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The diffraction spectum of a general family of linear quasiperiodic arrays

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Abstract. We study the diffraction spectrum and the structure factor of quasicrystalline, aperiodic, linear arrays with two arbitrary characteristic measure lengths, produced by a fairly general family of generating rules depending on two parameters. The calculation is performed by actually constructing the two-dimensional periodic structure whose projection will result in the desired linear aperiodic array. Distributions of some sequences of irrational numbers modulo 1 are derived as a byproduct of the main subject.

1. Introduction

A commonly accepted procedure for constructing quasicrystalline structures (such as sums of delta functions located at points which are distributed neither periodically nor randomly) is by projecting periodic structures from a higher-dimensional space. De Bruijn (1981a) was the first to propose an algebraic approach to describe the Penrose (1979) aperiodic patterns in two dimensions. He also showed that the same results can be obtained by projecting a five-dimensional cubic lattice onto a two-dimensional subspace. Kramer and Neri (1984) and Duneau and Katz (1985) later generalised these ideas to construct aperiodic fillings of an m-dimensional Euclidean space by projection of a periodic grid from an n-dimensional space, $1 \leq m < n$. Levine and Steinhardt (1984), on the other hand, have defined a set of geometric rules for generating quasicrystalline structures, which are based on the concept of quasi-periodicity.

A number of authors have recently set out to study various physical properties of quasicrystalline model systems. Lu *et al* (1985) investigated the phonon spectrum of harmonic oscillators and the energy spectrum of electrons on a linear Fibonacci chain. General properties of diffraction spectra of quasiperiodic lattices were studied by Elser (1985, 1986) and Zia and Dallas (1985). These works include, by way of illustration, the construction of a linear quasiperiodic array by projecting a given two-dimensional square periodic lattice on a line whose slope is an irrational number.

The purpose of this paper is to solve explicitly the inverse projection problem for a fairly general family of quasiperiodic arrays. By 'inverse problem' we mean that the linear array is specified by some generating procedure, depending on a small number of parameters. Then a two-dimensional periodic structure is constructed in such a way that its projection on a line will result in the desired quasiperiodic array. The Fourier coefficients of the periodic structure calculated on the projection line define the diffraction spectrum and the structure factor of the linear array. These are uniquely defined by the array specifying parameters.

We consider a linear array of pointlike 'atoms'. Adjacent points are separated by one of two characteristic lengths. Crucial to the solution of the proposed problem is our ability to write down an explicit formula for the coordinate x_j of the jth point in the array. This amounts to knowing how many line segments of each type there are among the first j segments of the sequence. A sequence of these line segments is isomorphic to a binary sequence of objects, say 0 and 1, which were extensively studied in the mathematical literature in connection with the theory of complementary sets of integers. A very incomplete list of relevant articles includes works by Fraenkel (1969), Gilbert (1963), Lambek and Moser (1954), de Bruijn (1981b), Stolarsky (1976) and Fraenkel *et al* (1978).

An infinite binary sequence of 0 and 1 is a very general object: it may be constructed at random, or specified by some deterministic algorithm, which in turn may depend on an infinite or a finite set of parameters. The occupation of a given site in a deterministic sequence may or may not depend upon the occupation of other sites. The sequence may be periodic or aperiodic. Even aperiodic sequences may exhibit a large variety of pattern regularities, etc.

In this paper we consider a deterministic rule for generating binary sequences which is fairly general in the sense that it depends on two parameters (v and w, see below). For some values of these parameters a variety of periodic patterns will result. For others, however, the rule will produce aperiodic sequences, which can be shown to be strongly related to quasiperiodic and almost periodic functions (Bohr 1951, Katznelson 1976, Avron and Simon 1981). Results from the theory of this type of binary sequence provide the necessary tools to establish the relation between the index of a site in the sequence and the index of the element occupying the given site, allowing the problem of Fourier transformation to be solved in closed form.

The rule is incorporated in a well known theorem from the theory of complementary sets of integers. This theorem has appeared in the literature in various forms and degrees of generality. The form best suited for our purpose is found in a paper by de Bruijn (1981b), theorem 5.3. We shall restate the theorem without proof, omitting some details which are unimportant in the present context, and allowing for some convenient changes of notation.

Theorem 1. Let N be the set of positive integers. Let v and w be real numbers, $v > 1$. Define the sequence $p(j)$ by

$$p(j) = [(j+1)/v + w] - [j/v + w] \qquad j \in N. \tag{1}$$

Then p is a sequence of 0 and 1. The sequence p takes its 1 on the set

$$S_1\colon \{j \mid j = [(k-w)v],\ k \in N\} \tag{2}$$

and its 0 on the set

$$S_0\colon \{j \mid j = [(l+w)u],\ l \in N\} \tag{3}$$

where u is defined by

$$1/v + 1/u = 1. \tag{4}$$

The sets S_1, S_0 satisfy $S_1 \cap S_0 = \varnothing$, $S_1 \cup S_0 = N$.

