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Quasicrystals and their Fourier transform

by N.G. de Bruijn

Department of Mathematics and Computing Science, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, the Netherlands

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1. INTRODUCTION

Quasicrystals form a very striking case of structures that were constructed theoretically before there was any idea that there is something in the physical reality corresponding to it. The source of the theoretical discovery lies in Penrose's non-periodic tilings of the plane with infinitely many copies of two pieces, whose angles are multiples of 36 degrees (R. Penrose [21], [22]; see M. Gardner [11] for a beautiful survey).

In analogy to this, the question was proposed to do something similar in three dimensions, where the role of the regular pentagon is taken over by the icosahedron. This possibility was indicated by A.L. Mackay ([19], [20]), and subsequently investigated by D. Levine and P.J. Steinhardt ([17]).

The dual method, with specialization to the multigrid construction, initiated in [5] (for a two-dimensional application with angles of 45 and 90 degrees, we refer to F. Beenker [1]) made it possible to give a fast description of such space fillings. The dual method was applied to the icosahedral case by P. Kramer and R. Neri [16]. Not long after that, the real surprise was that the work of Shechtman et al. ([24]) revealed certain metallic alloys of which the Bragg diffraction patterns show a five-fold symmetry that had never been observed before, and that was well known to be impossible with the ordinary periodic crystal structures.

Most authors refer to the multigrid method as the "projection method" or "strip method", on the basis of the geometrical interpretation given in [5], section 1 (vi). This may be very illuminating, but on the other hand it may mean a certain loss of generality. It may have caused most authors to restrict the multigrid method to the special form that the grid vectors are the same as the lattice vectors (with the terminology of section 10 of this paper, this means $D = V$). Gähler and Rhyner [10] treat the general case.

The question was proposed by D. Levine and P.J. Steinhardt ([17], [18]) whether the theoretical constructions would lead, by means of Fourier transforms, to diffraction patterns similar to those found by Shechtman et al. This turned out to be more or less the case. Also quite recently, V. Elser ([8], [9]), A. Katz and M. Duneau ([7], [14]), F. Gähler and J. Rhyner ([10]) produced theories leading to Fourier transforms in the form of an every where dense superposition of delta functions. Related work was published by R.K.P. Zia and W.J. Dallas ([26]), and by P.A. Kalugin et al. ([13]). All that work is of a quite algebraic nature, and seems to be quite general and very satisfactory from that point of view. But what seems to be lacking, is a systematic analytical foundation. The first thing one should require from the analytical point of view, is that when working with generalized functions (like infinite sums of delta functions), one should make it clear to what function space these objects belong. Also, when dealing with infinite processes, it has to be made clear what kind of convergence procedures are intended.

A reason for being careful in this respect is that the Fourier transforms of the crystal patterns (even in the so-called one-dimensional case) are superpositions of infinitely many delta functions, everywhere dense, but by no means absolutely convergent, not even in a sense that the deltas in a bounded region give an absolutely convergent contribution to the Fourier transform.

When studying quasicrystals, or in particular the Penrose patterns, one is invariably confronted with a particular kind of zero-one-sequences that will be called Beatty sequences in this paper, following the survey paper [25] by K.B. Stolarsky. Some authors have refered to these sequences as "one dimensional quasicrystals", but a clear description of how to specialize a general notion of quasicrystals in order to get these sequences seems to be lacking. Such a specialization will be indicated in this paper (section 14).

Different readers may look for different things in this paper, and therefore it will be explained here what the various parts are, and what can be read independently.

The paper contains the following items.

(i) A description of the Beatty sequences (sections 2, 3, 4).

(ii) A description of multigrid-produced quasicrystals (section 10), with particular emphasis on what happens if $D^T V$ is singular.

(iii) A way to get Beatty sequences as one-dimensional quasicrystals (section 15).

(iv) A description of a theory of generalized functions suitable for the Fourier analysis of superpositions of infinitely many Dirac delta functions (sections 5, 6, 7, 8). Such superpositions will be called "Dirac combs" in this paper. In general the distribution of the deltas is everywhere dense.

These sections give all their attention to the case of a single variable. Extensions to several variables will not be exposed in that detail.

(v) The Fourier analysis of the Beatty sequences (section 9, revisited in section 14).

(vi) The Fourier analysis of a substantial class of Dirac combs in several variables, a class that is mapped into itself by Fourier transform (section 11). This may be considered as the key result of this paper.

(vii) Application of that result to the Fourier analysis of quasicrystals (sections 12, 13).

(viii) Indication of how symmetries of quasicrystals reflect in symmetries of their Fourier transforms (section 16).

(ix) Approximate equality of different quasicrystals and approximate almost periodicity of a single quasicrystal (section 17).

The order in which these subjects have been treated is induced by the idea that some experience with a single variable might give a better understanding in matters with many variables. This is from an analytic point of view; from an algebraic or geometric point of view one would rather not treat Beatty sequences before quasicrystals, since Beatty sequences are no obvious specializations of quasicrystals. Readers who want to get to the Fourier analysis of quasicrystals as fast as possible, might be advised to go through sections 5, 6, 7, 8, 10, 11, 12. Readers who might not at all be interested in Fourier analysis, might just read sections 10, 16 and 17, or just sections 2, 3, 4. And they might look into sections 14 and 15.

The paper will not mention topics like tilings, fitting conditions, deflation, Ammann bars, which may be important for the study of quasicrystals in general, but seem to be unnecessary for their Fourier theory.

2. BEATTY SEQUENCES

We follow the notation of [4] (although the name Beatty sequences was not used there).

If x is a real number then $\lfloor x \rfloor$ (the "floor" of x) is the largest integer $\leq x$, and $\lceil x \rceil$ (the "roof" of x) is the least integer $\geq x$.

$\mathbb{Z}$ is the set of all integers. We use notations like $\mathbb{Z}/\alpha$ to denote the set of all numbers of the form k/α where k is an integer; $\mathbb{Z}-\mathbb{Z}/\alpha$ is the set of all numbers of the form $n-m/\alpha$, where n and m are integers, etc.

The letters α and γ denote fixed real numbers, with $\alpha>1$. If $n\in\mathbb{Z}$ then $L(n)$ is defined by

$$L(n)=\gamma+n/\alpha, \tag{2.1}$$

and $p(n)$, $q(n)$ by

$$p(n)=\lceil L(n+1)\rceil-\lceil L(n)\rceil, \tag{2.2}$$

$$q(n)=\lfloor L(n+1)\rfloor-\lfloor L(n)\rfloor. \tag{2.3}$$

Since $\alpha > 1$ we have $0 < L(n+1) - L(n) < 1$, and therefore $p(n)$ and $q(n)$ take no other values than 0 and 1. We consider p and q as mappings of the set $\mathbb{Z}$ into the set $\{0, 1\}$, but they can also be called doubly infinite sequences of zeros and ones.

According to Theorem 5.3 of [4] the sequence p takes its 1's on the set $\lfloor(\mathbb{Z}-\gamma)/\alpha\rfloor$ and its 0's on $\lceil(\mathbb{Z}+\gamma)\alpha/(\alpha-1)-1\rceil$, whereas q takes its 1's on $\lceil(\mathbb{Z}-\gamma)\alpha-1\rceil$ and its zeros on $\lfloor(\mathbb{Z}+\gamma)\alpha/(\alpha-1)\rfloor$. In other words:

(2.4) $\quad p(\lfloor(m-\gamma)\alpha\rfloor) = 1, \; p(\lceil(m+\gamma)\alpha/(\alpha-1)-1\rceil) = 0,$

(2.5) $\quad q(\lceil(m-\gamma)\alpha-1\rceil) = 1, \; q(\lfloor(m+\gamma)\alpha/(\alpha-1)\rfloor) = 0,$

for all m, moreover (i) every integer n has either the form $\lfloor(m-\gamma)\alpha\rfloor$ or the form $\lceil(m+\gamma)\alpha/(\alpha-1)-1\rceil$, and (ii) every integer n has either the form $\lceil(m-\gamma)\alpha-1\rceil$ or the form $\lfloor(m+\gamma)\alpha/(\alpha-1)\rfloor$. And (since $\alpha > 1$) different m's produce different values of $\lfloor(m-\gamma)\alpha\rfloor$. The same thing can be said for the other expressions: note that also $\alpha/(\alpha-1) > 1$.

3. CASES WHERE p AND q ARE DIFFERENT (WITH α IRRATIONAL)

In most cases p and q are just the same, but let us devote some attention to the exceptions. We have $\lfloor x\rfloor = \lceil x-1\rceil$ unless x is an integer, so the exceptions stem from cases where $L(n)$ or $L(n+1)$ is an integer.

Let us first take the case where is α irrational.

If $\gamma \notin \mathbb{Z} - \mathbb{Z}/\alpha$ then we have $p(n) = q(n)$ for all integers n, so p and q are identical sequences.

If $\gamma \in \mathbb{Z} - \mathbb{Z}/\alpha$ then there is exactly one pair K, N such that $\gamma = K - N/\alpha$. In that case we have

(i) $L(n) \in \mathbb{Z}$ if and only if $n = N$. Actually $L(N) = K$.

(ii) $p(n) = q(n)$ for all integers n, except for the cases $n = N-1$ and $n = N$. There we have

(3.1) $\quad p(N-1) = 0, \; p(N) = 1, \; q(N-1) = 1, \; q(N) = 0.$

(iii) For the expressions $(m-\gamma)\alpha$ that occur in (2.4) we have: if $m \in \mathbb{Z}$ then $(m-\gamma)\alpha \in \mathbb{Z}$ if and only if $m = K$. Actually $(K-\gamma)\alpha = N$.

Likewise, in connection with (2.5), $(m+\gamma)\alpha/(\alpha-1) \in \mathbb{Z}$ if and only if $m = N-K$, and there we have $(m+\gamma)\alpha/(\alpha-1) = N$. So (2.4) and (2.5) reconfirm (3.1).

4. THE CASES WHERE α IS RATIONAL

For the sake of completeness we also discuss the case that α is rational, in spite of the fact that it will not be considered in further sections.

Let $\alpha = r/s$, $0 < s < r$, $s \in \mathbb{Z}$, $r \in \mathbb{Z}$, and assume that r and s are relatively prime. Obviously p and q are periodic mod r: $p(n) = p(n+r)$, $q(n) = q(n+r)$ for all integers n.

