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WHICH DISTRIBUTIONS OF MATTER DIFFRACT ? AN INITIAL INVESTIGATION

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Abstract - We report on a preliminary investigation of the connections between quasiperiodic tilings, algebraic number theory, and cut-and-project sets. We substantially answer the question "which 1-dimensional tilings obtained by inflation rules are quasiperiodic" by showing that in general the characteristic equation of the inflation rule should have one root of absolute value greater than one and the rest of absolute value less than one. We also show that the vertices of such a tiling are contained in a cut-and-project set.

INTRODUCTION

The discovery of first one alloy [1] and then several others (see this volume) which are nonperiodic and yet sufficiently ordered to "diffract" -- i.e. show spots in their diffraction patterns -- raises many questions. One direction of research is to understand in as much detail as possible the structure of these alloys and why they form. Another is to predict what other such diffraction patterns may form. At one extreme of the latter direction lies the purely mathematical question of determining which distributions of matter diffract. This paper represents a preliminary investigation of that question, restricting itself to the question of which one-dimensional distributions of the form

$$\rho(x) = \sum_k \delta(x - x_k)$$

have their Fourier transforms of the form

$$\hat{\rho}(\xi) = \sum_{\lambda \in \Lambda} a_\lambda \delta(\xi - \lambda) + g(\xi),$$

where δ denotes the Dirac delta, $g(\xi)$ is some function (possibly 0), and Λ is a set which is not contained in the integral multiples of any single frequency (that is, there is no λ such that $\Lambda = \lambda\mathbb{Z}$). We further require that the points $\{x_k\}$ be generated by an inflation rule. (As was observed at least as early as [2] and has recently been emphasized by Bak [3], every density ρ which has a formal expression as

$$\rho(x) = \sum_{\lambda \in \Lambda} m_\lambda e^{2\pi i x \lambda},$$

where Λ is some finitely generated $\mathbb{Z}$ -module, is the slice by a line of a periodic "density" in a higher dimensional space, and conversely every periodic density in a higher dimensional space gives rise to lower dimensional quasiperiodic densities. This expansion is purely formal and ignores questions of convergence -- questions which are quite relevant, as noted below. We consider only densities which result from inflation rules primarily because that has been a major framework of discussion for quasicrystals.)

We find that the nature of the substitution rule, rather than the relative sizes of the tiles whose distribution it specifies, is what is important: the characteristic polynomial of the rule must in general have just one root greater than 1 in absolute value.

We have recently become aware of the work of Yves Meyer [4,5] who looked at similar questions from a somewhat different point of view. He identified several important facts, among them the importance of models (sets resulting from the cut-and-project technique), of algebraic numbers in conjunction with models, and of questions of convergence (for example, if one requires $\hat{\rho}$ to be a locally finite measure, then Λ must be contained in ξZ for some ξ). See also [6].

A preliminary version of this paper was the subject of an exposé at the Special Session on Quasicrystals at the October 1985 Amherst meeting of the American Mathematical Society, and a more complete version will appear in [7].

AN EXAMPLE: THE FIBONACCI QUASICRYSTAL

Define a tiling of R by means of points

$$x_k = k + (\tau - 1) [k/\tau], \quad k \in Z$$

where $\tau = (1 + \sqrt{5})/2$ is the "golden mean" and satisfies the quadratic equation

$$\tau^2 = \tau + 1$$

and $[.]$ denotes the greatest integer function. Since $x_{k+1} - x_k$ equals either 1 or τ , the $\{x_k\}$ are the vertices of a tiling using tiles of size 1 and τ . We put unit masses at the points $\{x_k\}$ to obtain the density

$$\rho(x) = \sum_k \delta(x - x_k).$$

This tiling can be obtained by the cut-and-project method by using the line $\{(t, z): z \in R\}$ in R^2 and the strip formed by translating the unit square along the line, and its Fourier transform (formally $\hat{\rho}(\xi) = \sum_k e^{2\pi i \xi x_k}$) can be computed via this construction. It is of the form

$$\hat{\rho}(\xi) = \sum_{\lambda \in \Lambda} a_\lambda \delta(\xi - \lambda),$$

and Λ consists of the points $(n - m/\tau)/p$, where $p = 2 - 1/\tau$ and m and n are integers.