The symbol $[x]$ denotes the greatest integer not exceeding x. Although the original theorem was formulated for $j, k, l \in Z$, the set of all integers, in this paper however, it is convenient to consider only the positive integers. The sequence p is sometimes referred to as a 'Beatty sequence' (Stolarsky 1976), while the sets S_1 and S_0 are classified as 'non-homogeneous complementary systems' (see, e.g., Fraenkel 1977, Boshernitzan and Fraenkel 1981). In the case $w=0$, an additional restriction must be put on v, namely $v \neq 2$; otherwise equations (2) and (3) fail to generate complementary sets. It turns out that $v=2$ is a 'singular' value of the parameter (see § 2). Its exclusion does not alter in any way the general scope of this work. If j denotes the position index of an element in the sequence p, then according to equations (2) and (3), k and l are the number of 1 and 0, respectively, among the first j elements of the sequence. Obviously $k+l=j$.

Equations (2) and (3) can be inverted to give k and l as functions of j:

$$k=[(j+1)/v+w] \qquad j \in N \tag{5}$$

$$l=[(j+1)/u-w] \qquad j \in N. \tag{6}$$

These expressions allow us to write an explicit formula for x_j. k and l are monotonic staircase functions of j increasing by one every time an element 1 (or 0, respectively) is encountered along the sequence. Asymptotically $k=j/v+\mathrm{O}(1)$, $l=j/u+\mathrm{O}(1)$, and the functions follow average slopes of $1/v$ and $1/u$, respectively, never deviating from the slope by more than one unit of the ordinate. If v and u are irrational numbers then the deviation never vanishes at integer values of j, except 0. The following description will help a better understanding of the matter. Suppose that somebody has prepared for us the beginning of a particular $p(j)$ sequence up to position j, drawn the lines of irrational slope $1/v$ and $1/u$ on a checkered sheet of paper and indicated the partial staircases $k(j)$ and $l(j)$. Now he asks us to continue the sequence without knowing v and w. Let us try adding a 1 in position $j+1$. Then a unit must be added to k, while l remains constant. If this action does not cause k to deviate from $1/v$ by more than one unit of ordinate, the choice was right. Otherwise, let k stay level for another step and put a 0 in position $j+1$ instead. The choice is unique and the procedure of forcing the stairs to follow the slopes as closely as possible is guaranteed to produce the correct sequence *ad infinitum.* The elements 0 and 1 will as a result be distributed 'as evenly as possible' along the sequence. It is not known whether other deterministic rules exist for generating binary sequences which are quasiperiodic *and* possess explicit expressions for $k(j)$ and $l(j)$.

In § 2 we discuss properties of the sequences $p(j)$ in order to gain a better insight into their nature. In § 3 we present in some detail the construction of the diffraction spectrum and the structure factor for arrays of line segments isomorphic to $p(j)$. Finally, we present in § 4 results about distributions of certain sequences of irrational numbers modulo 1. Although apparently unrelated to the main subject of this paper, these results were obtained while carrying out various computer experiments with linear Fibonacci sequences and their connection with the Fourier transform and the diffraction spectrum will be shown.

2. Properties of the sequence $p(j)$

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

$$|z(M, j_1) - z(M, j_2)| < \varepsilon. \tag{7}$$

For the sequence $p(j)$, the function $z(M, j)$ is obtained from (6): $z(M, j) = \{[(j+M)/u + w] - [j/u + w]\}/M$. Using the inequality $a - b - 1 < [a] - [b] < a - b + 1$, it suffices to choose $M_0(\varepsilon) = 2/\varepsilon$ in order to satisfy (7). The condition is also satisfied independently of v and u, a result which follows from the fact that $l(j)$ and $k(j)$ are 'linear on the average'. Uniform average density is, of course, a trivial property of periodic and of uniformly random binary sequences. If, however, v is irrational, the sequence $p(j)$ will be quasiperiodic due to property (7) which distinguishes this from other types of aperiodicity.

Example 1. $v = 4.656\,871\,196\ldots > 2$, $u = 1.273\,457\,813\ldots < 2$, $w = 0$. The sequence is

$$0001000010001000010000100010000100001 0001\ldots.$$

(b) In a sequence $p(j)$ one of the binary constituents, 0 or 1, always appears isolated, while the other comes in strings of consecutive elements. Assume that two consecutive 1 appear at positions j and $j+1$. Then according to (2) we must have $[(k+1-w)v] - [(k-w)v] = 1$. The arguments of the greatest integer functions in this equation must therefore satisfy $0 < (k+1-w)v - (k-w)v < 2$, or, since $v > 1$, one must have

$$1 < v < 2. \tag{8}$$

An attempt to derive a similar condition for two consecutive 0 leads to $1 < u < 2$, which means, of course, $v > 2$. We conclude that consecutive 0 and 1 cannot coexist in a $p(j)$ sequence. The rule is

$1 < v < 2$, $u > 2$: consecutive 1 and isolated 0 (this sequence will be called 1-dominant);

$1 < u < 2$, $v > 2$: consecutive 0 and isolated 1 (this sequence is called 0-dominant).

