ω . The value of β , on the other hand, may be estimated with increasing accuracy by looking at ever longer segments. ω governs the beginning of the sequence.

Due to property (d) one may regard a 1-dominant p sequence as a succession of two kinds of tile: a long tile (L) composed of h digits 1 followed by a 0, and a short tile (S) composed of $h - 1$ digits 1 followed by a 0, where $h = [\beta]$. The following shorthand notation will be used: $h1 + 0$ and $(h - 1)1 + 0$, respectively. In example E1 we have 11110 and 1110. Depending upon the value of ω there may be an incomplete tile at the beginning. The specification of these two kinds of tile, however, is not unique, for we can use appropriate permutations of the digits on the tiles. In example E1 the following specifications are equally valid: 11011 and 1011. For some permutation, the first tile will be complete.

Definition. A covering tile is a tile which can be placed somewhere on a given p sequence in such a way that the binary digits on the tile exactly match those underneath.

Thus 11110, 1110, 0111011 are covering tiles for the sequence in example E1, while 11010, 1001 are not.

Definition. A binary covering partition (BCP) is defined by a set of two different covering tiles, one short, the other long, an infinite supply of which will enable the covering of a given p sequence without gaps. As a consequence of property (d), if β is irrational (i.e. the p sequence is non-periodic), then the set of two is minimal. The following are BCP for the sequence in example E1: (1, 1110), (1110, 11110), (11110, 111011110), etc. Partitions obtained through permutations of digits within the tile will not be counted as different.

Definition. A BCP will be called elementary (EBCP) if the non-dominant digit occurs at most once in any tile.

In the examples above, the first two are EBCP, while the third is not. The significance of this distinction will be clarified subsequently. We shall concern ourselves with BCP and EBCP for p sequences only. There are in general four possible EBCP for a fixed value of h , two of which are of the 1-dominant type, with $h = [\beta] \geq 2$:

$$\begin{aligned} \text{EBCP1: } \{S = (h - 1)1 + 0, L = h1 + 0\} \\ \text{EBCP2: } \{S = 1, L = (h - 1)1 + 0\} \end{aligned} \tag{16}$$

and two of the 0-dominant type, complementary to (16), with $h = [\alpha] \geq 2$:

$$\begin{aligned} \text{EBCP1c: } \{S = (h - 1)0 + 1, L = h0 + 1\} \\ \text{EBCP2c: } \{S = 0, L = (h - 1)0 + 1\}. \end{aligned} \tag{17}$$

(f) The distribution of short and long tiles of an EBCP as a function of β .

Consider first EBCP1: $\{S = (h - 1)1 + 0, L = h1 + 0\}$. Denote by $w_h(\beta)$ the fraction of $h1 + 0$ tiles in the infinite sequence. By property (d), $w_h = 1$ at $\beta = h + 1$ and decreases monotonically to zero at $\beta = h$ and $\beta = h + 2$. A schematic representation of a few $w(\beta)$ is shown in figure 2. The following relationships hold:

$$w_{h-1}(\beta) + w_h(\beta) = 1 \quad h < \beta < h + 1 \quad h = 2, 3, \dots \quad (18)$$

$$w_{h+1}(\beta + 1) = w_h(\beta). \quad (19)$$

At $\beta = h - 1$ there are only S tiles $(h - 1)1 + 0$ and the density of 1 is $(h - 1)/h$. As β increases, extra 1 must be accommodated and this will be realised ‘as evenly as possible’, meaning that the L tiles $h1 + 0$ will be isolated among the short ones, until β reaches the value $h + \frac{1}{2}$. At this point the density of 1 is $(h - \frac{1}{2})/h = h/2h + (h - 1)/2h$, i.e. the proportions of S and L tiles are equal. From now on the L tiles prevail, while the S tiles will appear isolated among ever larger clusters of long tiles. At $\beta = h + 1$ the tiles $h1 + 0$ become short and new long tiles $(h + 1)1 + 0$ make their way into the sequence.

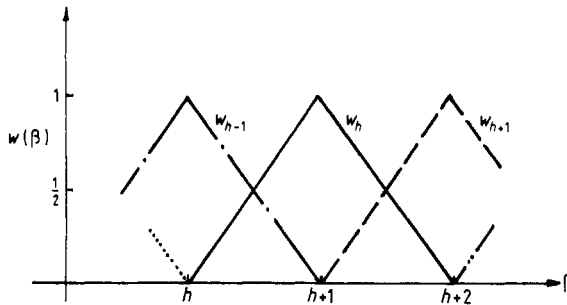


Figure 2. The distribution of long and short tiles of an EBCP1.

The important fact to be realised from this description is that one of the two kinds of tile present in the sequence always occurs isolated. In just the way $\beta = 2$ was a turning point between 0-dominant and 1-dominant sequences, the point $\beta = h + \frac{1}{2}$ marks the transition from short-tile-dominant to long-tile-dominant sequences for the EBCP under consideration. Moreover, an analysis analogous to that carried out for property (d), albeit somewhat more involved, shows that strings of tiles of the dominant type always come in two sizes: r and $r - 1$, $r = 2, 3, \dots$. The rule is as follows.

In the half unit interval $h < \beta < h + \frac{1}{2}$: for $h + 1/(r + 1) < \beta < h + 1/r$ there are isolated L tiles, and strings of $r - 1$ and r consecutive S tiles, $r = 2, 3, \dots$.

In the half unit interval $h + \frac{1}{2} < \beta < h + 1$: for $h + (r - 1)/r < \beta < h + r/(r + 1)$ there are isolated S tiles and strings of $r - 1$ and r consecutive L tiles, $r = 2, 3, \dots$.