If $\gamma \notin \mathbb{Z}/r$ then $p(n) = q(n)$ for all integers n, so p and q are identical sequences.

If $y \in \mathbb{Z}/r$, then $y = t/r$ with some $t \in \mathbb{Z}$. We now take integers w and N such that $t = wr - Ns$, $0 \le w < s$ (this is possible since r and s are relatively prime). We note

(i) $L(n) \in \mathbb{Z}$ if and only if $n - N \in r\mathbb{Z}$ (i.e., $n \equiv N \pmod{r}$).

(ii) $p(n) = q(n)$ for all $n \in \mathbb{Z}$, except for the cases where $n \equiv N$ or $n \equiv N-1 \pmod{s}$. For all $y \in \mathbb{Z}$ we have

$$(4.1) \qquad p(N-1+ry) = 0,\ p(N+ry) = 1,\ q(N-1+ry) = 1,\ q(N+ry) = 0.$$

(iii) For the expression $(m-\gamma)\alpha$ occurring in (2.4) we note, if $m \in \mathbb{Z}$, that $(m-\gamma)\alpha \in \mathbb{Z}$ if and only if $m \in w + s\mathbb{Z}$. And if $m = w + sy$ with $y \in \mathbb{Z}$ we have $(m-\gamma)\alpha = N + yr$.

Likewise, in connection with (2.5) we note that $(m+\gamma)\alpha/(\alpha-1) \in \mathbb{Z}$ if and only if $m \in N - w + (r-s)\mathbb{Z}$. And if $m = N - w + (r-s)y$ with $y \in \mathbb{Z}$ then $(m+\gamma)\alpha/(\alpha-1) = N + yr$.

So (2.4) and (2.5) reconfirm (4.1).

5. GENERALIZED FUNCTIONS

The paper [3] elaborately treated a class of generalized functions of Gelfand-Shilov type, particularly well suited for Fourier analysis. In this section we explain the main things needed in the present note.

The basis of this theory is a set S of very smooth functions, for which all kinds of analytical operations are very easy. By algebraical operations this set is extended to a set S^*, the elements of which are called *generalized functions*. Usually such a set of generalized functions would be introduced as a kind of dual of S, by means of the inner product in S. In [3] a different point of view was taken, using "smoothing operators" N_α. Nevertheless it is possible to get the same set of generalized functions by means of dualization, but that still uses the smoothing operators (see section 6 below).

A complex analytic function f, analytic in the whole complex plane, is called *smooth* if positive numbers A, B, M exist such that

$$(5.1) \qquad |f(x+iy)| \le M \exp(-Ax^2 + By^2)$$

for all real numbers x and y. The set of all such f is called S. If $f \in S$, $g \in S$, we have the inner product

$$(5.2) \qquad (f, g) = \int_{-\infty}^{\infty} f(x)\overline{g(x)}\,dx$$

(the bar over $g(x)$ denotes complex conjugate).

If α is a positive number, the smoothing operator N_α is defined for all $f \in S$ by

$$(5.3) \qquad N_\alpha f = h, \text{ where } h(z) = \int_{-\infty}^{\infty} K_\alpha(z,t) f(t)\,dt,$$

and

$$K_\alpha(z,t) = (\sinh \alpha)^{-\frac{1}{2}} \exp(-\pi((z^2+t^2)\cosh \alpha - 2zt)/\sinh \alpha).$$

These smoothing operators have the property

(5.4) $$N_\alpha(N_\beta f) = N_{\alpha+\beta} f$$

for all positive real numbers α, β and all $f \in S$.

In S we have the Fourier transform $\mathscr{F}$, defined by $\mathscr{F}f = g$, where

$$g(z) = \int_{-\infty}^{\infty} e^{-2\pi izt} f(t)dt \text{ for all complex } z.$$

It satisfies Parseval's theorem: $(\mathscr{F}f, \mathscr{F}g) = (f, g)$ for all $f \in S$, $g \in S$. And the Fourier transform commutes with the smoothing operators: $\mathscr{F}N_\alpha f = N_\alpha \mathscr{F}f$ for all $f \in S$, $\alpha > 0$.

If in the definition of $\mathscr{F}$ we replace $-2\pi izt$ by $2\pi izt$ we get the operator $\mathscr{F}^*$. It is the inverse of $\mathscr{F}$.

We now explain the notion of generalized function. We consider a mapping F of the set of all positive numbers into S. So for every $\alpha > 0$ the value $F(\alpha)$ is a smooth function. This mapping F is taken as an element of S^* if and only if

(5.5) $$N_\alpha F(\beta) = F(\alpha + \beta)$$

for all $\alpha > 0$, $\beta > 0$.

The elements of S^* are called *generalized functions*. At first, this is confusing: we think of generalized functions as something that generalizes the idea of a (real or complex-valued) function on the real line, and the F's are defined on the positive half-line with values in S. The connection is made by means of an embedding that gives a mapping of S into S^*. If $f \in S$, then its embedding into S^* is denoted emb (f). Its values are as follows: if emb (f) is called G, then for all $\alpha > 0$ we have $G(\alpha) = N_\alpha f$. So emb (f) is not a function on the real line, but a function defined on the positives, with values in S.

If f and g are different elements of S, then emb (f) and emb (g) are different elements of S^*.

If $F \in S^*$, $f \in S$ then we can define a kind of inner product (F, f); for its definition we refer to section 18 of [3]. It has the usual linearity properties of a complex inner product. It is related to the inner product in S by means of the theorem $(\text{emb}(f), g) = (f, g)$ for all $f \in S$, $g \in S$. Moreover we mention the property that if $(F, g) = 0$ for all $g \in S$, then $F = 0$. Analogously, if $(F, g) = 0$ for all $F \in S^*$, then $g = 0$ (it suffices to specialize F to emb (g)).

We can also define (f, F), just as the complex conjugate of (F, f).

Many operators on S can be "extended" to S^* (see [3], section 19). If K is an operator on S then the operator L on S^* is called an extension of K if $L(\text{emb}(f)) = \text{emb}(K(f))$ for all $f \in S$. As an example we can extend the Fourier operator (and keep calling it $\mathscr{F}$). We mention that it keeps the inner product property $(\mathscr{F}F, \mathscr{F}f) = (F, f)$ for all $F \in S^*$, $f \in S$.

6. QUASI-BOUNDED LINEAR FUNCTIONALS

The contents of this section will not be used in further sections; the only purpose is to indicate the link with usual distribution theory.

A linear mapping L of S into the complex numbers will be called *quasi-bounded* if for every $\alpha>0$ there exists a positive number C_α such that for all $f\in S$ we have

$$|L(N_\alpha f)|\le C_\alpha (f,f)^{\frac{1}{2}}.$$

To every $F\in S^*$ there corresponds a quasi-bounded linear functional M_F, defined by

$$M_F(f)=(F,\bar{f}) \text{ for all } f\in S.$$

Conversely, every quasi-bounded linear functional M can be obtained this way (see [3], section 22).

This opens the way to describe S^* in the more usual way of distribution theory: as a set of linear functionals on a set S of "test functions". It shows that S^* is essentially the same as one of the classes defined by Gelfand and Shilov ([12], IV).

7. CONVERGENCE IN S AND S^*

In S we can work with a very strong kind of convergence. We say that a sequence $f_1, f_2, \ldots$ of elements of S is S-convergent to 0 if there are positive numbers A and B such that

$$f_n(x+iy)\exp(Ax^2-By^2)\to 0$$

uniformly for all x and y. And we say that f_n is S-convergent to f if f_n-f is S-convergent to 0. It is denoted by $f_n\xrightarrow{S} f$.

We next take a sequence $F_1, F_2, \ldots$ in S^*, and we want to say what it means that it is S^*-convergent to F (again in S^*). We remind that an element of S^* is always a mapping of the positives into S, so it makes sense to require that for given $\alpha>0$ the sequence $F_1(\alpha), F_2(\alpha), \ldots$ is S-convergent to $F(\alpha)$. If this happens for every positive α, i.e., if

$$F_n(\alpha)\xrightarrow{S} F(\alpha) \text{ for all } \alpha>0$$

then we say that F_n is S^*-convergent to F, which we shall write as

$$F_n\xrightarrow{S^*} F. \tag{7.1}$$

It is not hard to show that the limit of an S^*-convergent sequence is unique.

There is an easy criterion for establishing this kind of convergence (see Theorem 24.4 in [3]). It says that the sequence $F_1, F_2, \ldots$ is S^*-convergent if and only if for every $h\in S$ the sequence of inner products $(F_1,h),(F_2,h),\ldots$ is convergent.

We now express some material not contained in [3].

It is not hard to get to the modification that we have (7.1) if and only if (F_n,h) converges to (F,h) for every h (this is easily derived from the previous statement by considering the mixed sequence $F_1, F, F_2, F, F_3, \ldots$).

As an application we mention that if F_n is S^*-convergent to F then the sequence of its Fourier transforms $\mathscr{F}F$ is S^*-convergent to $\mathscr{F}F$. It suffices to consider $F=0$. If $h \in S$ we now have $(F_n, \mathscr{F}^*h) \to 0$, whence $(\mathscr{F}F_n, h) \to 0$ for all $h \in S$.

We shall also have to deal with the notion of *absolutely S^*-convergent series*. If $F_1, F_2, \ldots$ are generalized functions, and if for every $h \in S$ the series $(F_1, h)+$ $+(F_2, h)+\ldots$ is absolutely convergent, then there is a unique $F \in S^*$ such that $F_1+\ldots+F_n$ is S^*-convergent to F, and, moreover, in whatever order the terms of the series are rearranged, it remains S^*-convergent to F. Because of this we say that $F_1+F_2+\ldots$ is absolutely S^*-convergent, and that its sum is F.

The converse is also true: if the series is absolutely S^*-convergent then for every $h \in S$ the series $\sum (F_n, h)$ is absolutely convergent (for we know that if the convergence of a series of complex terms is unaffected by reorderings, then it converges absolutely).

If $\sum F_n$ is absolutely S^*-convergent with sum F then the series of Fourier transforms $\sum \mathscr{F}F_n$ is absolutely S^*-convergent too, with sum $\mathscr{F}F$. This easily follows from $(\mathscr{F}F, h)=(F, \mathscr{F}^*h)$.