Notice that the parameter w plays no role in establishing this property.

(c) The interchange between v and u in (1) produces the complementary sequence, i.e. 0 are interchanged with 1. The following properties will be specifically derived for 0-dominant sequences and can be readily translated to 1-dominant by use of property (c).

(d) The number of consecutive 0. What must be the value of v in order to have strings of h consecutive 0, preceded and followed by isolated 1? The sites of these 1 will be $h+1$ places apart, which means that there must exist some values of k such that $[(k+1-w)v] - [(k-w)v] = h+1$. From this follows

$$h < v < h+2. \tag{9}$$

The next question is: given v in the interval (9), are there strings of 0 of different lengths $h+g$, $g = \pm 1, \pm 2, \ldots$, also present in the sequence? By the same argument there must be values of k for which $[(k+1-w)v] - [(k-w)v] = h+g+1$, from which it follows that

$$h+g < v < h+g+2. \tag{10}$$

Intervals (9) and (10) will partially overlap in two instances: $g = 1$ or $g = -1$. This means that for any value of v in the interval

$$h < v < h+1 \tag{11}$$

the corresponding 0-dominant sequence will contain strings of consecutive 0 of sizes $h=[v]$ and $h-1=[v-1]$ only, separated by isolated 1 (see example 1 with $[v]=4$). Notice again that the parameter w plays no role in shaping this property either.

(e) What then is the role of w? Let us take in example 1, say, $w=-0.4$ instead of 0. The new sequence will be

$$0100001000010001000010000100010000100\ldots.$$

By properties (a) and (d) this sequence has exactly the same density of 0 and the same string structure as the former. However, the strings of 4 and 3 consecutive 0 follow each other in a different way. The role of w is to rearrange the binary elements of the sequence while preserving the string structure and the average density; w is called the 'shift parameter'. As a matter of fact, there are as many different $p(j)$ sequences with the same string structure (v) as there are points w on a line, i.e. an uncountable infinity of them. This can be proven as follows. For two different values w and w', construct the sets S_1 and S_1' according to equation (2): S_1: $j=[(k-w)v]$, $k\in N$, and S_1': $j'=[(k-w')v]$, $k\in N$. What is the condition on w and w' for these sets to be identical? We must have, of course, $[(k-w)v]=[(k-w')v]$, $k\in N$. If this equality is true for some k, then

$$[kv-wv]<kv-w'v<[kv-wv]+1. \tag{12}$$

Writing $[a]=a-\{a\}$, where the curly brackets denote the fractional part of the argument, we obtain from (12) after rearranging terms:

$$v(w'-w)<\{kv-wv\}<1+v(w'-w). \tag{13}$$

By a famous theorem of Weyl (1916), if θ_1 is irrational, and θ_2 is a real number, then the set $\{k\theta_1+\theta_2\}$, $k\in N$ is uniformly and densely distributed in the open interval (0, 1). The sets S_1 and S_1' will be identical when (13) is satisfied for all $k\in N$, i.e. if and only if $w'=w$. Otherwise, there exist finite values of k for which either end of inequality (13) will eventually be violated. We conclude that two $p(j)$ sequences with the same v, but different w, will eventually differ starting from some finite position j. This property has important consequences on the nature of the Fourier transform of the corresponding array of segments (see § 3.3).

The parameter v determines the global structure of a $p(j)$ sequence. By looking at finite segments taken from the middle of an infinite $p(j)$ sequence there is no way one can tell what is the value of w. The value of v, on the other hand, can be estimated with increasing accuracy by looking at ever longer segments.

3. The diffraction spectrum of $p(j)$

3.1. The quasiperiodic linear array

The following double inequality can be derived from equation (5):

$$-(1+vw)<j-vk<v-(1+vw) \tag{14}$$

and will be used subsequently.

Consider now two characteristic line segments. Without loss of generality one can choose the shorter of the two as unit length. The other will be σ, a real number ($\sigma>1$). Construct a sequence of segments isomorphic to $p(j)$ by matching

$$\begin{aligned}&(\text{segment } \sigma)\rightarrow(\text{element } 1)\\&(\text{segment } 1)\rightarrow(\text{element } 0).\end{aligned} \tag{15}$$

The total length of the first j segments is

$$x_j = k\sigma + (j-k)\cdot 1 = j + k(\sigma - 1) \qquad j = 1, 2, \ldots . \tag{16}$$