Suppose we have an alphabet with two letters a and b . Let T be the substitution

$$Ta = ab, \quad Tb = a.$$

Let $C_n = T^n a$. Thus

$$C_0 = a, \quad C_1 = ab, \quad C_2 = aba, \quad C_3 = abaab, \quad \dots$$

and in general $C_{n+1} = C_n C_{n-1}$. Let a be a tile (interval) of length τ and b a tile of length 1. Then the Fibonacci tiling is obtained as $\lim_{n \rightarrow \infty} C_n$ by choosing the origin appropriately.

ANOTHER INFLATION RULE WHICH PRODUCES QUASIPERIODICITY

The preceding example leads to the study of inflation rules obtained by starting with a finite alphabet A and a mapping $T: A \rightarrow W(A)$, the words (of finite length) in A . One is interested in $T^n w$, as $n \rightarrow \infty$, for w a word in A .

We present an argument for a special inflation rule on an alphabet with three letters a, b, c which shows that the largest root of the associated characteristic equation being a Pisot-Vijayaraghavan (P-V) number is sufficient for the tiling to be of the type we are seeking.

Define T by $Ta = aac$, $Tb = ac$, $Tc = b$. Write $C_n = T^n a$, so that

$$C_0 = a$$

$$C_1 = aac$$

$$C_2 = aacaacb$$

$$C_3 = aacaacbaacaacb$$

and in general $C_{n+1} = C_n^2 (C_{n-2}^{-1} C_{n-1})$. (The last formula could be found by writing a , b , and c in terms of C_0 , C_1 , and C_2 , then writing C_3 in terms of C_0 , C_1 , C_2 and using induction.) The associated characteristic equation is

$$x^3 = 2x^2 + 1 + x;$$

it is also the characteristic equation of the matrix of T , which is

$$\begin{pmatrix} 2 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Let c_n be the number of letters in C_n , and let

$u_1(k)$ = the number of occurrences of a in the first k letters of C_n (for $c_n \geq k$)

$u_2(k)$ = the number of occurrences of b in the same k letters

$u_3(k)$ = the number of occurrences of c in the same k letters.

Note that

$$u_1(c_{n+1}) = 2u_1(c_n) + u_1(c_{n-2}),$$

$$u_1(k) = u_1(c_n) + u_1(k - c_n) \quad \text{if } c_n \leq k \leq 2c_n$$

$$u_1(k) = 2u_1(c_n) - u_1(c_{n-2}) + u_1(k - 2c_n + c_{n-2}) \quad \text{if } 2c_n < k < c_{n+1};$$

the same holds for u_2 and u_3 . (These formulas will be used to compute the recurrence relation for f_n below.)

We let l_1 be the length of a tile corresponding to a , l_2 the length of a tile corresponding to b , and l_3 the length of a tile corresponding to c . Then we deal with $\rho(x) = \sum_k \delta(x - x_k)$ where

$$x_k = l_1 u_1(k) + l_2 u_2(k) + l_3 u_3(k), \quad k = 0, 1, 2, \dots$$

(To obtain a quasiperiodic sequence that goes to infinity in both directions, one can translate C_n by C_{n-1} . Then within any finite region the limit of the sequence to the right of the origin is the same as before, while there are two different limits to the left, one from using only odd n and one from using only even n .)

If $\hat{\rho}$ has an atomic part at ξ_0 then

$$\Psi_N(\xi) = \sum_{k=0}^{N-1} e^{2\pi i \xi x_k}$$

should have $\Psi_N(\xi_0)/N$ approach a nonzero constant as N goes to infinity. So the question is for which ξ the limit as $N \rightarrow \infty$ of $\Psi_N(\xi)/N$ exists and is nonzero.