8. DIRAC COMBS

If b is a real number, then the "Dirac delta function at b" is the element of S^* defined by

$$\delta_b(\alpha)(t)=K_\alpha(t, b)$$

for all $\alpha>0$ and all complex values of t.

For all $g \in S$ we have $(g, \delta_b)=g(b)$, which shows that our definition corresponds to the usual idea of what a delta function should be. It is proved as follows. There is a $\beta>0$ and an $h \in S$ with $g=N_\beta h)$ ([3], Theorem 10.1). Now with the above definition of $\delta_b(\alpha)$ and the definition of inner product ([3], section 18) we get $(g, \delta_b)=(h, \delta_b(\alpha))=(N_\alpha h)(b)=g(b)$.

Dirac combs can be introduced by means of absolutely convergent series of Dirac deltas, with the aid of the following theorem.

THEOREM 8.1. *Let $x_1, x_2, \ldots$ be a sequence of real numbers, and let $c_1, c_2, \ldots$ be complex numbers. Assume that for every $\varepsilon>0$*

$$\sum c_n \exp(-\varepsilon x_n^2) \tag{8.1}$$

converges absolutely. Then

$$\sum c_n \delta_{x_n} \tag{8.2}$$

is absolutely S^*-convergent.

Its sum can be called a "Dirac comb".

REMARK. The x_n do not necessarily tend to infinity, so boundedness of the c_n would not be always sufficient for (8.1).

PROOF. According to a remark at the end of section 7 it suffices to show that for every $h \in S$

(8.3) $\sum c_n(h, \delta_{x_n})$

converges absolutely. The inner product equals $h(x_n)$, and by the definition of S we have positive numbers M and A such that $|h(x)| \leq M \exp(-Ax^2)$ for all real x. Applying (8.1) with $\varepsilon = A$ we get the absolute convergence of (8.3).

In the case that $x_n = n$ for all n, the condition of Theorem 8.1 can be simplified a little. Instead of (8.1) we can just require, for every separate ε, that $c_n \exp(-\varepsilon n^2)$ is bounded.

We now show a result on some Dirac combs whose Fourier transform again looks like a Dirac comb.

THEOREM 8.2. Let $A(k)$ be complex numbers and $\sigma(k)$ be real numbers, for all $k \in \mathbb{Z}$. We put

(8.4) $$W(n, K) = \sum_{|k| \leq K} A(k) \exp(2\pi i n \sigma(k)).$$

Assume that there is a positive number M such that for all n and all positive $K \in \mathbb{Z}$

(8.5) $$|W(n, K)| \leq M$$

and that for every $n \in \mathbb{Z}$ we have a number $V(n)$ with

(8.6) $$\lim_{K \to \infty} W(n, K) = V(n).$$

Then $\sum_{n \in \mathbb{Z}} V(n)\delta_n$ is absolutely S^*-convergent. It represents an element G of S^*. The S^*-convergent series $\sum_{m \in \mathbb{Z}} \delta_{m+\sigma(k)}$ represents an element of S^* for every k. If $K \to \infty$, then

(8.7) $$\sum_{|k| \leq K} A(k)\Big(\sum_{m \in \mathbb{Z}} \delta_{m+\sigma(k)}\Big)$$

is S^*-convergent to the Fourier transform $\mathscr{F}G$ of G.

REMARK. We do not claim that the double series

$$\sum_{k \in \mathbb{Z}} \sum_{m \in \mathbb{Z}} A(k)\delta_{m+\sigma(k)}$$

is absolutely S^*-convergent. In the examples we have to deal with, $A(k)$ is of the order of $1/k$, which gives no absolute convergence.

PROOF. From (8.5) and (8.6) it follows that $|V(n)| \leq M$, so both $\sum_n W(n, K)\delta_n$ and $\sum_n V(n)\delta_n$ are absolutely S^*-convergent.

If $K \to \infty$ we have

(8.8) $$\sum_{n \in \mathbb{Z}} W(n, K)\delta_n \xrightarrow{S^*} \sum_{n \in \mathbb{Z}} V(n)\delta_n.$$

This can be shown by taking inner products with an arbitrary function $h \in S$. With some $C>0$, $\varepsilon>0$ we have $|h(n)| \leq C \exp(-\varepsilon n^2)$ for all $n \in \mathbb{Z}$, so

$$\lim_{K\to\infty} \sum_{n\in\mathbb{Z}} W(n,K)\bar{h}(n) = \sum_{n\in\mathbb{Z}} V(n)\bar{h}(n)$$

since term-wise the limit of $W(n,K)$ equals $V(n)$, and the convergence is dominated by $\sum_{n\in\mathbb{Z}} MC \exp(-\varepsilon n^2)$.

According to section 7 we can take Fourier transform on both sides of (8.8). So $\mathscr{F}G$ is the S^*-limit of

$$(8.9) \qquad \mathscr{F}\Big(\sum_{n\in\mathbb{Z}} W(n,K)\delta_n\Big).$$

The particular Dirac comb $\sum_{n\in\mathbb{Z}} \delta_n$ is its own Fourier transform. This is a reformulation of Poisson's formula (see [3] section 27.18). In a similar way, a simple transformation of Poisson's formula leads to

$$(8.10) \qquad \mathscr{F} \sum_{n\in\mathbb{Z}} \delta_{n+a} \exp(2\pi ibn) = \exp(-2\pi iab) \sum_{n\in\mathbb{Z}} \delta_{n+b} \exp(-2\pi ina)$$

(for all real a, b). We only need the case $a=0$, $b=\sigma(k)$.

Using (8.4) we now evaluate (8.9) as (8.7), which proves the theorem.

It is not hard to show that, under the assumptions of theorem 8.2, $\mathscr{F}G$ is also the S^*-limit (if $\nu\to\infty$) of

$$(8.11) \qquad \sum_{k\in\mathbb{Z}} A(k) \exp(-k^2/\nu) \sum_{m\in\mathbb{Z}} \delta_{m+\sigma(k)}.$$

For a proof we have to make an appeal to the dominated convergence of

$$\sum_{n\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} A(k) \exp(-k^2/\nu + 2\pi in\sigma(k))\bar{h}(n).$$

The convergence procedure in (8.11) is of the same type as the one we shall meet later in theorem 12.1.

9. FOURIER ANALYSIS OF DIRAC COMBS OF BEATTY SEQUENCES

We take real numbers α and γ, with $\alpha>1$, and consider the sequence p defined by (2.2). If to every n with $p(n)=1$ we attach the delta δ_n and form the sum of all of them, we get the Dirac comb of p, and for q we have a similar thing.

We shall present two methods for evaluating the Fourier transform of this Dirac comb. We restrict ourselves to irrational values of α; the rational case would be slightly more troublesome.

In the first method we take deltas for both the zeros and the ones of the sequence, and we provide the zeros with weight 0, the ones with weight 1. So the Dirac combs C_p of p and C_q of q can be expressed by

$$C_p = \sum_{n\in\mathbb{Z}} p(n)\delta_n, \quad c_q = \sum_{n\in\mathbb{Z}} q(n)\delta_n.$$

We define U as a real-valued function of a real variable by

$$U(x) = \lfloor x \rfloor - x + \tfrac{1}{2} \text{ if } x \notin \mathbb{Z}$$
$$U(x) = \quad 0 \qquad \text{if } x \in \mathbb{Z}.$$

We can express the Dirac combs of p and q in terms of U, but we have to be careful in the exceptional cases. According to section 3, the simple case is the one with $\gamma \notin \mathbb{Z} - \mathbb{Z}/\alpha$, where we have $p = q$. Here $L(n)$ (see (2.1)) is never an integer, so we can write

$$(9.1) \qquad \lfloor L(n) \rfloor = U(L(n)) + L(n) - \tfrac{1}{2}, \quad \lceil L(n) \rceil = U(L(n)) + L(n) + \tfrac{1}{2}.$$

Therefore $C_p = C_q = R$, where

$$(9.2) \qquad R = \sum_{n \in \mathbb{Z}} U\left(\gamma + \frac{1}{\alpha} + \frac{n}{\alpha}\right)\delta_n - \sum_{n \in \mathbb{Z}} U\left(\gamma + \frac{n}{\alpha}\right)\delta_n + \frac{1}{\alpha} \sum_{n \in \mathbb{Z}} \delta_n.$$

Note that by Theorem 8.1 the three series are all absolutely S^*-convergent.

In the cases where $\gamma \in \mathbb{Z} - \mathbb{Z}/\alpha$ we have $\gamma = K - N/\alpha$, with $K \in \mathbb{Z}$, $N \in \mathbb{Z}$ (see section 3). If $n = N$ we have instead of (9.1)

$$\lceil L(N) \rceil = \lfloor L(N) \rfloor = U(L(N)) + L(N),$$

whence

$$(9.3) \qquad C_p = R + \tfrac{1}{2}\delta_N - \tfrac{1}{2}\delta_{N-1},$$

$$(9.4) \qquad C_q = R - \tfrac{1}{2}\delta_N + \tfrac{1}{2}\delta_{N-1}.$$

We now turn to the question how to determine $\mathscr{F}R$. We know that $\sum_{n \in \mathbb{Z}} \delta_n$ is transformed into itself, so it suffices to evaluate $\sum U(\gamma + n/\alpha)\delta_n$ (the other term can be treated by taking $\gamma + 1/\alpha$ instead of γ).

We have for all real x

$$(9.5) \qquad U(x) = \sum_{1}^{\infty} \sin(2\pi kx)/(\pi k).$$

Let us write $B(k) = (2\pi ik)^{-1}$ $(k \neq 0)$, $B(0) = 0$. So

$$U(\gamma + n/\alpha) = \lim_{K \to \infty} \sum_{|k| \le K} B(k) \exp(2\pi ik(\gamma + n/\alpha)).$$

It is well known that the partial sums of (9.5) are uniformly bounded (for the exact bound see [23], vol 2, Abschnitt VI, nr. 25). So we can apply theorem 8.2, with the result

$$\mathscr{F} \sum_{n \in \mathbb{Z}} U(\gamma + n/\alpha)\delta_n = \lim_{K \to \infty} \sum_{|k| \le K} B(k) e^{2\pi ik\gamma} \sum_{m \in \mathbb{Z}} \delta_{m + k/\alpha},$$

where the limit has to be taken in the sense of S^*-convergence.