When β equals the upper end of one of the intervals defined above—a rational number—the sequence becomes periodic, with a period of r consecutive tiles of the dominant type plus one non-dominant.

Example E2. $\alpha = 1.435\ 258\ 49 \dots < 2$, $\beta = 3.297\ 485\ 34 \dots > 2$, $\omega = 0$, $[\beta] = 3$. The sequence $p(\alpha, \omega, j)$ is

1101101101110110110111011011011011101101101110110110110110110110
 11011011101101101110...

For the EBCP1 under consideration $S = 110$, $L = 1110$, $h = 3$ and the following sequence

of S and L tiles results:

$$\text{SSSLSSLSSSLSSLSSSLSSLSSSLSSLSSSLSSSL} \dots \tag{20}$$

Thus $3 + \frac{1}{4} < \beta < 3 + \frac{1}{3}$, $r = 3$, and there are strings of three and two consecutive S tiles and isolated L tiles.

Next, consider EBCP2: $\{S = 1, L = (h - 1)1 + 0\}$. Denote by $w_S(\beta)$ the frequency of S tiles and by $w_L(\beta)$ that of L tiles, in the interval $h < \beta < h + 1$. We already know that the frequency of tiles $h1 + 0$ varies from zero to one in this interval. Translated to EBCP2 under consideration, this means that

$$w_S(h) = 0 \quad w_L(h) = 1 \quad w_S(h + 1) = w_L(h + 1) = \frac{1}{2} \tag{21}$$

The frequencies are schematically represented in figure 3. In this case the short tiles $S = 1$ always occur isolated throughout the unit interval, while the L tiles form strings of $r - 1$ and r consecutive tiles which coexist in the interval

$$h + 1/r < \beta < h + 1/(r - 1) \quad r = 2, 3, \dots$$

Applying EBCP2 to the sequence in example E2 we obtain the following sequence of $S = 1$ and $L = 110$ tiles:

$$\text{LLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLL} \dots \tag{22}$$

Here $r = 4$, $3 + \frac{1}{4} < \beta < 3 + \frac{1}{3}$, and have strings of four and three consecutive L tiles.

Now one can substitute in (20) and (22) $L = 1, S = 0$ or $L = 0, S = 1$ and obtain four different, albeit pairwise complementary p sequences. We have just described in detail the process of inflation mentioned in the introduction; its consequences are very interesting. The succession of L and S tiles defined by the corresponding EBCP is completely isomorphic to any of two complementary p sequences of 0 and 1. The latter may in turn be partitioned according to any of two appropriate EBCP (1 or 2) whose tiles can be put into one-to-one correspondence with 'supertiles' covering the original sequence. These supertiles evidently constitute a BCP of the original sequence. One type of supertile will be dominant occurring in strings of s and $s - 1$ consecutive supertiles, the other will be isolated. As an illustration consider the L, S sequence (22). Choose $L = 0, S = 1$. The resulting p sequence is

$$000100010000100010001000010001000100001 \dots$$

This sequence is 0-dominant and we can choose either EBCP1c or EBCP2c with $h = 4$. If we choose EBCP1c then the L, S sequence at this level is SSSLSSLSSL... To each S and L of this sequence there correspond the following 'supertiles' of the original sequence, respectively: $S \rightarrow 1101101101, L \rightarrow 1101101101101$. If, on the other hand we

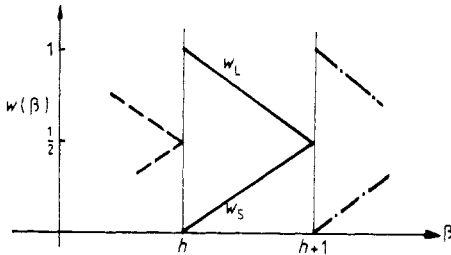


Figure 3. The distribution of long and short tiles of an EBCP2.

choose EBCP2c, then the L, S sequence at the same level is LLSLLLSLLLSL To each S and L of this sequence there correspond the following 'supertiles' of the original p sequence, respectively: $S \rightarrow 110$, $L \rightarrow 1101101101$. Both are BCP of the original p sequence.

Continuing the inflation process one can identify an infinite number of BCP of the original sequence with ever larger supertiles, the succession of which at each level is isomorphic to some p sequence of 0 and 1. In fact, a EBCP of a successively inflated sequence at any stage necessarily corresponds to a BCP of the original. At each level there is a fourfold choice involving the identification of L and S with 0 and 1, and subsequently choosing EBCP1 or 2. The two possible initial EBCP of a given p sequence will therefore generate together a tree of p sequences with four branches at each node. This is the content of property (f). If the original p sequence is periodic, successive inflation steps will eventually end up in a periodic p sequence with period 1.

Note that although strongly interrelated, the EBCP1 and EBCP2 have been treated separately for they generate distinct trees.

(g) Identical 'neighbourhoods' at finite distances. Given a p sequence $p(\alpha, \omega, j)$, choose a site j' and a finite segment of length D (a neighbourhood) starting at j' . There exists a site j'' at a finite distance from j' such that

$$p(\alpha, j' + d - 1) = p(\alpha, j'' + d - 1) \quad d = 1, 2, \dots, D$$

where we have omitted ω , for it plays no role. Moreover, $|j'' - j'| = O(D)$, i.e. the distance $|j'' - j'|$ varies linearly with D .