Abbreviate $t_n = x_{c_n}$ and $f_n = \Psi_{c_n}(\xi)$. Note that

$$t_n = l_1 u_1(c_n) + l_2 u_2(c_n) + l_3 u_3(c_n)$$

and

$$t_{n+1} = 2t_n \cdot t_{n-2} + t_{n-1}.$$

One computes

$$\begin{aligned} f_{n+1} - f_n &= \sum_{k=c_n}^{c_{n+1}-1} e^{2\pi i \xi x_k} \\ &= e^{2\pi i \xi x_{c_n}} + \dots + e^{2\pi i \xi (x_{c_n} + x_{c_{n-1}})} \\ &\quad + e^{2\pi i \xi (2x_{c_n} - x_{c_{n-2}} + x_{c_{n-2}})} + \dots + e^{2\pi i \xi (2x_{c_n} - x_{c_{n-2}} + x_{c_{n-1}-1})} \\ &= e^{2\pi i \xi t_n} (e^{2\pi i \xi x_0} + \dots + e^{2\pi i \xi x_{c_{n-1}}} \\ &\quad + e^{2\pi i \xi (2t_n - t_{n-2})} (e^{2\pi i \xi x_{c_{n-2}}} + \dots + e^{2\pi i \xi x_{c_{n-1}-1}})). \end{aligned}$$

Therefore f_n satisfies

$$f_{n+1} = (1 + e^{2\pi i t_n \xi}) f_n + e^{2\pi i (2t_n - t_{n-2}) \xi} (f_{n-1} - f_{n-2}).$$

Suppose that $\lim_{n \rightarrow \infty} f_n/c_n$ exists and is not 0 for some ξ . Then divide the above recurrence relation for f_{n+1} by c_{n+1} and take the limit as $n \rightarrow \infty$. The common (nonzero)

values of $\lim_{n \rightarrow \infty} f_{n+1}/c_{n+1} = \lim_{n \rightarrow \infty} f_n/c_n$ etc. can be cancelled, leaving that $\sigma = \lim_{n \rightarrow \infty} e^{2\pi i t_n \xi}$ exists and satisfies

$$1 = (1 + \sigma) \lim_{n \rightarrow \infty} c_n/c_{n+1} + (\sigma^2/\sigma) (\lim_{n \rightarrow \infty} c_{n-1}/c_{n+1} - \lim_{n \rightarrow \infty} c_{n-2}/c_{n+1}).$$

Since also

$$1 = 2 c_n/c_{n+1} + c_{n-1}/c_{n+1} - c_{n-2}/c_{n+1}$$

for every integer n greater than 1, we have $\sigma = 1$. That is,

$$(*) \quad \lim_{n \rightarrow \infty} e^{2\pi i t_n \xi} = 1$$

at every ξ for which $\lim_{n \rightarrow \infty} f_n/c_n \neq 0$.

So the question becomes whether the solution of the linear recurrence

$$t_{n+1} = 2t_n \cdot t_{n-2} + t_{n-1}$$

can satisfy (*) for some ξ and if so, for which ξ 's.

Let $\theta_1, \theta_2, \theta_3$ be the roots of the characteristic equation

$$x^3 - 2x^2 - x + 1 = 0,$$

with $|\theta_1| > |\theta_2| > |\theta_3|$. Note that for $i = 1, 2, 3$,

$$\theta_i^{n+1} = 2\theta_i^n - \theta_i^{n-2} + \theta_i^{n-1},$$

so that t_n and θ_i^n satisfy the same linear recurrence relation for each $i = 1, 2, 3$, and any solution $\{t_n\}$ to the recurrence relation can be written as a linear combination of the θ_i^n . Since θ_1 is the only root of the characteristic equation which has absolute value greater than 1, $t_n - \tau\theta_1^n$ tends to 0 exponentially as $n \rightarrow \infty$ for some τ , and this means that for (*) to hold we need

$$(**) \quad \langle \xi \tau \theta_1^n \rangle \rightarrow 0$$

exponentially as $n \rightarrow \infty$ (here $\langle \cdot \rangle$ denotes the signed distance to the nearest integer -- i.e. $\langle x \rangle = \{x\}$ if $\{x\} < 1/2$ and $\langle x \rangle = \{x\} - 1$ if $1/2 \leq \{x\} < 1$). A theorem of Thue (refined by Pisot) [8] states that if (**) occurs then $\xi\tau \in Q(\theta_1)$ and $\text{trace}(\xi\tau\theta_1^\nu)$ is an integer for $\nu = 0, 1, \dots, \deg \theta_1$. In particular,

$$\xi\tau \in (1/\sqrt{\Delta}) \mathbb{Z}[\theta_1]$$

where Δ is the discriminant of $Q(\theta_1)$ ($\Delta = ((\theta_1 - \theta_2)(\theta_2 - \theta_3)(\theta_1 - \theta_3))^2$; here $\Delta = 49$).