Using (9.2) we get the Fourier transform of R:

$$(9.6) \qquad \mathscr{F}R = \lim_{K \to \infty} \sum_{|k| \le K} c(k) \sum_{m \in \mathbb{Z}} \delta_{m + k/\alpha}$$

in the sense of S^*-convergence, with

$$c(k)=e^{2\pi i\gamma k}(e^{2\pi ik/\alpha}-1)/(2\pi ik) \text{ if } k\neq 0,$$

$$c(0)=1/\alpha.$$

The term with $c(0)$ is caused by the last one of the three series in (9.2).

We can write this in a single formula:

$$(9.7)\qquad c(k)=\int_{\gamma}^{\gamma+1/\alpha} e^{2\pi ikt}dt.$$

If $\gamma\notin\mathbb{Z}-\mathbb{Z}/\alpha$ then (9.6) presents the Fourier transform of the Dirac combs of p and q; in the exceptional case $\gamma=K-N/\alpha$ we have to add (in case of p) or subtract (in case of q) the Fourier transform of $\frac{1}{2}\delta_N-\frac{1}{2}\delta_{N-1}$, which is the function whose value at x is

$$(e^{-2\pi iNx}-e^{-2\pi i(N-1)x})/2.$$

We next explain the second method. Instead of taking the zeros and ones with coefficients 0 and 1, we now just look at the ones. According to (2.4) the n with $p(n)=1$ can be parametrized by means of $\lfloor(m-\gamma)\alpha\rfloor$, where m runs through $\mathbb{Z}$. With $x_m=\lfloor(m-\gamma)\alpha\rfloor$, $c_m=1$ the condition (8.1) is satisfied, so by Theorem 8.1 the series $\sum\delta_{x_m}$ is absolutely S^*-convergent. Its sum is the Dirac comb of p.

Similarly, the Dirac comb of q is $\sum\delta_{y_m}$ with $y_m=\lceil(m-\gamma)\alpha-1\rceil$.

These Dirac combs can also be represented as the sum of an absolutely convergent double series. We introduce functions P and Q, mapping reals to reals, by

$$P(x)=1\ (0\le x<1),\ P(x)=0\ (x\ge 1 \text{ or } x<0),$$

$$Q(x)=1\ (0<x\le 1),\ Q(x)=0\ (x>1 \text{ or } x\le 0).$$

If n is an integer, and u is a real number, the condition $\lfloor u\rfloor=n$ is equivalent to $P(u-n)=1$, and $\lfloor u\rfloor\neq n$ is equivalent to $P(u-n)=0$. Similarly, $\lceil u-1\rceil=n$ is equivalent to $Q(u-n)=1$, and $\lceil u-1\rceil\neq n$ is equivalent to $Q(u-n)=0$. So the Dirac comb of p is the sum of the absolutely S^*-convergent double series

$$(9.8)\qquad \sum_{m\in\mathbb{Z}}\sum_{n\in\mathbb{Z}} P((m-\gamma)\alpha-n)\delta_n,$$

and the one of q is the sum of

$$(9.9)\qquad \sum_{m\in\mathbb{Z}}\sum_{n\in\mathbb{Z}} Q((m-\gamma)\alpha-n)\delta_n.$$

We restrict ourselves to the case that $\gamma\notin\mathbb{Z}-\mathbb{Z}/\alpha$ (the material for dealing with the exceptional case $\gamma\in\mathbb{Z}-\mathbb{Z}/\alpha$ can be found in section 3, part (iii)). Now $(m-\gamma)\alpha-n$ is never an integer, so we can safely replace $P(x)$ and $Q(x)$ by $Y(x/\alpha)$, where

$$Y(t)=0\ (t<0 \text{ or } t>1/\alpha),$$

$$Y(t) = 1 \quad (0 < t < 1/\alpha),$$

$$Y(0) = \tfrac{1}{2}, \quad Y(1/\alpha) = \tfrac{1}{2}.$$

It is now required to find the Fourier transform of R, where

$$(9.10) \qquad R = \sum_{n \in \mathbb{Z}} \Big(\sum_{m \in \mathbb{Z}} Y(m - (\gamma + n/\alpha)) \Big) \delta_n.$$

In spite of the fact that the sum over m contains at most one non-zero term, we apply Poisson's summation formula to it. If $X = \mathscr{F}Y$ this gives

$$\sum_{m \in \mathbb{Z}} Y(m - a) = \sum_{k \in \mathbb{Z}} e^{-2\pi iak} X(k)$$

for all real values of a, so (replacing k by $-k$)

$$\sum_{m \in \mathbb{Z}} Y(m - (\gamma + n/\alpha)) = \lim_{K \to \infty} \sum_{|k| \le K} c(k) e^{2\pi ink/\alpha}$$

where $c(k)$ is given by (9.7). As in the first method, it can be remarked that the partial sums are uniformly bounded. So by Theorem 8.2 we again get to (9.6).

We note that this second method can also be treated as a special case of theorem 10.1.

10. QUASICRYSTALS PRODUCED BY MULTIGRIDS

The multigrid method was developed in [5] for the particular two-dimensional case that produces the Penrose tilings, but the method can immediately be applied to other cases. It was explained in [5] how tilings can be obtained from their dual figures, and what special forms of the dual have to be chosen in order to produce the Penrose tilings. These special duals were the "pentagrids". A pentagrid in the plane is a superposition of 5 ordinary grids (consisting of sets of equidistant lines). In the present section we shall take the number m instead of the number 5, and instead of the dimension 2 we take n; instead of the lines we take hyperplanes of dimension $n-1$.

We shall assume $0 < n < m$. The case $n = m$ can be treated in the same way, but it would be notationally inconvenient to handle both cases simultaneously.

We shall use matrix notation. By $M(a, b)$ we denote the set of all matrices with a rows and b columns. Vectors in a-space will be taken as columns, i.e., as elements of $M(a, 1)$. The set $Z(a)$ will be the set of all a-vectors with integral coordinates.

The transpose of a matrix A will be written as A^T.

We start from m real numbers $\gamma_1, \dots, \gamma_m$ and $2m$ elements $d_1, \dots, d_m$, $\upsilon_1, \dots, \upsilon_m$ in $R(n)$; the restriction will be made that the d's span $R(n)$, and that none of them is the zero vector. A condition about the υ's will be made at the end of this section (see (10.12)).

The γ's and d's lead to a multigrid in the following way. If $1 \le j \le m$, the grid Γ_j is the set of all n-vectors z such that $(d_j, z) + \gamma_j \in \mathbb{Z}$, where (d_j, z) denotes the inner product of d_j and z. The set $\{\Gamma_1, \dots, \Gamma_m\}$ is called a *multigrid*. The υ's are not involved in building the grid, they will help to pass from the grid to the crystal pattern.

In [5] the vectors $d_1, \dots, d_m$ were the 5 fifth roots of unity in the complex plane; the sum of the γ's was assumed to be zero, but we shall not make that restriction here. Moreover, in [5] the v's were equal to the corresponding d's, and here we shall not make that assumption either. (These restrictions had the effect that the duals become the Penrose patterns.)

For arbitrary $k \in Z(m)$ we define the set $E(k)$. It is the set of all $z \in R(n)$ such that for $j = 1, \dots, m$

(10.1) $\quad k_j - 1 < (d_j, z) + \gamma_j < k_j$

($k_1, \dots, k_m$ are the coordinates of the vector k). If $E(k)$ is non-empty then $E(k)$ is called a *mesh*. In this case we say that k satisfies the *mesh condition*. To any k with $E(k) \neq \emptyset$ we attach the vector

(10.2) $\quad k_1 v_1 + \cdots + k_m v_m.$

The set of all these will be called the *crystal pattern*, and will be denoted by Cp.

We have excluded the case $m = n$, but we note that if $m = n$ and $d_1, \dots, d_m$ are linearly independent, we have $E(k) \neq \emptyset$ for all k, and Cp becomes a simple periodic structure. So our Fourier analysis of sections 11 and 12 may be modified to include the case of ordinary crystals.

Following [5], section 8, we phrase the mesh condition $E(k) \neq \emptyset$ by saying that z and $\lambda_1, \dots, \lambda_m$ exist with $0 < \lambda_1 < 1, \dots, 0 < \lambda_m < 1$ such that

(10.3) $\quad (d_j, z) + \gamma_j + \lambda_j = k_j \quad (j = 1, \dots, m).$

Let us express this in matrix notation. The column with entries γ_j is written as the vector γ ($\in R(m)$), and similarly we build the vector λ. The set of all vectors $\lambda \in R(m)$ with $0 < \lambda_1 < 1, \dots, 0 < \lambda_m < 1$ will be denoted $Cu(m)$ (Cu is mnemonic for "cube"). And $D \in M(m, n)$ will be the matrix whose rows are $d_1^T, \dots, d_m^T$. Similarly, $V \in M(m, n)$ will be the matrix with rows $v_1^T, \dots, v_m^T$.

Now the mesh condition $E(k) \neq \emptyset$ can be expressed as the existence of $z \in R(n)$ and $\lambda \in Cu(m)$ such that

(10.4) $\quad Dz + \gamma + \lambda = k.$

In this matrix notation, Cp is the set of all vectors

(10.5) $\quad V^T k$ with $k \in Z(m), E(k) \neq \emptyset.$

We form a Dirac comb by attaching a delta to every k with $E(k) \neq \emptyset$:

(10.6) $$\sum_{k \in Z(m) | E(k) \neq \emptyset} \delta_{V^T k}.$$

It is intended as a generalized function of n variables, but the convergence of the series has still to be investigated.

Expressing this in terms of this Dirac comb has the advantage that it covers the cases where sometimes different vectors k lead to one and the same vector (10.2); in such cases we should define Cp as a multiset rather than as a set. We shall see an example of this in section 14.

We shall transform (10.6) by means of (10.4) in the way used in [5], section 8. We take a matrix $W \in M(m, m-n)$ with the property that W has rank $m-n$ and $W^T D = 0$. Since D has rank n (the vectors $d_1, \dots, d_m$ were assumed to span $R(n)$), the columns of D and W span subspaces of dimension n and $m-n$, respectively, and these subspaces are each others orthogonal complement.

If q is any vector in $R(m)$ we have: there exists $z \in R(n)$ with $Dz = q$ if and only if $W^T q = 0$. Both conditions express that q lies in the space spanned by the columns of D.