Define $x_0 = 0$. The model system having pointlike identical 'atoms' located at x_j, $j = 0, 1, 2, \ldots$, can be mathematically described by a sum of delta functions:

$$G(x) = \sum_j \delta(x - x_j). \tag{17}$$

3.2. *The periodic structure in two dimensions*

Consider a rectangular lattice in the (X, Y) plane with periods L in the X direction and λL in the Y direction. The coordinates of the lattice points are $(mL, n\lambda L)$, m, n integers (figure 1). The x axis on which the function $G(x)$ will be constructed passes through the origin. Denote by $1/\eta$ its slope in the (X, Y) plane. The equation of the x axis is

$$Y = (1/\eta)X. \tag{18}$$

Let $\boldsymbol{b}$ be the unit vector in a direction perpendicular to the x axis

$$\boldsymbol{b} = \frac{1}{(1+\eta^2)^{1/2}}\begin{pmatrix} 1 \\ -\eta \end{pmatrix} \tag{19}$$

where $-\eta$ is its slope in the (X, Y) plane. Through every lattice point construct identical line segments (B) in direction $\boldsymbol{b}$. Their position relative to the corresponding lattice point is defined by two numbers γ, δ, such that the endpoint coordinates of the segment passing through the origin are $(\gamma, \eta\gamma)$, and $(\delta, -\eta\delta)$, respectively (figure 1). The total length of a segment is $d = (\gamma + \delta)/\cos\theta$. The assembly of all B segments forms a doubly periodic structure in the (X, Y) plane. Some segments will intersect the x axis, others will not. The purpose is to determine the five unknown parameters L, λ, η, γ, δ, in such a way that the periodic structure intercepts the x axis at x_j, $j = 0, 1, 2, \ldots$, and only at x_j.

Choose a lattice point $(mL, n\lambda L)$ and assume that its B segment intercepts the x axis (direction $\boldsymbol{a}$) at the point (X, Y). Denote by q the distance between (X, Y) and

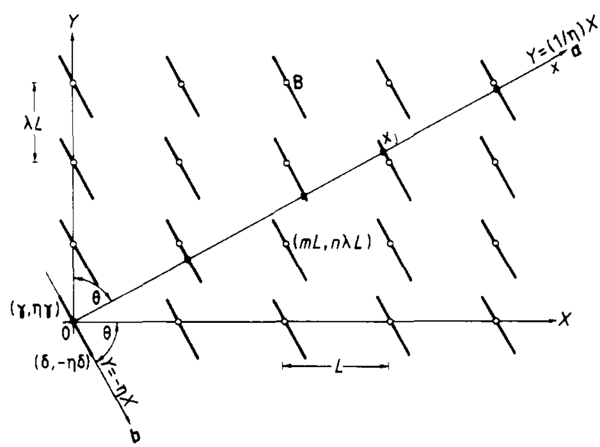

Figure 1. This shows the periodic rectangular lattice, the projections axis $\boldsymbol{a}$, the direction of projection $\boldsymbol{b}$ and the B segments.

$(mL, n\lambda L)$ (figure 2). Together with the origin 0, these points form a right triangle and we have the following vector equation:

$$\begin{pmatrix} X \\ Y \end{pmatrix} + \frac{q}{(1+\eta^2)^{1/2}} \begin{pmatrix} 1 \\ -\eta \end{pmatrix} = \begin{pmatrix} mL \\ n\lambda L \end{pmatrix}. \tag{20}$$

Solving the system of three equations (18) and (20) for q, X, Y, we obtain

$$q/(1+\eta^2)^{1/2} = L(m - n\lambda\eta)/(1+\eta^2) \tag{21}$$

$$X = L\eta(m\eta + n\lambda)/(1+\eta^2) \tag{22}$$

$$Y = L(m\eta + n\lambda)/(1+\eta^2). \tag{23}$$

If (X, Y) should be a point x_j of the sequence on the x axis, then the quantity

$$x = (X^2 + Y^2)^{1/2} = L\eta(m + n\lambda/\eta)(1+\eta^2)^{-1/2} \tag{24}$$

must be of the form (16). Put

$$L = (1+\eta^2)^{1/2}/\eta \tag{25}$$

$$\lambda/\eta = \sigma - 1 \tag{26}$$

and identify m with j and n with k. The values of m, n in a pair (m, n) corresponding to a lattice point which supports a B segment intercepting the x axis at x_j are, of course, not independent of each other; they must satisfy the double inequality (14). On the other hand, q must satisfy the double inequality

$$-\delta/\cos\theta < q < \gamma/\cos\theta. \tag{27}$$

Substitute (21) into (27) and compare the result with (14). Then, reverting to the usual meaning of rectangular brackets, and using equations (25) and (26), the following expressions are obtained for the unknown parameters:

$$\eta = [v/(\sigma-1)]^{1/2} \tag{28}$$

$$\lambda = [v(\sigma-1)]^{1/2} \tag{29}$$

$$L = \Delta^{1/2} \tag{30}$$

$$\delta = (\sigma-1)(1/v + w)/\Delta^{1/2} \tag{31}$$

$$\gamma = (\sigma-1)(1/u - w)/\Delta^{1/2} \tag{32}$$

where

$$\Delta = \sigma/v + 1/u = (\sigma - 1 + v)/v \tag{33}$$

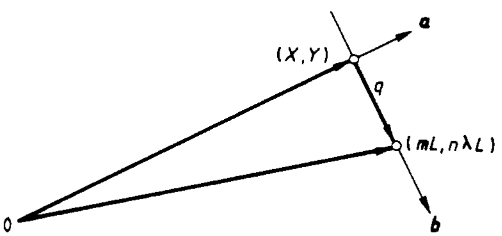

Figure 2. Auxiliary to equation (42).