We have only considered here the limit of Ψ_N when N is restricted to the sequence $\{c_n\}$, and one may ask what further restrictions occur if we deal with general N . One can prove that there are no further restrictions, but the argument is somewhat more complicated (as one has to use the various recurrence relationships for the $u_1(k)$, etc. according to the value of k).

This proves that the atomic part of the Fourier transform of a measure originating from the inflation rule T given initially in this section is carried by the set

$$(1/7\tau) \mathbb{Z}[\theta_1]$$

where θ_1 is the largest root of $x^3 - 2x^2 - x + 1 = 0$; in fact this set can be characterized as the set Λ of ξ 's such that $\langle \xi \tau \theta_1^n \rangle \rightarrow 0$ for a suitable $\tau \in Q(\theta_1)$. It is clear that Λ is an additive group which is of rank 3. See Figure 1.

GENERAL INFLATION RULES

Similar considerations apply for general inflation rules. What is crucial is that the formulas for the number of times each letter appears in the tiling are related to the characteristic equation for the matrix of the transformation, with the sum of the exponents of C_1 being the coefficient of the corresponding power of x in the characteristic equation. This can always be done, though the formulas may be very complicated.

We assume we have a quasicrystal which is generated by a substitution rule. We have now r tiles with lengths $l_1, \dots, l_r$ and corresponding counting functions $u_1(k), \dots, u_r(k)$. Let

$$p(x) \equiv x^r - (a_1 x^{r-1} + \dots + a_r)$$

be the characteristic equation of the inflation rule. We assume that there is a unique largest root θ_1 and that no roots have absolute value 1. We define s by

$$|\theta_1| > |\theta_2| \geq \dots \geq |\theta_s| > 1 > |\theta_{s+1}| \geq \dots \geq |\theta_r|.$$

If C_n is the n^{th} iterate of the inflation rule applied to a single tile, then the location of the corresponding end-point is

$$t_n = l_1 u_1(c_n) + \dots + l_r u_r(c_n),$$

with c_n being the length of C_n .

Now the main point is that, as in the preceding section, the recurrence relations for the c_n and f_n imply that if ξ is in Λ then $\langle \xi t_n \rangle \rightarrow 0$ as $n \rightarrow \infty$. We analyze the condition $\langle \xi t_n \rangle \rightarrow 0$ in a manner similar to that of [8], Chapter VIII, p. 133. The details are contained in [7]. The net result is that one can write

$$t_n = \tau_1 \theta_1^n + \dots + \tau_r \theta_r^n$$

for all integers $n \geq 0$ and some $(\tau_i; i = 1, \dots, r)$; if $s = 1$, we find that as in the previous example $\xi \tau_1$ belongs to a certain $\mathbb{Z}$ -module of rank r . Moreover, if $a_r = \pm 1$, then θ_1 is a unit and

$$\xi \tau_1 \in (1/p'(\theta_1)) \mathbb{Z}[\theta_1],$$

which is an important restriction on the set of frequencies. On the other hand, if $s \geq 2$ there are further non-trivial severe restrictions on ξ . We illustrate this with the case $r = 3$, $s = 2$; this case is fairly typical of what occurs in general.

Assume that $\xi^* \neq 0$ and ξ are in the atomic part Λ of the Fourier spectrum. Our analysis implies in particular that there exist rational numbers b_0, b_1, b_2 such that

$$\xi/\xi^* = b_0 + b_1 \theta_1 + b_2 \theta_1^2 = b_0 + b_1 \theta_2 + b_2 \theta_2^2.$$

Suppose that ξ/ξ^* were not rational; then either b_1 or b_2 would be nonzero. But the above set of equalities implies (by factoring out $\theta_1 - \theta_2 \neq 0$) that

$$b_1 + b_2(\theta_1 + \theta_2) = 0.$$

Thus $\theta_1 + \theta_2$ would also have to be rational. Since $\theta_1 + \theta_2 + \theta_3 = a_1$ is an integer, θ_3 would have to be rational.