According to (10.4) we can now say that, for any $k \in Z(m)$, we have $E(k) \neq \emptyset$ if and only if there exists a $\lambda \in Cu(m)$ such that

$$(10.7) \quad W^T(k - \lambda - \gamma) = 0.$$

In order to see this, we have to note that, for all $x \in R(m)$, the condition $W^T x = 0$ in equivalent to the existence of $z \in R(n)$ with $Dz = x$.

Let us define the set $P(W, \gamma)$. It is the subset of $R(m-n)$ consisting of all vectors of the form $W^T(\lambda + \gamma)$, where λ runs through $Cu(m)$:

$$(10.8) \quad P(W, \gamma) = \{ W^T(\lambda + \gamma) | \lambda \in Cu(m) \} \subset R(m-n).$$

Since W has rank $m-n$, it is easy to show that $P(W, \gamma)$ does not fall in any hyperplane with dimension less than $m-n$. Therefore $P(W, \gamma)$ is the interior of a polytope. The closure of $P(W, \gamma)$ is the convex hull of the set of points $W^T(\mu + \gamma)$, where μ runs through the set of 2^m vertices of the cube $Cu(m)$.

By means of (10.7) we conclude that the mesh condition $E(k) \neq \emptyset$ is equivalent to $W^T k \in P(W, \gamma)$.

We denote the characteristic function of $P(W, \gamma)$ by ϱ, so

$$(10.9) \quad \varrho(x) = 1 \text{ if } x \in P(W, \gamma),\ \varrho(x) = 0 \text{ otherwise.}$$

Now we have

$$(10.10) \quad \varrho(W^T k) = 1 \text{ if } E(k) \neq \emptyset,\ \varrho(W^T k) = 0 \text{ otherwise.}$$

It follows that (10.6) can be written as

$$(10.11) \quad \sum_{k \in Z(m)} \varrho(W^T k) \delta_{V^T k}.$$

This presents the Dirac comb of a quasicrystal in a form that enables us to evaluate the Fourier transform.

A word may be added here about the role of W. There is a certain amount of arbitrariness in it: W had just to satisfy $W^T D = 0$, and had to have rank $m-n$. So $P(W, \gamma)$ does not depend on D and γ only: it definitely depends on the particular choice of W. But the condition $W^T k \in P(W, \gamma)$ depends on D and γ only, since it is equivalent to $E(k) \neq \emptyset$.

We have not formulated a condition on V yet. If V has rank less than n, then the vectors $v_1, \ldots, v_m$ are linearly dependent, and the whole crystal pattern would belong to a lower dimensional subspace of $R(n)$. We of course want to exclude that, but we shall even impose the stronger condition that the matrix $V^T D$ ($\in M(m,m)$) is non-singular:

(10.12) rank $(V^T D) = n$.

This obviously guarantees that $v_1, \ldots, v_m$ span $R(n)$ as well as that $d_1, \ldots, d_m$ span $R(n)$.

Let us build the matrix N ($\in M(m,m)$) by taking as its first n columns the n columns of V, and as its last $m-n$ columns the $m-n$ columns of W. From (10.12) we can derive that N is non-singular:

(10.13) rank $(N) = m$.

A way to prove this, and to see what liberty we have with W, is to transform D in standard form by means of non-singular matrices A ($\in M(m,m)$) and B ($\in M(n,n)$):

$$D = A\begin{pmatrix} I \\ 0 \end{pmatrix} B,$$

where $I \in M(n,n)$, $0 \in M(m-n,n)$. Now

$$A^T V = \begin{pmatrix} K_{11} \\ K_{21} \end{pmatrix}, \quad A^T W = \begin{pmatrix} K_{12} \\ K_{22} \end{pmatrix}, \quad A^T N = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}$$

with $K_{11} \in M(n,n)$, $K_{12} \in M(n,m-n)$, $K_{21} \in M(m-n,n)$, $K_{22} \in M(m-n,m-n)$. From $D^T W = 0$ we get $K_{12} = 0$, and now (10.12) gives rank $(K_{11}) = n$. Since we required that rank $(W) = m-n$, we have rank $(K_{22}) = m-n$. Therefore rank $(A^T N) = m$, and (10.13) follows.

The significance of condition (10.12) is that it guarantees that the quasicrystal more or less fills the space $R(n)$:

THEOREM 10.1. If (10.12) holds then there is a positive number r such that in $R(n)$ every sphere with radius r contains at least one point of the quasicrystal Cp.

PROOF. We denote the norm of any vector z by $|z|$ (both in $R(m)$ and in $R(n)$).

If $k \in R(m)$ and $z \in E(k)$ (which implies that k satisfies the mesh condition) then the point $V^T k$ of the quasicrystal satisfies (according to (10.4))

(10.14) $|V^T Dz - V^T k| \leq s$,

if s is the supremum of the set of all numbers $V^T(\lambda + \gamma)$ with $\lambda \in Cu(m)$.

Now take any $r > s$. Consider any sphere with radius r; let y be its center. Since $V^T D$ is non-singular, there is an $x \in R(m)$ with $V^T Dx = y$. This x may accidently fall on a grid hyperplane, but we can find a point z which lies inside a mesh such that $|V^T D(z-x)| < r-s$. If $k \in R(m)$ is such that $z \in E(k)$, we have $|y - V^T k| < r$ by (10.14). This proves the theorem.

THEOREM 10.2. If (10.12) does not hold then Cp lies between two parallel hyperplanes in $R(n)$.

PROOF. Assuming rank $(V^TD)<n$, all points V^TDz fall in some hyperplane of dimension $n-1$, so by (10.14) all points of Cp have a distance at most s to that hyperplane.

11. SOME SPECIAL DIRAC COMBS IN HIGHER DIMENSIONAL SPACES

As in section 10, m and n are integers, $0<n<m$. The cases $n=0$ and $n=m$ might be admitted too, but that would give notational inconveniences. The results for these cases will be mentioned at the end of this section.

We take matrices $V\in M(m,n)$, $W\in M(m,m-n)$. The matrix $N\in M(m,m)$ is built by taking as its first n columns the n columns of V, and as its last $m-n$ columns the columns of W.

We require that N is non-singular. So the V, W, N of section 10 would satisfy these conditions. The matrix D will not appear in the present section.

If p is any positive number then S^p is the set of all smooth functions of p variables (see [3] section 7). We shall write such functions as functions of a variable in $R(p)$.

The analog of S^* for the case of p variables will be written as S^{p*} (see [3] section 21).

The notion of S^*-convergence is extended to the higher dimensional cases in the obvious way, and Theorem 8.1 is extended to this case if we replace $\exp(-\varepsilon x^2)$ by $\exp(-\varepsilon x^Tx)$.

We are now ready to prove the following theorem:

THEOREM 11.1. If m, n, W, V are as described above, and if $f\in S^{m-n}$, then

$$(11.1)\qquad \sum_{k\in Z(m)} f(W^Tk)\delta_{V^Tk}$$

is absolutely S^*-convergent and represents an element of S^{n*}. If g is the Fourier transform of f ($g=\mathscr{F}f$), then the Fourier transform of the generalized function (11.1) is again the sum of an absolutely S^*-convergent delta series, viz.

$$(11.2)\qquad |\det(N)|^{-1}\sum_{k\in Z(m)} g(-U^Tk)\delta_{R^Tk},$$

where R and U are derived from the matrix N^{-T} (N^{-T} is the inverse of N^T) in the same way as V and W are obtained from N. In other words, R is the matrix whose first n columns are the columns of N^{-T}, and U's columns are the last $m-n$ columns of N^{-T}. And $|\det N|$ is the absolute value of the determinant of N.

PROOF. The absolute S^*-convergence of (11.1) is shown by means of the m-dimensional analogue of Theorem 8.1. We have to show the convergence of

$$(11.3)\qquad \sum_{k\in Z(m)} |f(W^Tk)|\exp(-\varepsilon k^TVV^Tk).$$

Since f is smooth, we have, with some δ and some C

$$|f(W^Tk)| < C \exp(-\delta k^T W W^T k).$$

From the fact that N is non-singular we easily derive that $VV^T + WW^T$ is positive definite, so there is an $\eta > 0$ such that $k^T(VV^T + WW^T)k \geq \eta k^T k$ for all $k \in R(m)$. This shows the absolute S^*-convergence of (11.3).

Since the Fourier transform of a smooth function is smooth again, the series (11.2) is absolutely S^*-convergent too.

Let us denote (11.1) by F and (11.2) by G; both F and G are in S^{n*}. We have to show

(11.4) $\mathscr{F}F = G.$

This can be done by showing that

(11.5) $(h, F) = (\mathscr{F}h, G)$

for all $h \in S^n$. Both sides can be written as sums over $k \in Z(m)$:

$$(h, F) = \sum_{k \in Z(m)} h(V^T k) \bar{f}(W^T k),$$

and if $\mathscr{F}h$ is denoted by j:

$$(j, G) = |\det(N)|^{-1} \sum_{k \in Z(m)} j(R^T k) \bar{g}(-U^T k).$$

Now (11.5) can be obtained by application of the Poisson summation formula. We put, for $x \in R(m)$,

(11.6) $\varphi(x) = h(V^T x) \bar{f}(W^T x),$

(11.7) $\psi(x) = |\det(N)|^{-1} j(R^T x) \bar{g}(-U^T x),$

and will show

(11.8) (i) $\varphi \in S^m, \quad \psi \in S^m,$

(11.9) (ii) if $\chi = \mathscr{F}\varphi$ then $\psi = \chi$.

Then application of Poisson's formula

$$\sum_{k \in Z(m)} \varphi(k) = \sum_{k \in Z(m)} \psi(k)$$

will finish the proof of (11.4).

In order to show $\varphi \in S^m$ we have to prove an inequality

(11.10) $|\varphi(x+iy)| \leq C \exp(-Ax^T x + By^T y)$

for all $x, y \in R(m)$. As h and f are smooth, we have with some C, A, B

$$|h(V^T(x+iy))| \leq C \exp(-Ax^T VV^T x + By^T VV^T y),$$

$$|f(W^T(x+iy))| \leq C \exp(-Ax^T WW^T x + By^T WW^T y).$$

Since $VV^T + WW^T$ is positive definite, we get to (11.10) (with new values of C, A, B). This settles (11.9), since we can give the same proof for ψ.