is the weighted average length of the segments σ and 1. Do not worry about the apparent dimensional inconsistency of some of the expressions above: all quantities are dimensionless.

The preceding equations show that the periodic lattice and the direction of projection are completely determined by v and σ. Since $\delta+\gamma$ is also independent of w, this parameter only affects the proportion into which the lattice point divides a B segment. In other words, by keeping v and σ fixed, and changing w, the B segments will collectively slide relative to their supporting lattice points. As a result, the sequence of intercepts on the x axis will change while preserving the relative frequency of the two types of segment.

3.3 The Fourier transform

Adjacent to every B segment of the lattice define a rectangular domain R of length d and width ε (figure 3). Define the function

$$g_\varepsilon^{(R)}(X, Y)=\begin{cases}1/\varepsilon d & \text{if } (X, Y)\in R\\ 0 & \text{if } (X, Y)\notin R.\end{cases} \tag{34}$$

Then, the sum of $g_\varepsilon^{(R)}$ over the lattice is a doubly periodic function

$$g_\varepsilon(X, Y)=\sum_{m,n} g_\varepsilon^{(R)}(X-mL, Y-n\lambda L) \tag{35}$$

with periods L, λL, such that

$$\int_0^L\int_0^{\lambda L} g_\varepsilon(X, Y)\,\mathrm{d}X\,\mathrm{d}Y=1. \tag{36}$$

On the x axis we have

$$X=x\sin\theta=x/\Delta^{1/2} \qquad Y=x\cos\theta=x[(\sigma-1)/v\Delta]^{1/2}. \tag{37}$$

Recalling the definition of $G(x)$ in equation (17), we can write

$$G(x)=\lim_{\varepsilon\to 0} g_\varepsilon(x/\Delta^{1/2}, x[(\sigma-1)/v\Delta]^{1/2}). \tag{38}$$

The function $g_\varepsilon(X, Y)$, on the other hand, can be expanded in a double Fourier series

$$g_\varepsilon(X, Y)=\sum_{m,n} c_{mn}^{(\varepsilon)}\exp[2\pi\mathrm{i}(mX/L+nY/\lambda L)]. \tag{39}$$

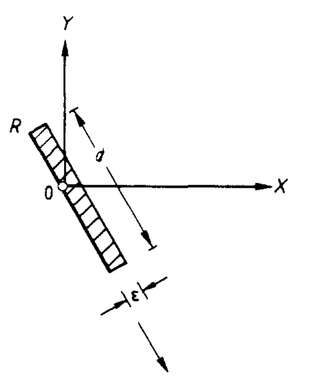

Figure 3. The function $g_\varepsilon^{(R)}(X, Y)$.

On the x axis we have

$$m(X/L)+n(Y/\lambda L)=x(m+n/v)/\Delta. \tag{40}$$

Therefore, on the x axis

$$g_\varepsilon(x/\Delta^{1/2}, x[(\sigma-1)/v\Delta]^{1/2})=\sum_{m,n} c_{mn}^{(\varepsilon)} \exp[2\pi i x(m+n/v)/\Delta]. \tag{41}$$

The Fourier coefficients of $G(x)$ are defined by

$$\begin{aligned}F(s)&=\lim_{T\to\infty}\frac{1}{T}\int_0^T G(x)\exp(2\pi i s x)\,dx\\ &=\lim_{\varepsilon\to 0}\lim_{T\to\infty}\frac{1}{T}\int_0^T g_\varepsilon(x/\Delta^{1/2}, x[(\sigma-1)/v\Delta]^{1/2})\exp(2\pi i s x)\,dx\\ &=\lim_{\varepsilon\to 0}\sum_{m,n} c_{mn}^{(\varepsilon)}\lim_{T\to\infty}\frac{1}{T}\int_0^T \exp[2\pi i x(s+(m+n/v)/\Delta)]\,dx.\end{aligned} \tag{42}$$

It follows that

$$F(s)=\begin{cases}\lim_{\varepsilon\to 0} c_{mn}^{(\varepsilon)} & \text{if } s=s_{mn}(v,\sigma)=-(m+n/v)/\Delta\\ 0 & \text{if } s\neq s_{mn}(v,\sigma);\ m,n=0,\pm 1,\pm 2,\ldots.\end{cases} \tag{43}$$

The spectrum s_{mn} is parametrised by two sets of integers m, n and is infinitely dense on the s line provided that v is irrational. This well known general property is governed by the linear combination $m+n/v$, where v, of course, is one of the specifying parameters of the quasiperiodic sequence: quasiperiodicity implies an infinitely dense spectrum of Bragg peaks of zero width. The parameter σ which specifies the relative size of the segments appears in the denominator Δ, which plays the role of a scaling factor. The location of spectral lines is independent of the parameter w, which means that the whole uncountably infinite set of sequences with common v, σ, but different w, produce identically located peaks.