The proposition is proven by performing a finite number s of successive inflation transformations as follows: let q denote the inflation stage. The initial sequence is $q = 0$, i.e. $\alpha_0 = \alpha$, $D_0 = D$, $p_0 = p(\alpha_0, j)$. Select a EBCP of p_0 and mark the smallest finite sequence of whole tiles which completely includes D_0 . These tiles form the 'extended segment' $E_0 \supseteq D_0$. Inflate p_0 by means of one of the two complementary reverse (inflation) SRR based upon this EBCP. A new sequence $p_1(\alpha_1, j)$ is obtained at stage $q = 1$. Mark the segment D_1 of p_1 which maps E_0 . Select a EBCP of p_1 and extend the segment D_1 to $E_1 \supseteq D_1$, if necessary. Repeat the process until, after a finite number of stages $q = s$, D_s has reduced to one binary digit. This bit is the mapping in p_s of a larger segment $F_0 \supseteq D_0$ of the original sequence p_0 . Move on p_s to the nearest bit of the same kind, an operation requiring a finite number of steps on p_s . This second bit will be the mapping in p_s of another segment F'_0 of p_0 such that $F_0 \cap F'_0 = \emptyset$, which is certain to contain an exact replica of D_0 . Furthermore, all the binary digits of the same kind map in p_s disjoint segments F'_0 of p_0 which contain replicas of D_0 . Let E_q also denote the bit length of the extended segment E_q at stage q . Then clearly, $E_q/E_{q+1} < \gamma_q$, where $\gamma_q = \max(\alpha_q + 1, \beta_q + 1)$. It follows that the product $\prod_{q=0}^s \gamma_q$ is an upper bound for $|j'' - j'|/D_0$. An analogous property of Penrose tilings has been referred to by the name of 'local isomorphism' (Gardner 1977).

3. Simple replacement rules (SRR) and self-similarity

Definition. A deflation simple replacement rule (DSRR) is a rule under which the 0 and 1 are replaced by the tiles of a EBCP. There are two possibilities for each EBCP, a total of eight rules, four of which are, according to (16) and (17), complementary to the other four. An inflation simple replacement rule (ISRR) is the reverse of the corresponding DSRR.

According to property (e) established in the preceding section, both deflation and inflation SRR transform a p sequence into a p sequence, the latter action being possible only if the corresponding EBCP exists. In this section we shall derive the parameters α', β', ω' of the transformed sequence as functions of α, β, ω of the original one. It is easier to do this using DSRR, the results for a ISRR being obtained by inverting the corresponding formula.

A classification of the DSRR is in order. They will be labelled 1, 2, 1c, 2c corresponding to the EBCP involved. The additional label L(S) indicates that the dominant element of the original sequence is replaced by the L tile (S tile) of the EBCP. The complete list of DSRR as functions of $h \geq 2$ is

$$\text{DSRR1L: } \{1 \rightarrow h1 + 0; 0 \rightarrow (h - 1)1 + 0\} \tag{23}$$

$$\text{DSRR1S: } \{1 \rightarrow (h - 1)1 + 0; 0 \rightarrow h1 + 0\} \tag{24}$$

$$\text{DSRR2L: } \{1 \rightarrow (h - 1)1 + 0; 0 \rightarrow 1\} \tag{25}$$

$$\text{DSRR2S: } \{1 \rightarrow 1; 0 \rightarrow (h - 1)1 + 0\} \tag{26}$$

$$\text{DSRR1cL: } \{0 \rightarrow h0 + 1; 1 \rightarrow (h - 1)0 + 1\} \tag{27}$$

$$\text{DSRR1cS: } \{0 \rightarrow (h - 1)0 + 1; 1 \rightarrow h0 + 1\} \tag{28}$$

$$\text{DSRR2cL: } \{0 \rightarrow (h - 1)0 + 1; 1 \rightarrow 0\} \tag{29}$$

$$\text{DSRR2cS: } \{0 \rightarrow 0; 1 \rightarrow (h - 1)0 + 1\}. \tag{30}$$

Derivation of α', β', ω' for DSRR1L. No particular assumption need be made about the dominance type of the original p sequence. Perform DSRR1L, (23). The first j elements of the original sequence transform into j' elements, among which there are

$$1: k' = kh + (j - k)(h - 1) = jh - j + k \tag{31a}$$

$$0: l' = j \tag{31b}$$

$$\text{total: } j' = k' + l' = jh + k = jh + j - l. \tag{31c}$$

According to (23) it is clear that element j' is a zero. If the transformed sequence should be a p sequence then j', l' must, for some β', ω' , satisfy the relation

$$j' = [l'\beta' + \omega'\beta'] \quad l' = 1, 2, \dots \tag{32}$$

First assume that $j \in C_1$; then $k = [(j + 1)/\alpha + \omega]$, by (5). Substitute (31b) and (31c) into (32) and then (5) for k . The following equation is obtained:

$$[j/\alpha + 1/\alpha + \omega] = [j(\beta' - h) + \omega'\beta'] \quad j \in C_1. \tag{33}$$

Next assume that $j \in C_0$; then $l = [(j + 1)/\beta - \omega]$, by (6). Substitute again (31b) and (31c) into (32) and then (6) for l . The result is $j - [j/\beta + 1/\beta - \omega] = [j(\beta' - h) + \omega'\beta']$. Using the identity $j - [a] = [j - a + 1]$, and the relation (2) we obtain equation (33) for $j \in C_0$. Hence, equation (33) must be satisfied for $j \in C_0 \cup C_1 = N$. By lemma L, we must have therefore

$$\beta' = h + 1/\alpha = h + 1 - 1/\beta \tag{34}$$

$$\omega' = (1 + \alpha\omega)/\alpha\beta' = (1 + \alpha\omega)/(h\alpha + 1). \tag{35}$$

Hence

$$\alpha' = 1 + \alpha/(h\alpha - \alpha + 1). \tag{36}$$

Clearly $\beta' > 2$, i.e. the transformed sequence is 1-dominant irrespective of the type of original sequence.