Finally (11.9) is a matter of change of variables in an m-fold integral. We have for $u \in R(m)$

$$\chi(u) = \int h(V^T x)\bar{f}(W^T x) e(-u^T x) dx$$

where the integral is taken over $R(m)$, with abbreviation

$$\exp(2\pi i t) = e(t).$$

It will be convenient to use projection operators onto n-dimensional and $(m-n)$-dimensional subspaces, with matrices

$$P = \begin{pmatrix} I \\ 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 \\ I \end{pmatrix}.$$

In the first formula, I is the unit matrix in $M(n, n)$, 0 is the zero matrix in $M(m-n, n)$; in the second formula 0 is the zero matrix in $M(m-n, m-n)$ and I is the unit matrix in $M(m-n, m-n)$. Obviously

(11.11) $V = NP, \quad W = NQ.$

We now change coordinates by $N^T x = y$:

$$\chi(u) = |\det(N)|^{-1} \int h(P^T y)\bar{f}(Q^T y) e(-u^T N^{-T} y) dy.$$

Putting $P^T y = y_1$, $Q^T y = y_2$ and noting

$$u^T N^{-T} y = u^T N^{-T}(PP^T + QQ^T) y = u^T N^{-T} P y_1 + u^T N^{-T} Q y_2$$

we can write the integral as a product of two, both of Fourier type. We find

$$\chi(u) = |\det(N)|^{-1} j(P^T N^{-1} u)\bar{g}(-Q^T N^{-1} u).$$

Just like (11.11) we have

(11.12) $R = N^{-T} P, \quad U = N^{-T} Q$

whence

$$P^T N^{-1} u = R^T u, \quad Q^T N^{-1} u = U^T u.$$

So by (11.7) we now have established (11.9). This finishes the proof of the theorem.

We obtain an extension of Theorem 11.1 by straightforward application of the same method; we just mention the result:

THEOREM 11.2. Let m, n, W, V, R, U, N, f, g be as in theorem 11.1, and let $p \in R(m)$, $q \in R(m)$. Then the series

(11.13) $\sum_{k \in Z(m)} e(-q^T k) f(W^T(k+p)) \delta_{V^T(k+p)}$

is absolutely S^*-convergent, and it Fourier transform is

$$(11.14)\quad |\det(N)|^{-1} \sum_{k\in Z(m)} e(-(k-q)^T p) g(-U^T(k-q))\delta_{R^T(k-q)}.$$

We also mention to what this theorem degenerates in the cases $n=0$ and $n=m$. In the case $n=m$ we get that the Fourier transform of

$$(11.15)\quad \sum_{k\in Z(m)} e(-q^T k)\delta_{N^T(k+p)}$$

equals

$$(11.16)\quad |\det(N)|^{-1} \sum_{k\in Z(m)} e(-(k-q)^T p)\delta_{N^{-1}(k-q)}.$$

This can be considered as the formula that covers the case of ordinary (periodic) crystals.

The case $n=0$ just leads to a form of Poisson's formula for m variables:

$$(11.17)\quad \begin{cases} \sum_{k\in Z(m)} e(-q^T k) f(N^T(k+p)) = \\ = |\det(N)|^{-1} \sum_{k\in Z(m)} e(-(k-q)^T p) g(-N^{-1}(k-q)). \end{cases}$$

12. APPLICATION TO THE FOURIER TRANSFORM OF A QUASICRYSTAL

The theorems of section 11 cannot be applied directly to the Fourier transform of (10.11), since the ϱ in (10.11) is by no means smooth: it is the characteristic function of a polytope $P(W,\gamma)$, and therefore not even continuous.

We can deal with (10.11) by considering it as the limit of an S^*-convergent sequence of smooth functions of the type (11.1) with smooth f's. For these f's we can take smoothings of ϱ, by means of the smoothing operators of (5.3). If ν is a positive integer, we take

$$(12.1)\quad f_\nu = N_{1/\nu}\varrho.$$

It is not hard to show that $f_\nu(x)\to\varrho(x)$ for every x, possibly except for the boundary points of the polytope. And the convergence is dominated in the following sense: there are positive constants C and A such that

$$(12.2)\quad |f_\nu(x)| \le C\exp(-Ax^T x)$$

for all $x\in R(n)$ and for all positive integers ν.

Before going on, we have to say something about the exceptional cases. There will be a strong analogy with the exceptional cases $\gamma\in\mathbb{Z}-\mathbb{Z}/\alpha$ in section 9.

Let us say that the vector γ is singular if there exists a $k\in Z(m)$ such that $W^T k$ falls on the boundary of $P(W,\gamma)$. If γ is not singular it is called regular. We note that regularity of γ is a matter of γ and D (cf. the remark at the end of section 11).

In section 9 we treated the exceptional cases in detail, but here we avoid all difficulties by just assuming that γ is regular. Not much is excepted that way, for in the sense of Lebesgue measure we can say that almost all γ are regular.

In the particular case treated in [5] (with $m=5$, $n=2$) we were able to show that this condition is equivalent to the regularity of the pentagrid. (For the case of general m and n we might say that the multigrid is singular if there is a point lying on more than n grid hyperplanes).

So from now on we assume that γ is regular. Consequently, we have $f_\nu(W^Tk) \to f(W^TK)$ for all $k \in Z(m)$. By means of (12.2) we can now handle the S^*-convergence of F_ν to F, where

$$F_\nu = \sum_{k \in Z(m)} f_\nu(W^Tk)\delta_{V^Tk}$$

and F is the generalized function described by (10.11).

We claim that $F_\nu \xrightarrow{S^*} F$. To this end we have to show that, for any $h \in S^n$, the inner product (F_ν, h) converges to (F, h) in the ordinary sense. This is a matter of dominated convergence. If $\nu \to \infty$, every term of the series for (F_ν, h) converges to the corresponding term of the series for (F, h), and the terms are dominated by

$$(12.3) \quad C \exp(-AW^Tkk^TW)|h(V^Tk)|.$$

If we sum (12.3) over all $k \in Z(m)$, we can show that we get a convergent series of non-negative numbers; the method for this was explained for the case of (11.10).

As $F_\nu \xrightarrow{S^*} F$, we also have for the Fourier transforms $\mathscr{F}F_\nu \xrightarrow{S^*} \mathscr{F}F$. And each $\mathscr{F}F_\nu$ is of the form (11.2). For all ν, the series for $\mathscr{F}F_\nu$ has the deltas at the same places, but we cannot claim that $\mathscr{F}F$ is the sum of an absolutely S^*-convergent series (like the one for F). And there is, in general, no dominated convergence like we had with $F_\nu \xrightarrow{S^*} F$.

In this respect there is a close analogy with the case of (9.6). In (9.6) the S^*-convergence looks simpler: just by means of expanding partial sums. For the present case such a thing is not attempted. In section 8 it was shown that the convergence by partial sums implies the one by means of smoothing operators (see (8.11)). The latter kind of convergency may be slightly weaker, but it is probably quite adequate for most applications.

We note that the coefficients of the series for $\mathscr{F}F_\nu$ are easily described. In (11.2) we have to work with g_ν instead of with g, where

$$g_\nu = \mathscr{F}f_\nu = \mathscr{F}N_{1/\nu}f = N_{1/\nu}\mathscr{F}f.$$

The discontinuous function f is a generalized function anyway, and so is its Fourier transform $\mathscr{F}f$. And we have $N_{1/\nu}\mathscr{F}f \xrightarrow{S^*} \mathscr{F}f$ if $\nu \to \infty$.

Let us now phrase the result as a theorem:

THEOREM 12.1. If $0<n<m$, and γ is regular, then the Fourier transform of the Dirac comb (10.6) of the pattern Cp (see (10.2)) is the limit of the S^*-convergent sequence $F_1, F_2, \ldots$, where F_ν is the sum of the absolutely

S^*-convergent series

$$(12.4)\qquad |\det(N)|^{-1} \sum_{k\in Z(m)} g_\nu(-U^T k)\delta_{R^T k},$$

with the notation of theorem 11.1, and $g_\nu = N_{1/\nu}\mathscr{F}\varrho$, where ϱ is the characteristic function of the polytope $P(W, \gamma)$ in $R(m-n)$ (see (10.8), (10.9)).

13. A GENERALIZATION

The limit procedure explained in section 12 involved approximation of the characteristic function of a polytope by smooth functions. The particular polytope was $P(W, \gamma)$, obtained in a particular way from a multigrid. But we might consider polytopes in general. The generalization we get, means that we have a theorem of the form of theorem 11.1 (or of theorem 11.2), with f replaced by the characteristic function ϱ of some polytope P in $R(m-n)$, and g replaced by the Fourier transform of that ϱ. In the latter case ((11.2) or (11.14)) we have to take the limit of g_ν, where $g_\nu = N_{1/\nu}\mathscr{F}\varrho$.

We need not exclude the cases where $W^T k$ falls on the boundary for some $k \in Z(m)$, if we just replace ϱ by the *adapted characteristic function* ω.

This ω is defined as follows:

$$(13.1)\qquad \omega(x) = \lim_{r\to 0} \mathrm{vol}(\mathrm{Sph}(x, r)\cap P)/\mathrm{vol}(\mathrm{Sph}(x, r)).$$

Here $\mathrm{Sph}(x, r)$ is the interior of a sphere with center x and radius r, and "vol" stands for volume. Roughly speaking, $\omega(x)$ expresses what percentage of the volume around x belongs to the polytope P. In the exterior and in the interior of P we just have $\omega(x) = \varrho(x)$.

For example, if P is a cube in 3-space, then $\omega(x) = \frac{1}{2}$ on the faces, $\frac{1}{4}$ on the edges, and $\frac{1}{8}$ on the vertices.

14. APPLICATION TO BEATTY SEQUENCES

Let us take $m=2$, $n=1$, and apply section 13, where P is the interval on the real line with end-points γ and $\gamma+1/\alpha$. (γ and α are real parameters). The adapted characteristic function ω satisfies

$$\omega(x) = 1\ (\gamma < x < \gamma + 1/\alpha),$$

$$\omega(\gamma) = \omega(\gamma + 1/\alpha) = \tfrac{1}{2},$$

$$\omega(x) = 0 \text{ otherwise.}$$

Furthermore we take

$$V = \begin{pmatrix}1\\0\end{pmatrix},\quad W = \begin{pmatrix}-1/\alpha\\1\end{pmatrix},\quad R = \begin{pmatrix}1\\1/\alpha\end{pmatrix},\quad U = \begin{pmatrix}0\\1\end{pmatrix},$$

so $\det(N) = 1$. The series (11.1) (with f replaced by ω) turns into

$$(14.1)\qquad \sum_{h\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} \omega(k - h/\alpha)\delta_h.$$

Let us restrict ourselves to the case that $\alpha>1$ and $\gamma\notin\mathbb{Z}-\mathbb{Z}/\alpha$. So $k-h/\alpha$ lies never on the boundary of P. For any given h, the number of k with $\omega(k-h/\alpha)=1$ is easily seen to be equal to $\lceil\gamma+(h+1)/\alpha\rceil-\lceil\gamma+h/\alpha\rceil$. So according to (2.2) the series (14.1) represents $\sum p(h)\delta_h$.