If θ_3 is not rational (the usual occurrence), then either ξ/ξ^* must always be rational, or the hypothesis that there is a nonzero element of Λ is invalid. The latter case in general occurs unless the relative tile sizes obey a specific relationship in accordance with our analysis. Both cases imply that Λ is contained in the set of integral multiples of single frequency, contrary to our stated aim.

In general, the above argument implies that if there are points $\xi^* \neq 0$ and ξ in Λ then

$$\xi/\xi^* \in Q(\theta_1) \cap \dots \cap Q(\theta_s);$$

quite often we can check that $Q(\theta_1) \cap \dots \cap Q(\theta_s) \neq Q(\theta_1)$. For if $Q(\theta_1) = Q(\theta_2)$ and if $p(x)$ is irreducible then θ_2 is a rational function of θ_1 , and this implies non-trivial conditions on $p(x)$. In particular, if $p(x)$ is irreducible, of prime degree, and is not Galois and if Λ is not contained in $\xi' \mathbb{Z}$ for any ξ' , then we must have $s = 1$ (that is, θ_1 is a P-V number).

AN INFLATION RULE WHICH DOES NOT PRODUCE QUASIPERIODICITY

Let $r = 3$ and let the inflation rule be

$$Ta = aaaaab, \quad Tb = bbbbc, \quad Tc = a.$$

Then $T^{n+1}a = C_{n+1} = C_n^5 (C_{n-1}^{-5} C_n)^4 C_{n-2}$, and the fundamental recurrence relation is

$$c_{n+1} = 9c_n - 20c_{n-1} + c_{n-2}.$$

The recurrence relation for f_n is

$$f_{n+1} = (1 + e^x + e^{2x} + e^{3x} + e^{4x})f_n + e^{5x-5y}(1 + e^{x-5y} + e^{2(x-5y)} + e^{3(x-5y)})(f_n - (1 + e^y + e^{2y} + e^{3y} + e^{4y})f_{n-1}) + e^{9x-20y}f_{n-2},$$

where $2\pi i f_n$ is abbreviated by x and $2\pi i f_{n-1}$ is abbreviated by y . The matrix of T is

$$\begin{pmatrix} 5 & 1 & 0 \\ 0 & 4 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

and its characteristic equation is

$$x^3 - 9x^2 + 20x - 1 = 0.$$

The roots of the characteristic equation are irrational and are approximately 5.166, 3.7828, and .05117. Therefore by the preceding section the purely atomic part of the spectrum of ρ is contained in the integral multiples of a single frequency. Whether or not there is more than just 0 in Λ depends on the tile sizes. Note that if the spectrum were a purely atomic measure, ρ would be periodic, which is clearly not the case. Therefore there must be a diffuse spectrum as well. An approximation to the atomic part of the Fourier transform for different tile sizes is given in Figs. 2 and 3.

INFLATION RULES, P-V NUMBERS, AND CUT-AND-PROJECT SETS

We assume here that we have a given inflation rule, and that the characteristic equation for this inflation rule has one root of absolute value greater than one and the others of absolute value less than one. We show that if the tile sizes are chosen properly (not just the trivial case of all tile sizes the same!) then there is a cut-and-project set containing the points $\{x_k\}$, where the notation is as before. We illustrate the argument by considering the cubic case again.

We have

$$x_k = l_1 u_1(k) + l_2 u_2(k) + l_3 u_3(k).$$

If these points are to be contained in the projection onto the line E of $Z^3 \cap S$ for a strip $S = I \times E'$, where I is a square of side length $2K$ and E' is to be chosen, we need

$$(1) \quad -K \leq r_1 u_1(k) + r_2 u_2(k) + r_3 u_3(k) < K$$

$$(2) \quad -K \leq r_1 u_1(k) + r_2 u_2(k) + r_3 u_3(k) < K$$

where

$$\begin{pmatrix} l_1 & l_2 & l_3 \\ r_1 & r_2 & r_3 \\ s_1 & s_2 & s_3 \end{pmatrix}$$

is the matrix of the linear transformation of R^3 which takes E to the first coordinate axis and I to the space orthogonal to the first coordinate axis. We might as well require that the transformation take the unit vectors directing E and the sides of I to unit vectors. There are then six conditions on the nine entries of the matrix.