For complete self-similarity under DSRR1L we must have $\beta' = \beta$ and $\omega' = \omega$. The first condition leads to a quadratic equation: $\beta^2 - (h + 1)\beta + 1 = 0$, whose positive root $\tilde{\beta}$ is the desired result:

$$\tilde{\beta} = (\Delta + h + 1)/2 \quad \Delta = [(h + 1)^2 - 4]^{1/2} \tag{37}$$

$$\tilde{\alpha} = (\Delta + h - 1)/2(h - 1). \tag{38}$$

The equation for ω is $\omega = (1 + \tilde{\alpha}\omega)/\tilde{\alpha}\tilde{\beta}$. Hence

$$\tilde{\omega} = 1/\tilde{\beta} = (-\Delta + h + 1)/2. \tag{39}$$

Notice that $[\tilde{\beta}] = h$.

Using this model calculation the reader should have no difficulty in carrying out detailed derivations for other types of DSRR. The results for the first four DSRR (23)–(26) are summarised in table 1. The formulae for the corresponding complementary DSRR (27)–(30) can be obtained by simultaneous interchanges $\alpha \leftrightarrow \beta$, $\alpha' \leftrightarrow \beta'$, $\omega \leftrightarrow -\omega$, $\omega' \leftrightarrow -\omega'$, $\tilde{\alpha} \leftrightarrow \tilde{\beta}$ and $\tilde{\omega} \leftrightarrow -\tilde{\omega}$ in the listed expressions. A total of eight different sequences are obtained by DSRR, four of which are complementary to the other four.

Self-similarity is impossible under DSRR2S, for $\beta' = \beta$ exists only in the trivial case $h = 1$, which is the identity replacement rule.

Let us point out that expressions like (34) and (36) can be obtained easily, although perhaps less rigorously, from the asymptotic relations $j/k \sim \alpha$, $j/l \sim \beta$. For example, if indeed the transformed sequence is a p sequence, then for large k' one must have $\alpha' = j'/k' = (jh + k)/(jh - j + k) = (h\alpha + 1)/(h\alpha - \alpha + 1)$, which, of course, is the same

Table 1. Parameters of deflated p sequences and of the corresponding self-similar sequences.

	DSRR1L(h)	DSRR1S(h)	DSRR2L(h)	DSRR2S(h)
Replacement	$1 \rightarrow h1 + 0$ $0 \rightarrow (h - 1)1 + 0$	$1 \rightarrow (h - 1)1 + 0$ $0 \rightarrow h1 + 0$	$1 \rightarrow (h - 1)1 + 0$ $0 \rightarrow 1$	$1 \rightarrow 1$ $0 \rightarrow (h - 1)1 + 0$
α'	$1 + 1/(h - 1 + 1/\alpha)$ $1 + 1/(h - 1/\beta)$	$1 + 1/(h - 1/\alpha)$ $1 + 1/(h - 1 + 1/\beta)$	$\frac{h + \alpha - 1}{h + \alpha - 2}$	$\frac{h + \beta - 1}{h + \beta - 2}$
β'	$h + 1 - 1/\beta$ $h + 1/\alpha$	$h + 1/\beta$ $h + 1 - 1/\alpha$	$h + 1/(\beta - 1)$ $h + \alpha - 1$	$h + \beta - 1$ $h + 1/(\alpha - 1)$
ω'	$(1 + \alpha\omega)/\alpha\beta'$ $(1 + \alpha\omega)/(h\alpha + 1)$	$(1 - \beta\omega)/\beta\beta'$ $(1 - \beta\omega)/(h\beta + 1)$	$-\omega\alpha/\beta'$ $-\omega\alpha/(h + \alpha - 1)$	$\omega\beta/\beta'$ $\omega\beta/(h + \beta - 1)$
Quadratic equation	$\beta^2 - (h + 1)\beta + 1 = 0$	$\beta^2 - h\beta - 1 = 0$	$\beta^2 - (h + 1)\beta + (h - 1) = 0$	
Δ^2	$(h + 1)^2 - 4$	$h^2 + 4$	$(h - 1)^2 + 4$	
$\tilde{\alpha}$	$\frac{\Delta + h - 1}{2(h - 1)}$	$\frac{\Delta + h + 2}{2h}$	$(\Delta - h + 3)/2$	
$\tilde{\beta}$	$(\Delta + h + 1)/2$	$(\Delta + h)/2$	$(\Delta + h + 1)/2$	
$\tilde{\omega}$	$1/\tilde{\beta}$	$1/\tilde{\beta}(\tilde{\beta} + 1)$	0	
$[\beta]$	h	h	h	

Δ is the positive root of Δ^2 .
For the complementary DSRR, see text.

as (36). Also notice that the global parameters of the transformed sequence α', β' are independent of the original shift parameter ω .

We shall now turn our attention to ISRR. The corresponding replacement rules are obtained from the expressions (23)–(30) simply by inverting the arrows. The value of h , however, may not be arbitrary: if the original sequence is 1-dominant, then it must be $h = [\beta]$, while for a 0-dominant original sequence it must be $h = [\alpha]$. The results are summarised in table 2 giving the parameters α', β', ω' of the transformed (inflated) sequence as functions of the parameters α, β, ω of the original 1-dominant sequence. If the original sequence is 0-dominant, the corresponding transformed parameters can be obtained from table 2 by interchanging $\alpha \leftrightarrow \beta, \alpha' \leftrightarrow \beta', \omega \leftrightarrow -\omega, \omega' \leftrightarrow -\omega'$. Notice that the inflated sequence produced by ISRR1L and ISRR1S are complementary to each other. So are those produced by ISRR2L and ISRR2S. Because of these relationships of complementarity among transformed sequences it follows that by applying the appropriate eight ISRR to a given p sequence *and* its complement, only four distinct inflated sequences can possibly result.