Its Fourier transform is evaluated by specializing (12.4). We note that the Fourier transform of our characteristic function ω satisfies $(\mathscr{F}\omega)(-k)=c(k)$ (see (9.7)), so the Fourier transform of $\sum p(h)\delta_h$ is the limit of

$$(14.2)\qquad \sum_{k\in\mathbb{Z}}\ \sum_{h\in\mathbb{Z}} (N_{1/v}\mathscr{F}\omega)(-k)\delta_{h+k/\alpha}.$$

The only difference with (9.6) lies in the convergence procedure. Instead of $K\to\infty$ for the cut-off point of the sum we now have the smoothing index $1/v$ tending to zero, like in (8.11).

15. ONE-DIMENSIONAL QUASICRYSTALS

We get one-dimensional quasicrystals if in section 10 we take $n=1$. We can admit any $m>1$, but here we shall just take $m=2$.

We take numbers $\alpha>1$, δ, v_1, v_2 and

$$D=\begin{pmatrix}1\\1/\alpha\end{pmatrix},\quad \gamma=\begin{pmatrix}0\\\delta\end{pmatrix},\quad V=\begin{pmatrix}v_1\\v_2\end{pmatrix}.$$

The multigrid consists of two grids: $\mathbb{Z}$ and $\alpha\mathbb{Z}-\alpha\delta$. We assume that these two grids have no point in common. The multigrid is the union:

$$Cp=\mathbb{Z}\cup\alpha(\mathbb{Z}-\delta).$$

Let us investigate the meshes. Every mesh is indexed by a vector k with $E(k)\neq\emptyset$ (section 10). This k is a column with entries k_1, k_2 (both integers). There are two kinds of meshes, according to whether the right end-point lies in $\mathbb{Z}$ or in $\alpha(\mathbb{Z}-\delta)$.

(i) If the right end-point is in $\mathbb{Z}$ then that end-point is k_1, and the next point of $\alpha(\mathbb{Z}-\delta)$ to its right is $\alpha(k_2-\delta)$. Hence

$$(15.1)\qquad \alpha(k_2-1-\delta)<k_1<\alpha(k_2-\delta).$$

(ii) If the right end-point is in $\alpha(\mathbb{Z}-\delta)$ then that end-point is $\alpha(k_2-\delta)$, and the next point of $\mathbb{Z}$ to its right is k_1. Hence

$$(15.2)\qquad k_1-1<\alpha(k_2-\delta)<k_1.$$

In both cases we deduce

$$(15.3)\qquad \alpha(k_2-\delta)-\alpha<k_1<\alpha(k_2-\delta)+1.$$

We note that k_1+k_2 increases by 1 if we pass from a mesh to the next one. So if we put $k_1+k_2-1=x$ then every x occurs just once. Eliminating k_2 from (15.3) we get

$$k_1=\lceil(x-\delta)\alpha/(\alpha+1)\rceil,\quad k_2=x+1-k_1.$$

Now we know all vectors that satisfy the mesh condition, and we can build the Dirac comb of the quasicrystal:

(15.4) $\sum_{x\in\mathbb{Z}} \delta_{v_1 k_1 + v_2 k_2}.$

Let us now specialize v_1 and v_2. First we show what happens if rank $(V^T D) < 1$. Taking $v_1 = 1$, $v_2 = -\alpha$ we get

$$v_1 k_1 + v_2 k_2 = (1+\alpha)(\lceil (x-\delta)\alpha/(\alpha+1)\rceil - (x+1)\alpha/(\alpha+1)),$$

and this is bounded. This is a special case of theorem 10.2.

Next we take $v_1 = 1$, $v_2 = 0$. For any $y \in \mathbb{Z}$, the number of $x \in \mathbb{Z}$ with $\lceil a(x-\delta)/(\alpha+1)\rceil = y$ equals

$$\lfloor y(\alpha+1)/\alpha + \delta \rfloor - \lfloor (y-1)(\alpha+1)/\alpha + \delta \rfloor$$

and this is $1 + q(y)$, where

$$q(y) = \lfloor y/\alpha + \delta \rfloor - \lfloor (y-1)/\alpha + \delta \rfloor.$$

So the Dirac comb of the quasicrystal equals

(15.5) $\sum_{y\in\mathbb{Z}} \delta_y + \sum_{y\in\mathbb{Z}} q(y)\delta_y,$

and here the second term is the Dirac comb of the Beatty sequence q.

Next we take a general $v_2 \in \mathbb{Z}$, $v_2 \neq 0$ and $v_1 = v_2 + 1$. Then

$$v_1 k_1 + v_2 k_2 = \lceil \beta x - \lambda \rceil,$$

where $\beta = v_2 + \alpha/(\alpha+1)$, $\lambda = -v_2 + \delta\alpha/(\alpha+1)$. If $v_2 > 0$ we have $\beta > 1$, and $\lceil \beta x - \lambda \rceil$ runs through the set of all integers z where the Beatty sequence

$$\lfloor (\lambda + z)/\beta \rfloor - \lfloor (\lambda + z - 1)/\beta \rfloor \quad (z \in \mathbb{Z})$$

takes the value 1 (see [4], theorem 5.3). It follows that the Dirac comb of the quasicrystal is just the Dirac comb of that Beatty sequence.

By suitable choice of v_2 and α we can get every Beatty sequence this way.

The positive values of v_2 take care of the intervals (1,3/2), (2,5/2), (3,7/2),... for β. In the case that $v_2 < 0$ we rather take $-x$ as the parameter running through $\mathbb{Z}$, and $\beta = -v_2 - \alpha/(\alpha+1)$. This covers the intervals (3/2,2), (5/2,3)..... The missing points (multiples of 1/2) need not be considered for a Beatty sequence, since they are not irrational.

16. QUASICRYSTAL SYMMETRY

We shall devote some attention to the question how symmetries of a quasicrystal reflect in symmetries of the Fourier transform.

First we change our notation: instead of the vector γ we shall use the vector θ:

(16.1) $\theta = \gamma + \xi$, where $\xi^T = (\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2})$.

In order to study symmetry, we introduce some transformations.

If h is some positive integer, if $A \in R(h,h)$, and f is a real-valued function on $R(h)$, then $\Phi_A f$ is the function defined by

(16.2) $\quad (\Phi_A f)(x) = f(Ax) \quad (x \in R(h)).$

From now on we assume that A is non-singular.

If S is a subset of $R(h)$, and χ_S is its characteristic function, then we note that

(16.3) $\quad \Phi_A \chi_S = \chi_{A^{-1}S}$

($A^{-1}S$ is the set of all $A^{-1}x$ with $x \in S$).

If $v \in R(h)$ then the delta function at v transforms like this:

(16.4) $\quad |\det(A)| \cdot \Phi_A \delta_v = \delta_{A^{-1}v}.$

As to the Fourier operator $\mathscr{F}$ (on S^h) we note that

(16.5) $\quad \Phi_{A^{-T}} \mathscr{F} = |\det(A)| \mathscr{F} \Phi_A.$

We now first study the meshes of section 10. The mesh determined by the vector $k \in Z(m)$ can be denoted by $E(k, D, \theta)$: it is the set of all $z \in R(n)$ for which $\mu \in Du(m)$ exists with $Dz + \theta + \mu = k$. Here $Du(m)$ is the set $Cu(m) - \xi$, which is symmetric with respect to the origin.

Let the matrix $A \in M(m,m)$ now be a *signed permutation*: it is non-singular, and in every row it has just one non-zero entry, which is always either 1 or -1. This A leaves $Du(m)$ invariant as well as $Z(m)$. We easily obtain, if $e \in M(n,n)$ is non-singular,

(16.6) $\quad E(k, D, \theta) = eE(Ak, ADe, A\theta).$

For the characteristic function ϱ of (10.9) we write $\varrho_{W,\theta}$. If $A \in M(m,m)$ is a signed permutation we have

(16.7) $\quad \varrho_{W,\theta} = \varrho_{A^T W, A^{-1}\theta},$

and for any non-singular $c \in M(m-n, m-n)$

(16.8) $\quad \Phi_c \varrho_{W,\theta} = \varrho_{Wc^{-T},\theta}.$

We also indicate what happens to V, W, N, R, U under transformation. Let $A \in M(m,m)$, $b \in M(n,n)$, $c \in M(m-n, m-n)$, all non-singular. Let V_1, W_1, N_1, R_1, U_1 be given by

$$V_1 = AVb, \quad W_1 = AWc, \quad N_1 = AN\begin{pmatrix} b & 0 \\ 0 & c \end{pmatrix},$$

$$R_1 = A^{-T} R b^{-T}, \quad U_1 = A^{-T} U c^{-T}.$$

Then we have the same situation all over again: V_1 and W_1 together form N_1, and likewise R_1 and U_1 together form N_1^{-T}.