The Fourier coefficients can be calculated by the standard procedure

$$\lim_{\varepsilon\to 0} c_{mn}^{(\varepsilon)}=\lim_{\varepsilon\to 0}\int_0^L\int_0^{\lambda L} g_\varepsilon(X,Y)\exp[-2\pi i(mX/L+nY/\lambda L)]\,dX\,dY. \tag{44}$$

However, it is more convenient to use the following lemma. Let $g_\varepsilon(X,Y)$ be the function defined in equation (35). Then, for any function $Z(X,Y)$, the following equality holds:

$$\lim_{\varepsilon\to 0}\int_0^L\int_0^{\lambda L} Z(X,Y)g_\varepsilon(X,Y)\,dX\,dY=(\delta+\gamma)^{-1}\int_{-\gamma}^{\delta} Z(X,-\eta X)\,dX. \tag{45}$$

Substituting for Z the imaginary exponential appearing in equation (44), and using equations (28)-(32), we obtain

$$c_{mn}=\frac{\Delta}{\sigma-1}\int_{-\gamma/L}^{\delta/L}\exp\left[-2\pi i\left(m-\frac{1}{\sigma-1}n\right)\xi\right]d\xi \tag{46}$$

$$\delta/L=(\sigma-1)(1/v+w)/\Delta \qquad \gamma/L=(\sigma-1)(1/u-w)/\Delta. \tag{47}$$

Writing $F(s_{mn})=A_{mn}\exp(i\Theta_{mn})$, we obtain the amplitude

$$A_{mn}=\frac{\sin(\pi\Omega)}{\pi\Omega} \tag{48}$$

and the phase

$$\Theta_{mn} = \pi\Omega(2w - 1 + 2/v) \tag{49}$$

where

$$\Omega = -s_{mn}[-(\sigma - 1), (\sigma - 1)/u] = [m(\sigma - 1) - n]/\Delta. \tag{50}$$

Only the phase Θ_{mn} depends on the shift parameter w. Therefore, the measurable structure factor $|F(s_{mn})|^2$ is completely determined by v and σ.

All sequences with equal v, σ, but different w produce identical spectral lines (location and intensity). The functional form of the amplitude A_{mn} implies that the smaller the value of Ω, the larger is the corresponding spectral line. Equation (50) shows that the strongest peaks are contributed by points in the (m, n) plane which are closest to a line of slope $(\sigma - 1)$. The intensity should decrease in directions away from the line. The distribution of intensities is thus governed by the relative size σ of the segments and not by the sequence parameters. The solution (45)-(47) is, of course, unique. However, the choice of the doubly periodic lattice and the x axis in the (X, Y) plane are not. For example, we may impose a particular direction for the x axis; then, in general, a non-orthogonal projection direction will result. Other options are available.

The set of frequently quoted Fibonacci sequences is obtained from the general sequence (equation (1)) by setting $v = \phi = (\sqrt{5} + 1)/2$, the golden mean, and arbitrary w. If, in addition, we choose $\sigma = \phi$, then the following values of parameters are obtained:

$$\eta = \phi \qquad \lambda = 1 \qquad \Delta = 3 - \phi \qquad L = (3 - \phi)^{1/2}. \tag{51}$$

These equations show that the doubly periodic lattice is square. The spectral lines are located at

$$s = s_{mn}(\phi) = -(m + n/\phi)/(3 - \phi) = -(m\phi + n)/\sqrt{5} \qquad m, n = 0, \pm 1, \pm 2, \ldots \tag{52}$$

a result which has been known for some time (Levine and Steinhardt 1984). From (50) we obtain

$$\Omega = (m/\phi - n)/(3 - \phi) = (m - n\phi)/\sqrt{5} \qquad m, n = 0, \pm 1, \ldots. \tag{53}$$

4. The distribution of $(x_j\phi^p)$ mod 1

The material presented in this section is only marginally related to the main topic of the paper. We obtain the distributions in the interval (0, 1) of certain infinite sequences of irrational numbers modulo 1, related to the Fourier transform of a Fibonacci sequence of the type discussed at the end of § 3.3. The distributions are quite interesting in themselves, although it is rather doubtful whether they might be encountered in another context.