Table 2. Parameters of inflated p sequences.

	ISRR1L	ISRR1S	ISRR2L	ISRR2S
Replacement	$[\beta]1+0 \rightarrow 1$ $[\beta-1]1+0 \rightarrow 0$	$[\beta]1+0 \rightarrow 0$ $[\beta-1]1+0 \rightarrow 1$	$[\beta-1]1+0 \rightarrow 1$ $1 \rightarrow 0$	$[\beta-1]1+0 \rightarrow 0$ $1 \rightarrow 1$
α'	$1/\{\beta\}$	$1/(1-\{\beta\})$	$1+\{\beta\}$	$1+1/\{\beta\}$
β'	$1/(1-\{\beta\})$	$1/\{\beta\}$	$1+1/\{\beta\}$	$1+\{\beta\}$
ω'	$\omega\beta - \{\beta\}$	$-\omega\beta + \{\beta\}$	$-\omega\beta/(1+\{\beta\})$	$\omega\beta/(1+\{\beta\})$

For the inflation of 0-dominant original sequences, see text.

4. Composite replacement rules (CRR) and self-similarity

In this section we consider only deflation rules, omitting the label D. The direct product of two SRR is defined as the result of applying the two SRR in succession. The SRR may be of any type, and have different values of $h \geq 2$. Example: SRR1S(3) \otimes SRR2L(2): $\{1 \rightarrow 10101, 0 \rightarrow 1010101\}$. The direct product of SRR is not commutative.

Definition. An r -step composite replacement rule is obtained by directly multiplying r SRR in ordered succession.

Due to the general properties of SRR, the application of an r -step CRR to a p sequence will result in a p sequence whose dominance type is determined by the last SRR in the product. The long and short replacement tiles of the CRR obviously constitute a BCP of the resulting deflated p sequence. Let the parameters of the original p sequence be $\alpha_0, \beta_0, \omega_0$. The parameters $\alpha_r, \beta_r, \omega_r$ can be calculated by successive substitution and may be cast in general form:

$$\alpha_r = \frac{a_1\alpha_0 + a_2}{a_3\alpha_0 + a_4} = \frac{(a_1 + a_2)\beta_0 - a_2}{(a_3 + a_4)\beta_0 - a_4} \tag{40}$$

$$\beta_r = \frac{b_1\beta_0 + b_2}{b_3\beta_0 + b_4} = \frac{(b_1 + b_2)\alpha_0 - b_2}{(b_3 + b_4)\alpha_0 - b_4} \tag{41}$$

where $a_1, a_2, \dots, b_1, b_2, \dots$ are integers depending on the set $h_i \geq 2, i = 1, 2, \dots, r$. Since the parameters α_r, β_r satisfy a relation of type (2), one has $b_1 = a_1 + a_2, b_2 = -a_2, b_3 = a_1 + a_2 - a_3 - a_4, b_4 = a_4 - a_2$. Furthermore

$$\omega_r = f_1(\alpha_0) + \omega_0 f_2(\alpha_0) \tag{42}$$

where both f_1 and f_2 are ratios of linear binomials in α_0 with the same denominator. Formulae (40) and (41) are not valid if the SRR in the product are all of type 2S, equation (26), or type 2cS, equation (30), in which cases the relations are linear.

This discussion leads to the following proposition. If a p sequence is known to be self-similar under some CRR, then its parameter $\tilde{\alpha} > 1$ must be a root of the quadratic equation derived from (40) by setting $\alpha_r = \alpha_0$: $a_3\alpha^2 - (a_1 - a_4)\alpha - a_2 = 0$. Then, by setting $\omega_r = \omega_0$ in (42), we obtain $\tilde{\omega} = f_1(\tilde{\alpha}) / (1 - f_2(\tilde{\alpha}))$. Conversely, if $\alpha = (P + Q^{1/2}) / 2R > 1, (P, Q > 0, R, \text{ integers})$ then there exists at least one CRR under which $p(\alpha, j)$ will be generically self-similar. We have $a_1 - a_4 = P, a_3 = R, a_2 = (Q - P^2) / 4R$ and the choice of the set of positive integers $\{r, h_1, \dots, h_r | h_i \geq 2\}$ may not be unique.

If the CRR is defined by an ordered succession $i = 1, 2, \dots, r$ of SRR of the same type (but not 2S or 2cS), with possibly different values h_i , then for 1-dominant SRR, β_r can be expressed as a function of β_0 in the form of a terminated continued fraction with all partial numerators equal to 1. Since β_{i+1} depends only on its predecessor β_i , the expressions in table 1 are used in a chain substitution process which eliminates all the intermediate β . For example, $\beta_1 = h_1 + 1/\beta_0$. Then $\beta_2 = h_2 + 1/\beta_1 = h_2 + 1/(h_1 + 1/\beta_0)$, etc. The same relations are found between α_r and α_0 for 0-dominant SRR. The common form is

$$\mu_r = c_r + \frac{1}{c_{r-1} + \frac{1}{c_{r-2} + \dots \frac{1}{c_1 + \frac{1}{\mu_0}}} \tag{43}$$

and its inverse

$$\mu_0 = -\frac{1}{c_1 + \frac{1}{c_2 + \dots \frac{1}{c_{r-1} + (c_r - \mu_r)}} \tag{44}$$

where μ_r, μ_0 and c_i are listed in table 3.