Since the $u_1(k)$, $u_2(k)$, and $u_3(k)$ obey the same linear recurrence relation as the roots θ_1 , θ_2 , and θ_3 of the characteristic equation, there exist $\{\rho_i, \sigma_i, \tau_i; i = 1, 2, 3\}$ so that

$$u_1(c_n) = \rho_1 \theta_1^n + \rho_2 \theta_2^n + \rho_3 \theta_3^n$$

$$u_2(c_n) = \sigma_1 \theta_1^n + \sigma_2 \theta_2^n + \sigma_3 \theta_3^n$$

$$u_3(c_n) = \tau_1 \theta_1^n + \tau_2 \theta_2^n + \tau_3 \theta_3^n;$$

we can explicitly compute the $\{\rho_i, \sigma_i, \tau_i\}$ from the recurrence relation and the initial conditions, using Cramer's rule. Since $|\theta_1| > 1$ and the other two roots are less than one in absolute value, the above inequalities require

$$(3) \quad r_1 \rho_1 + r_2 \sigma_1 + r_3 \tau_1 = 0$$

$$(4) \quad s_1 \rho_1 + s_2 \sigma_1 + s_3 \tau_1 = 0.$$

We thus have two additional conditions on the matrix of the transformation.

The conditions (3) and (4) are imposed by considering only the cases $k = c_n$. For the general case, let $L(k)$ be the length of $r_1 u_1(k) + r_2 u_2(k) + r_3 u_3(k)$. Then (3) implies that $L(c_n)$ is bounded by $\delta |\theta_2|^n$ for some constant δ . The recurrence relations for $u_1(k)$, $c_n < k \leq c_{n+1}$, imply that

$$L(k) \leq (2 + |\theta_2|^{-2}) \delta |\theta_2|^n + L(k')$$

for some $k' \leq c_n$. (The quantity in parentheses is for the specific cubic equation $x^3 = 2x^2 + x - 1$; a similar expression will hold for other cubics.) The resulting geometric series bounding $L(k)$ converges since $|\theta_2| < 1$. A similar argument holds for the length of the expression in (2). Thus there are no further restrictions: provided (3) - (4) hold, (1) - (2) will hold for a K which bounds the sums of the geometric series.

Thus such a matrix always exists.

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Figure 1. The atomic part of the Fourier transform is shown for a tiling with characteristic equation $x^3 = 2x^2 - x + 1$. The tile sizes used are the entries of the eigenvector for θ_1 , in order to mimic the simplest cut-and-project method. The values of $|f_n|/c_n$ are plotted for $n=10$ (which is sufficient since using the recurrence relations enables one to sum over many terms efficiently) at the 27 points $\xi = n_0 + n_1\theta_1 + n_2\theta_1^2$, where $|n_i| \leq 1$ for $i = 0,1,2$. The vertical axis is magnified by 10 and then chopped at 1. Note that the mass is nonzero at each ξ plotted, and Λ is of rank 3.

Figure 2. All is as in Fig. 1, except that the tiling has characteristic equation $x^3 = 9x^2 - 20x + 1$ and the vertical axis is magnified by a factor of 100 and then chopped at height 1. The tile sizes do not satisfy the constraints for Λ to be of rank 1 and as a result Λ is of rank 0 (there is just a one-pixel tick at each $\xi \neq 0$ plotted).

Figure 3. (a) Here the tile sizes are $l_1 = \theta_1 + \theta_2$, $l_2 = \theta_1^2 + \theta_2^2 - 5(\theta_1 + \theta_2)$, $l_3 = 2$; otherwise all is as in Fig. 2. These tile sizes are chosen in accordance with the analysis of the text, so that Λ can be of the largest possible rank, namely 1. Note that only when $n_1 = n_2 = 0$ is there a nonzero delta function at ξ .

(b) To show that the set carrying the atomic part of $\hat{\rho}$ is indeed of rank 1, $|f_n|/c_n$ is plotted at the integers $\xi = n_0$ for $-9 \leq n_0 \leq 10$. The central three peaks are the same as the three peaks in Fig. 2(a), but with a dilated x-axis and magnification only 10.