By operating the Fourier transform directly on $G(x)$ in equation (17) one obtains

$$F(s) = \lim_{J \to \infty} \frac{1}{J} \sum_{j}^{J} \exp(2\pi i x_j s). \tag{54}$$

At an early stage of this work we attempted to calculate $F(s)$ numerically by summing about 10^6 terms of (54) for some representative values of s. We chose the Fibonacci sequence: $v=\sigma=\phi$, $w=0$, $k=[(j+1)/\phi]$, $x_j=j+k/\phi$. The attempt, of course, was rather unsuccessful because the spectral lines are very narrow for sufficiently large values of J, and lie at irrational values of s which can only be approximately represented by computer words of finite length.

It was recognised, however, that the discrete infinite summation in (54) could be reduced to the integration of a (piecewise) continuous function over a finite interval if, for some fixed value of s, the distribution of the fractional parts

$$r_j=(x_js) \bmod 1=x_js-[x_js] \qquad 0<r_j<1 \tag{55}$$

were known. (The use of rectangular brackets for the greatest integer function should be clear from the context.) For then, subject to additional conditions, one could write $\exp(2\pi i x_j s)=\exp(2\pi i[x_js])\exp(2\pi i r_j)=\exp(2\pi i r_j)$ and therefore

$$F(s)=\int_0^1 h_s(r)\exp(2\pi i r)\,dr \tag{56}$$

where we have omitted the subscript j from r_j and $h_s(r)$ is the normalised distribution of r for a fixed value s. All that is required from $h_s(r)$ is that it be integrable on the interval (0, 1). The fractional parts r_j must fill densely the interval (0, 1), or at least a subinterval thereof.

We have investigated the important set of values $s=\phi^p$, where p is an integer: positive, negative or zero. This set is related to the property of self-similarity of the Fibonacci sequence. For this case it is easy to show that the fractional parts r_j are all different. If indeed one assumes that $r_j=r_l$ for $j\neq l$, a contradictory equation results between an integer and an irrational number. Let us now relabel the function h and denote by $h_p(r)$ the distribution of fractional parts $(x_j\phi^p) \bmod 1$, $j=1,2,\ldots$. We have generated sequences of several million terms j, and sorted the fractional parts along the interval (0, 1). The distributions $h_p(r)$ were found by computer experiment to be piecewise uniform, taking at most two constant values (including zero) on at most three subintervals whose union is (0, 1). The results are summarised in figure 4 and in table 1. The question is: are they rigorous?

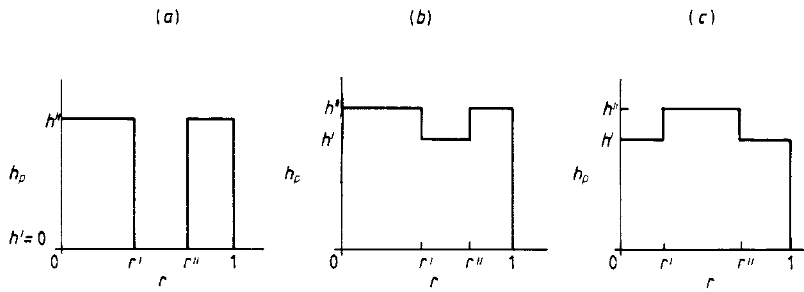

Figure 4. The distributions $h_p(r)$. (a) $p>0$; (b) $p<0$, odd; (c) $p\leqslant 0$, even.

No matter how elaborate a computer experiment may be, there is no way we can tell by it alone whether or not r is a densely distributed variable. If the distributions are indeed rigorous, then working from the analytic equation (44) for $F(s_{mn})=\lim c_{mn}^{(\varepsilon)}$, one must be able to recover an expression of the form (56) with an appropriate distribution $h_p(r)$. If this can be done then the above statement concerning the distributions of r would have attained indirect validation.

Table 1. The distribution $h_p(r)$.

Figure	p	r'	r''	$r''-r'$	$h''-h'$
4(a)	1	—	—	0	1
	$2q$	ϕ^{-2q}	$1-\phi^{-(2q+1)}$	$1-\phi^{-(p-1)}$	$\phi^{(p-1)}$
	$2q+1$	ϕ^{-2q}	$1-\phi^{-(2q+1)}$	$1-\phi^{-(p-2)}$	$\phi^{(p-2)}$
4(b)	<0, odd	$1-\phi^{-(p-1)}$	$1-\phi^{-p}$	$\phi^{-(p+1)}$	$\phi^{-(p+1)}$
4(c)	$\leqslant 0$, even	$1-\phi^{-(p-1)}$	$1-\phi^{-p}$	$\phi^{-(p+1)}$	$\phi^{-(p+1)}$

We can start from equation (46) by substituting the parameters corresponding to the Fibonacci sequence

$$c_{mn} = \lim_{\varepsilon \to 0} c_{mn}^{(\varepsilon)} = \frac{\phi^2+1}{\phi} \int_{-\gamma/L}^{\delta/L} \exp[-2\pi \mathrm{i}(m-n\phi)\xi]\, \mathrm{d}\xi \tag{57}$$

where $\delta/L = (\phi^2+1)^{-1}$, $\gamma/L = \phi^{-1}(\phi^2+1)^{-1}$. A change of variable $\xi = t/(2\phi-1)$ gives

$$c_{mn} = \int_{-1/\phi^2}^{1/\phi} \exp\left(-2\pi\mathrm{i}\frac{m-n\phi}{2\phi-1}t\right) \mathrm{d}t. \tag{58}$$

The general form of the Fibonacci spectrum s_{mn} was given in equation (52). It is easy to see that $s=\phi^p$ belongs to the spectrum and in fact the integers m, n are uniquely determined by p.