The condition for generic self-similarity under the corresponding CRR is obtained by equating $\mu_0 = \mu_r$ in (43). The following quadratic equation results:

$$\mu = c_r + \frac{1}{c_{r-1} + \dots \frac{1}{c_1 + \mu}} \tag{45}$$

Table 3.

	c_i	μ_d
SRR1L	$(-1)^{i-1}(h_i + 1)$	β_d
SRR1S	h_i	β_d
SRR2L	$h_i - 1$	$\beta_d - 1$
SRR1cL	$(-1)^{i-1}(h_i + 1)$	α_d
SRR1cS	h_i	α_d
SRR2cL	$h_i - 1$	$\alpha_d - 1$

In the last column the subscript d stands for 0 and r .

If we substitute μ from (45) into the tail of the terminated continued fraction (45) and repeat this operation an infinite number of times, we obtain the representation of the root of equation (45) by an infinite purely periodic continued fraction with the period $(c_r, c_{r-1}, \dots, c_1)$.

For the SRR types 1S and 2L (and their complements) where all integers $c_i \geq 1$, $i = 1, 2, \dots, r$, a very important consequence emerges from (45). Evidently, $[\mu] = c_r$ and $\mu > 1$. Substitute $\mu_0 = \mu_r = -1/\nu$ in (44). Then the quantity ν satisfies the equation

$$\nu = c_1 + \frac{1}{c_2 + \dots \frac{1}{c_r + \frac{1}{\nu}}} \tag{46}$$

i.e. it is represented by the purely periodic continued fraction with the period reversed: (c_1, c_2, \dots, c_r) . Evidently $[\nu] = c_1$, and $\nu > 1$. Equation (46) is related to (45) in the following obvious manner. If ν is a solution of (46) then $-1/\nu$ is a solution of (45). We conclude that $\nu = -1/\mu'$, where μ' is one of the solutions of (45). Now, μ' cannot be μ , the solution represented by the infinite continued fraction with period $(c_r, c_{r-1}, \dots, c_1)$, because both μ and $\nu > 0$. It follows that $\mu' = -1/\nu$ is the second solution of (45) called the algebraic conjugate of the quadratic irrational μ . Since $\nu > 1$, we have $-1 < \mu' < 0$. This shows that for SRR types 1S and 2L, μ is a quadratic irrational > 1 , whose algebraic conjugate satisfies $-1 < \mu' < 0$.

There is an important variant of Lagrange's famous theorem (Khinchin 1964) which states: a purely periodic continued fraction with positive integer partial denominators and partial numerators equal to 1 represents a quadratic irrational $\mu > 1$ whose algebraic conjugate satisfies $-1 < \mu' < 0$.

Conversely, every quadratic irrational $\mu > 1$ whose algebraic conjugate μ' satisfies $-1 < \mu' < 0$, is represented by a purely periodic continued fraction as above (see, e.g., Henrici 1977).

The last part of the theorem tells us that, given a quadratic irrational $\mu > 1$ whose algebraic conjugate satisfies $-1 < \mu' < 0$, we can obtain its period by the standard expansion algorithm, thus actually determining the ordered set $h_i, i = 1, 2, \dots, r$, which goes into the construction of the CRR.

5. Application: the one-dimensional diatomic quasicrystal

Let us begin with a brief review of the main results derived in the earlier paper (Aviram 1986) for the one-dimensional monatomic quasicrystal. Two characteristic line segments of length a and b , with $\sigma = a/b > 1$, were used to construct a sequence of line segments isomorphic to a given sequence $p(\alpha, \omega, j)$ by matching element 1 with segment a , and element 0 with segment b . (In the quoted paper we had dimensionless segments σ and 1; here, however, it will be more convenient to specify the lengths a and b .) The total length of the first j segments is $x_j = jb + k(\sigma - 1)b, j = 1, 2, \dots$. The model system of pointlike identical atoms located at x_j was mathematically described by a sum of delta functions:

$$G(x) = \sum_j \delta(x - x_j). \tag{47}$$

The weighted average separation between atoms was

$$\Delta = (a/\alpha + b/\beta) = b(\sigma - 1 + \alpha)/\alpha. \tag{48}$$

Provided that α, β are irrational, the Fourier transform $F(s) = \mathcal{F}G(x)$ is an infinitely dense denumerable set of Bragg peaks of zero width located on the s line at the points:

$$s = s_{mn} = (m + n/\alpha)/\Delta \quad m, n = 0, \pm 1, \pm 2, \dots \quad (49)$$

Then $F(s) = F(s_{mn}) = A_{mn} \exp(i\theta_{mn})$, where the amplitude and phase are given by

$$A_{mn} = \frac{\sin \pi \Omega_{mn}}{\pi \Omega_{mn}} \quad (50)$$

$$\theta_{mn} = -\pi \Omega_{mn} (2\omega + 2/\alpha - 1) \quad (51)$$

where

$$\Omega_{mn} = b(m(\sigma - 1) - n)/\Delta \quad m, n = 0, \pm 1, \pm 2, \dots \quad (52)$$

The spectrum s_{mn} , the amplitude A_{mn} and the phase θ_{mn} are all parametrised by two sets of integers m, n , and $F(s) = 0$ for $s \neq s_{mn}$.