Let us now list some transformations of the sum (11.1). We denote it by $\Delta(f, V, W)$:

(16.9) $\quad \Delta(f, V, W) = \sum_{k \in Z(m)} f(W^T k) \delta_{V^T k}.$

If $H \in M(m,m)$ is non-singular with integer elements, it leaves $Z(m)$ invariant, and we have

$$(16.10) \quad \Delta(f, HV, HW) = \Delta(f, V, W).$$

If $b \in M(n,n)$, $c \in M(m-n, m-n)$ are non-singular, then

$$(16.11) \quad |\det(b)| \cdot \Delta(f, Vb, Wc) = \Phi_{b^{-T}} \Delta(\Phi_{c^T} f, V, W).$$

Theorem 11.1 can be written as

$$(16.12) \quad \mathscr{F}\Delta(f, V, W) = |\det(N)|^{-1} \Delta(\mathscr{F}f, R, -U).$$

Finally we express the fact that (10.6) equals (10.11):

$$(16.13) \quad \sum_{k \in Z(m) | E(k, D, \theta) \neq \emptyset} \delta_{V^T k} = \Delta(\varrho_{W,\theta}, V, W).$$

In stylized form (not bothering about the kind of convergence) we express (12.4) as

$$(16.14) \quad \mathscr{F}\Delta(\varrho_{W,\theta}, V, W) = |\det(N)|^{-1} \Delta(\mathscr{F}\varrho_{W,\theta}, R, -U).$$

We are now fully equipped for the study of quasicrystal symmetry. The word symmetry can be taken in a wide sense: sometimes there is no symmetry in the sum but just in the set of deltas. The series on the right of (16.14) contains deltas at the elements of the set $R^T Z(m)$, i.e., the set of all $R^T k$ with $k \in Z(m)$. This set can be called the *spectrum* of the quasicrystal pattern.

As an example of the study of symmetry we present

THEOREM 16.1. If $A \in M(m,m)$ is a signed permutation, if $b \in M(n,n)$, $e \in M(n,n)$ are both non-singular, and if D and V satisfy

$$(16.15) \quad D = ADe, \quad V = AVb$$

then the spectrum $R^T Z(m)$ satisfies

$$(16.16) \quad b(R^T Z(m)) = R^T Z(m).$$

The proof is a direct consequence of the material above. We remark that $A = A^{-T}$ since signed permutations are always orthogonal. We can also prove (16.16) directly; just some matrix calculus shows that $bR^T = R^T A$ (the matrix A need not be a signed permutation for this; orthogonality suffices).

The examples that first come to mind are those with $V = D$, $e = b$, b orthogonal. For the "icosahedral case" we take $m = 6$, $n = 3$; $v_1, \ldots, v_6$ are unit vectors along the 6 main diagonals of an icosahedron. And b is an orthogonal matrix that leaves the icosahedron invariant, inducing a signed permutation among the v's; The result is that the spectrum is invariant under the icosahedral group.

17. APPROXIMATE EQUALITY AND APPROXIMATE ALMOST PERIODICITY OF QUASICRYSTALS

We recollect from section 10 that n, m, D, V, γ define a multigrid as well as a crystal pattern, and that to any k with $k \in Z(m)$ there corresponds a mesh of the multigrid (i.e., $E(k) \neq \emptyset$) if and only if $z \in R(m)$ exists such that $k - Dz - \gamma$ lies in the cube $Cu(m)$. The point of the crystal pattern corresponding to such a vector k is $V^T k$. The crystal pattern will be denoted by $Cp(\gamma)$.

To every mesh $E(k)$ we can associate a positive number, to be called the *tolerance* of the mesh. The mesh is the set of all $z \in R(n)$ that satisfy (10.1) for all j, and the tolerance is the largest number η such that there still exists a $z \in R(n)$ with

(17.1) $\quad k_j - 1 + \eta \leq (d_j, z) + \gamma_j \leq k_j - \eta$

for all j.

We can also speak of the tolerance of a point of the crystal pattern: it is just the tolerance of the mesh it originates from.

Throughout this section we shall assume that the multigrid is non-singular, i.e., that nowhere more than n grid hyperplanes pass through a point. Singular grids require a little more care (there we have to apply "infinitesimally small" distortions of the multigrid (see [5], section 12)).

Crystals patterns with different values of γ can sometimes be approximately equal. This can be based on the following theorem of Kronecker (see J.F. Koksma [15], p. 83):

THEOREM 17.1. Let n and m be positive integers, let $D \in M(m, n)$ and $\beta \in R(m)$. Then the following conditions (i) and (ii) are equivalent:

(i) For every positive ε there exists a vector $u \in R(n)$ and a vector $p \in Z(m)$ such that $|Du - \beta - p| < \varepsilon$.

(ii) Every $h \in Z(m)$ with $h^T D = 0$ satisfying $h^T \beta \in \mathbb{Z}$.

Assuming that β satisfies (ii), and considering two different vectors γ and γ', with $\gamma' = \gamma + \beta$, we shall show that the crystal patterns $Cp(\gamma)$ and $Cp(\gamma')$ are in a certain sense approximately equal.

Let k indicate a point of $Cp(\gamma)$, and let η be its tolerance. Then we can take any ε with $0 < \varepsilon < \eta$, and u, p according to (i). Taking z according to (17.1) we obtain that $k - Dz - \gamma - v \in Cu(m)$ for every vector v with $|v| < \eta$. With $v = Du - \beta - p$ we infer that $(k+p) - D(z+u) - \gamma' \in Cu(m)$. It follows that in the multigrid with parameter γ' the mesh $E(k+p)$ is non-empty (actually its tolerance is at least $\eta - \varepsilon$). This means that by the shift $V^T p$ the crystal pattern $Cp(\gamma)$ turns into $Cp(\gamma')$ as far as the points in $Cp(\gamma)$ with tolerance $> \varepsilon$ are concerned.

If we have any finite portion of $Cp(\gamma)$, we can take ε less than all tolerances in that portion. Choosing p accordingly, we find that after a shift $V^T p$ this whole portion occurs in $Cp(\gamma')$. It is in this sense that we say that $Cp(\gamma)$ and $Cp(\gamma')$ are approximately equal.

Sometimes (ii) holds for all β, and then we can say that all $Cp(\gamma)$'s are approximately equal to $Cp(0)$. But this is roughly speaking: it forgets about the little singularity troubles.

Let us take a few examples. First we take the pentagrid case of [5], where $n=2$, $m=5$. The vectors $d_1, \dots, d_5$ are five unit vectors forming a regular 5-star. Now the only possibilities for $h \in Z(5)$ with $h^T D = 0$ are the multiples of the vector with all its entries equal to 1. Kronecker's theorem now shows that if γ satisfies $\gamma_1 + \cdots \gamma_5 \in \mathbb{Z}$ then $Cp(\gamma)$ is approximately equal to $Cp(0)$.

In our next example, we take $n=3$, $m=4$, and the vectors $w_1, \dots, w_4$ are the unit vectors leading from the center of a regular tetrahedron to the four vertices. Again it is easy to check that the only vectors $h \in Z(4)$ with $h^T W = 0$ are the multiples of the vector with all its entries equal to 1. So the answer is as in the previous example: $\gamma_1 + \cdots + \gamma_4 \in \mathbb{Z}$ guarantees approximate equality of all $Cp(\gamma)$'s.

In the icosahedral case we have $n=3$, $m=6$, and the vectors w_j are taken in the directions of the six main diagonals of an icosahedron. It is not hard to check that now the only vector $p \in Z(6)$ with $p^T W = 0$ is the zero vector, and therefore all $Cp(\gamma)$'s are approximately equal.

We used the Kronecker theorem in order to compare quasicrystals with different values of γ. Another matter is the fact that all quasicrystals show a certain kind of self-repetition which we shall refer to as approximate almost periodicity. It is based on the following theorem.

THEOREM 17.2. *If $\varepsilon > 0$ and if $Q(\varepsilon, D)$ is the set of all $z \in R(n)$ such that the distance of Dz to the set $Z(m)$ is less than ε, then $Q(\varepsilon, D)$ is relatively dense in $R(n)$, which means that there exists a number $r > 0$ such that for every $c \in R(n)$ there is a point $z_0 \in Q(\varepsilon, D)$ with $|z_0 - c| < r$.*

PROOF. The theorem follows at once from the fact that

$$\sum_{1 \le j \le m} \cos\,(2\pi(d_j, z))$$

is a uniformly almost periodic function of z.

For the theory of uniformly almost periodic functions of a vector variable we refer to Besicovitch [2] ch. 1,12.

In [6] there is an alternative proof of this theorem (and of some generalizations) independent of the theory of almost periodic functions.

We shall apply theorem 17.2 to quasicrystals. We take $1 \le n < m$, D and V as in section 10 (with (10.12)), and we consider the multigrid as well as the crystal pattern they generate (see (10.2)). In order to facilitate the discussion, we still assume that nowhere more than n grid hyperplanes pass through a point.

We take any number $\varepsilon > 0$, and fix r according to theorem 17.2. Next we take

$c \in R(n)$ arbitrary, and we take $z_0 \in Q(\varepsilon, D)$ with $|z_0 - c| < r$. By the definition of $Q(\varepsilon, D)$ we can find $x_0 \in Z(m)$ with $|Dz_0 - x_0| < \varepsilon$. We shall now show that, in a certain weak sense, $V^T x_0$ is a kind of period of the crystal pattern.

Let $k \in Z(m)$ satisfy the mesh condition $E(k) \neq \emptyset$, and let η be the tolerance of the mesh $E(k)$. Assume that $\eta > \varepsilon$. We can take z such that $k - Dz - \gamma - - \upsilon \in Cu(m)$ for all υ with $|\upsilon| < \eta$. Putting $k' = k + x_0$, we claim that k' again satisfies the mesh condition, and that its tolerance is at least $\eta - \varepsilon$. That mesh contains the point $z + z_0$, and with $\upsilon = Dz_0 - x_0$ we easily see that $k' - D(z + z_0) - - \gamma \in Cu(m)$.

If $k \in Z(m)$ satisfies the mesh condition, then $V^T k$ is the corresponding point. Assuming that it has tolerance η, and $\eta > \varepsilon$, the point $V^T(k + x_0)$ again belongs to the crystal pattern, and its tolerance is at least $\eta - \varepsilon$. So $V^T x_0$ is a kind of period: if a point of the crystal pattern has tolerance $> \eta$ then a shift over $V^T x_0$ leads to another point of the crystal pattern.

If we take any finite subset of the crystal pattern, we can take ε less than all tolerances of the points of that subset. If z_0, x_0 are chosen as above, then our $V^T x_0$ produces a new finite subset of the crystal pattern, congruent to the old one.

It is easy to see that, for given $\varepsilon > 0$, the set of all $V^T x_0$ is relatively dense. We have $|Dz_0 - x_0| < \varepsilon$, so $V^T Dz_0 - V^T x_0$ is bounded. The $V^T Dz_0$'s are relatively dense, since the z_0's are relatively dense, and $V^T D$ is non-singular. Therefore the Vx's are relatively dense. It is because of this that we call the quasicrystal approximately almost periodic.

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