The argument of the exponent in equation (58) can be formulated as

$$(m-n\phi)/(2\phi-1) = -\phi s_{mn}(-1/\phi). \tag{59}$$

For the special form $s_{mn}=\phi^p$ under consideration we have

$$(m-n\phi)/(2\phi-1) = (-1/\phi)^{p-1}. \tag{60}$$

Let us illustrate the procedure for $p>0$. All other cases listed in table 1 are somewhat more elaborate but can be worked out following the same general idea. By making another change of variable $r=-(-1/\phi)^{p-1}t$, we obtain

$$c_{mn} = (-\phi)^{p-1} \int_{(-1/\phi)^p}^{(-1/\phi)^{p+1}} \exp(2\pi\mathrm{i}r)\, \mathrm{d}r. \tag{61}$$

The next, and final, step of calculation is the mapping of the integration range in (61) onto the interval (0, 1), possibly by allowing for a piecewise constant function which would multiply the integrand. If $p=2q$, then

$$\begin{aligned} c_{mn} &= \phi^{2q-1}\left(\int_{-\phi^{-(2q+1)}}^{0} + \int_0^{\phi^{-2q}}\right) \exp(2\pi\mathrm{i}r)\, \mathrm{d}r \\ &= \phi^{2q-1}\left(\int_0^{\phi^{-2q}} + \int_{1-\phi^{-(2q+1)}}^{1}\right) \exp(2\pi\mathrm{i}r)\, \mathrm{d}r \\ &= \int_0^1 h_p(r) \exp(2\pi\mathrm{i}r)\, \mathrm{d}r \end{aligned} \tag{62}$$

which is of the form (56) and where $h_p(r)$ is the function shown in figure 4(a) and table 1. For $p=2q+1$, the calculation is just as easy. Negative values of p, however, require additional manipulation at the stage of range mapping. For then the limits of integration are of the general form $\pm\phi^{-p}$, with $\phi^{-p}>1$. The integer parts of these limits may be discarded for they contribute nothing to the integral. A problem of normalisation also arises which can be dealt with by adding a suitable constant which multiplies a zero-valued integral over $(0, 1)$.

This calculation shows indeed that $h_p(r)$ is rigorously piecewise constant and r is densely distributed in $(0, 1)$.

5. Concluding remarks

We have presented the explicit solution for the diffraction spectrum of a fairly general family of linear quasiperiodic sequences of identical atoms separated by one of two characteristic lengths. The main limitation is that one of the binary elements always appears isolated in the sequence, to which, however, no particular significance should be attached for this happens to be an inherent property of the type of sequences under investigation, based on theorem 1. It is not known whether other generating rules exist which produce quasiperiodic sequences *and* permit an explicit solution of the Fourier transform in a closed form.

The solution is uniquely determined by three parameters of the problem: two of them, v and w, specify the sequence while the third, σ, is the ratio between two characteristic atom separation distances. The parameter v must be irrational and determines the string structure of the binary elements in the sequence. This is also the parameter which, up to a scaling factor, uniquely determines the location of the spectral lines. The parameter w governs the possible 'shuffling' of the binary elements along the sequence, while preserving the string structure. Finally, the parameter σ determines the distribution of intensities of the spectral lines. w and σ may be any real numbers. While the sequence and its Fourier transform are uniquely specified by v, w, σ, the two-dimensional periodic lattice from which the projection is constructed need not be so: there is some, although not much, freedom in deciding which of the lattice parameters would be specified in advance, but the natural choice is that presented in this paper. Perhaps the most significant explicit result of this work is that for every fixed v and σ, there exists an uncountable infinity of *different* sequences exhibiting identical measurable diffraction patterns, i.e. locations and intensities, the only difference being in the phase. This provides strong support to analogous assertions about quasiperiodic tilings of two- and three-dimensional spaces with pentagonal and icosahedral symmetries, respectively. It is not easy to find a physical system which lends itself to description by a one-dimensional model of quasiperiodic arrays. Nevertheless, it seems useful to investigate a number of questions which the present work has left unanswered: (a) the possibility of relaxing the inherent restriction of isolated elements typical of the investigated sequences; (b) a way of taking into account different atoms in each type of segment (cell); and (c) ternary sequences in one dimension.

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