The spectral lines are zero width Bragg peaks densely filling the reciprocal one-dimensional s -space; their positions s_{mn} are expressed as linear combinations of two integers m, n taken in an irrational ratio α , unique for all spectral lines of a given quasicrystal. Except for the fact that they enter the scaling factor Δ common to all s_{mn} , the characteristic lengths a and b do not affect the locations of the spectral lines which are governed by the sequence parameter α . The set of spectral lines is denumerable, and in an arbitrarily small neighbourhood of any given line there are infinitely many other spectral lines. The distribution of amplitudes A_{mn} , on the other hand, is governed through Ω_{mn} by the ratio σ of the characteristic lengths and not by α . Both s_{mn} and A_{mn} are independent of the shift parameter ω which affects only the phase θ_{mn} . A one-dimensional diatomic quasicrystal will now be constructed by taking advantage of an inflation transformation. Consider a sequence of segments of lengths a and b , isomorphic to a given p sequence (figure 4 (top), based on example E2). The coordinates of the endpoints are x_j . Inflate the sequence by any appropriate replacement rule, simple or composite. Figure 4 (middle) shows the result of this operation for ISRR1L, whereby a sequence of segments a' and b' , $\sigma' = a'/b' > 1$, is obtained. The endpoint coordinates x'_j form a subset of (x_j) . Let the sites x'_j be occupied by atoms of one species (open circles), while the remaining sites of the original sequence are occupied by another species (crosses), figure 4 (bottom). This model system may be described by the expression

$$G(x) + G'(x) = Q \sum_j \delta(x - x_j) + (Q' - Q) \sum_{j'} \delta(x - x'_{j'}) \quad (53)$$

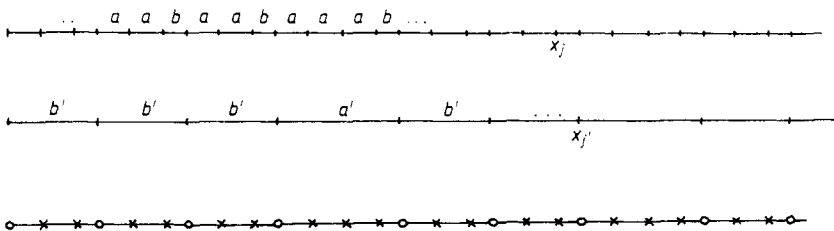


Figure 4. The construction of a diatomic one-dimensional quasicrystal.

where Q, Q' are the scattering amplitudes of the two species. The Fourier transform being a linear operation, we have for this model system

$$F(s) = \mathcal{F}G(x) + \mathcal{F}G'(x). \tag{54}$$

All we have to do in this instance therefore is to add with appropriate weights the Fourier transforms of two monatomic one-dimensional quasicrystals. Both quasicrystals are generated by p sequences related to each other by an inflation transformation. An interesting property of such a diatomic quasicrystal has been announced in the introduction: the positions of the spectral lines in the one-dimensional reciprocal s -space are exactly the same as if all sites were occupied by a single species, and there are no more, and no less, lines than in the case of single species occupancy. The intensities, however, are different.

Let us illustrate this by a simple model calculation based on ISRR1L. The inflated segments are

$$a' = [\beta]a + b \qquad b' = [\beta - 1]a + b. \tag{55}$$

Using the inflated parameters α', β', ω' from the appropriate column of table 2, we calculate the weighted average separation between atoms of species Q' (open circles in figure 4):

$$\Delta' = (a'/\alpha' + b'/\beta') = \rho\Delta \tag{56}$$

where $\rho \equiv \rho(\beta) = \beta$. By taking $\mathcal{F}G'(x)$, we obtain the location of the spectral lines of this species alone:

$$s_{m'n'} = (m' + n'/\alpha')/\Delta' \\ = ((m' - [\beta - 1]n') + (-m' + [\beta]n')/\alpha)/\Delta \qquad m', n' = 0, \pm 1, \pm 2, \dots \tag{57}$$

Set

$$m = m' - [\beta - 1]n' \qquad n = -m' + [\beta]n'. \tag{58}$$

Then $s_{m'n'}$ in (57) coincides with (49), and since the linear transformation (58) is never singular, there is a one-to-one correspondence between (m, n) and (m', n') : the spectrum $s_{m'n'}$ is identical to s_{mn} . The inverse of (58) is

$$m' = [\beta]m + [\beta - 1]n \qquad n' = m + n. \tag{59}$$

Write $\mathcal{F}G'(x) = A_{m'n'} \exp(i\theta_{m'n'})$. Then, applying to this species the general formulae (50)–(52) and using (59), we obtain

$$\Omega_{m'n'} = b'(m'(\sigma' - 1) - n')/\Delta' \\ = b(m(\sigma - 1) - n)/(\Delta\beta) = \Omega_{mn}/\psi \tag{60}$$

where $\psi \equiv \psi(\beta) = \beta$. Similarly, we have

$$\theta_{m'n'} = \theta_{mn} + \pi\Omega_{mn}/\varphi \tag{61}$$

where $\varphi \equiv \varphi(\beta) = \beta/(\beta - 1)$, and

$$A_{m'n'} = \frac{\sin \pi\Omega_{mn}/\psi}{\pi\Omega_{mn}/\psi}. \tag{62}$$

The Fourier transform of the whole diatomic quasicrystal is then

$$F(s_{mn}) = \exp(i\theta_{mn}) \left(Q \frac{\sin \pi \Omega_{mn}}{\pi \Omega_{mn}} + (Q' - Q) \frac{\sin \pi \Omega_{mn} / \psi}{\pi \Omega_{mn} / \psi} \exp(i\pi \Omega_{mn} / \varphi) \right)$$

$$m, n = 0, \pm 1, \pm 2, \dots \quad (63)$$

Notice from (61) that the phase difference $\theta_{m'n'} - \theta_{mn}$ is independent of ω . It follows that, just as in the monatomic case, the experimentally measurable quantity $|F(s_{mn})|^2$ is completely independent of the shift parameter of the basic sequence $p(\alpha, \omega, j)$. The general form of equations (56), (60)–(63) is the same for all ISRR listed in table 2 and their complements, the only difference residing in the values of the scaling functions ρ, ψ, φ . In addition, it is easy to see that, as long as we choose the matching of inflated segments in such a way that $a'/b' > 1$, ISRR1L and 1S give identical diatomic quasicrystals and so do ISRR2L and 2S. The same is true for the corresponding pairs of complements. The results are summarised in table 4, under the assumption that the following matching is conserved for all original sequences: $1 \rightarrow a, 0 \rightarrow b, a/b > 1$.

Table 4. Scaling functions for ISRR.

	ISRR1L, 1S	ISRR2L, 2S	ISRR1Lc, 1Sc	ISRR2Lc, 2Sc
Replacement	$a' = [\beta]a + b$ $b' = [\beta - 1]a + b$	$a' = [\beta - 1]a + b$ $b' = a$	$a' = [\alpha]b + a$ $b' = [\alpha - 1]b + a$	$a' = [\alpha - 1]b + a$ $b' = b$
m'	$[\beta]m + [\beta - 1]n$	$m + n$	$[\alpha]m + n$	m
n'	$m + n$	$[\beta - 1]m + [\beta - 2]n$	m	$[\alpha - 1]m + n$
ρ	β	$\beta / (1 + \{\beta\})$	α	$\alpha / (1 + \{\alpha\})$
ψ	β	$-\beta / (1 + \{\beta\})$	$-\alpha$	$\alpha / (1 + \{\alpha\})$
φ	$\beta / (\beta - 1)$	$\beta / [\beta - 1]$	$-\alpha / (\alpha - 1)$	$-\alpha / [\alpha - 1]$

As for inflation under a composite replacement rule, it can be shown that the double indices (m', n') of the spectrum of species Q' are always related to (m, n) by non-singular linear transformations. This situation leads to the conclusion that the spectral lines are located as if the quasicrystal were monatomic, no matter what inflation transformation was used in order to locate the atoms of species Q' . In order to appreciate the significance of this result, let us recall what happens in the periodic case. The spectrum of an infinite one-dimensional array of pointlike identical atoms *equally* separated by a distance a is a periodic array of Bragg peaks of zero width, equal amplitude and equally separated in the reciprocal space by a distance $1/a$. Now, if we replace, say, every third atom with an atom of another species (scattering amplitude), we obtain a periodic diatomic one-dimensional crystal whose spectral lines are equally separated in the reciprocal space by a distance $1/3a$, with every third line having a different amplitude from the other two. In other words, the periodic diatomic crystal exhibits *more* spectral lines per unit length of reciprocal space than in the case of single species occupancy, a situation very much unlike that obtained for the diatomic quasicrystal. It should be realised, however, that this interesting property of quasicrystals is characteristic of the particular subset of sites chosen for species Q' , namely the

sites surviving an inflation operation. Other choices will almost certainly destroy this property.

The general idea of this section may be carried one stage further, whereby the sequence of inflated segments a' and b' is inflated once more. The resulting segments a'' , b'' produce a new sequence of sites $x_{j''}$ which form a subset of (x_j) . A triatomic quasicrystal may thus be constructed with the addition of a third species Q'' ; the spectral lines as before will be located as if the whole quasicrystal were monatomic, etc.

6. Concluding remarks

The major part of this paper was dedicated to the investigation of the properties of quasiperiodic p sequences undergoing deflation and inflation operations under simple replacement rules. A set of formulae relating the parameters of the transformed sequence to the original one were derived; it was shown that a p sequence always transforms into a p sequence under repeated application of SRR. The condition for self-similarity under a particular replacement rule, simple or composite, is that the parameter α be a quadratic irrational greater than one. This property is strongly related to the theory of purely periodic continued fractions.

The results were then used in order to construct a diatomic one-dimensional quasicrystal whose diffraction spectrum was calculated. The spectral lines lie at the same locations as if the whole quasicrystal were monatomic, which is a direct consequence of the particular way in which two atomic species share the sites of the quasicrystal between themselves. Moreover, polyatomic one-dimensional quasicrystals may be constructed by successive inflation transformations, the spectral lines being invariably located at the same places in the Fourier space. Only the intensities and phases are affected in the process.

Finally, a comment on the inverse problem is in order. The crystallographer—or perhaps, the quasicrystallographer for that matter—is usually interested in extracting from the diffraction spectrum some information about the relative positions of atoms in the crystal. Although this work may have shed some light on the way in which a mathematical model of a rather particular diatomic one-dimensional quasicrystal would respond to the probing of a diffracting beam, the practical problem is far from being resolved. As the monatomic one-dimensional quasicrystal isomorphic to a p sequence depends on only two parameters, one may hope to deduce something of its structure from an analysis of positions and relative intensities of the strongest peaks. The analysis of a diatomic quasicrystal, however, is further complicated by additional parameters such as scattering amplitudes, the inflation rule, etc.

Numerous experimental and theoretical investigations of three-dimensional quasicrystals—in particular, the icosahedral phase of rapidly cooled alloys (Schectman *et al* 1984)—are currently under way. It is not as yet clear how the present work could be extended to higher dimensions.

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