Mathematical Quasicrystals with Toric Internal Spaces, Diffraction and Rarefaction

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Abstract

Aperiodic crystals viewed as Delone sets of points on the real line, having an average lattice, are studied as congruence model λ-sets (physical space is Euclidean and the equivalent of the internal space is toric) in the context of cut-and-congruence λ-schemes, a new concept. When windows are finite point sets, the fractal rates of occupancy, at infinity, of the affine lattices associated with such Delone sets are shown to be simply related to the scaling exponents of the Fourier transform of the autocorrelation measure, completing results of Hof. These fractal rates of occupancy are named rarefaction laws. The case of the Thue-Morse quasicrystal, as a Meyer set, is explicitly developed. We present the arithmetics of 3-rarefaction phenomenon, the fractality of the Fourier transform of the autocorrelation measure. This new approach provides explicit formulae for singular continuous peaks and allows to discuss their possible extinction. In particular, this gives a possible sieve among Delone sets to be crystals in the new definition of a *crystal* by the IUCr in 1992. Ponctual scaling laws and the Bombieri-Taylor argument are considered.

1. Introduction

Two basic objects are naturally and commonly called by the modelling of quasicrystals: cut-and-project schemes and model sets, formed from them with suitable choices of windows and parameters. These objects work fairly well and beautifully for many quasicrystal structures. Comparison to experimental data in real and Fourier spaces is often good, and a large part of the positions of the atomic sites in the structure is provided [1]. It is assumed that window boundaries are of Lebesgue measure zero, for instance when windows are a finite union of polytopes in the internal space obeying a finite symmetry group G which leaves also the spectrum invariant. This condition on window boundaries suffices to know that the spectra of model sets are only pure point [2]. With respect to the definition of what is a *crystal* nowadays [3], we obtain, by using such model sets, *crystals*, that is coloured Delone sets for which no singular continuous or absolutely continuous component exist in their Fourier spectrum. However, there exist various classes of Delone sets which are more general than model sets, so-called mathematical quasicrystals [4], [5], [6], generically named in an general attempt to cover

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the field of aperiodic crystals. In section 2, we recall briefly these notions. Just above the class of model sets is the class of Meyer sets [5], [6]. A Meyer set is already not necessarily a *crystal*.

There is a lack of criteria for saying that a Delone set is deprived of diffuse (continuous) measures in its spectrum. Of course, it is a formidable task to find such criteria, if any [7], [8]. This objective seems unreachable at present. In this contribution, which is a summary of [9], given Λ a Delone set on the real line, we show that scaling exponents of the diffracting intensity at $k = 2\pi/\lambda$ arise from rarefaction laws at infinity on the affine lattices of period λ which intersect Λ, under some assumptions. The concept of *rarefaction law* is a new one [9]. In other words, we provide a geometrical origin to the scaling behaviour of the diffracting intensity. This is quite surprising and lead to study arithmetically such rarefaction laws. When rarefactions laws are combined over all these affine lattices of period λ, it is possible to discuss the existence of only δ-peaks in the spectrum of Λ as it will be shown. Therefore, the present results shed a new light on the existence of such criteria, giving an answer to the Bombieri-Taylor argument. In section 3, we recall cut and congruence λ-schemes and congruence model λ-sets introduced in [9] in the context of toric spaces (which play the role of internal spaces in the classical cut-and-project schemes). In section 4, we provide some new results concerning the spectrum of the Thue-Morse quasicrystal from p-rarefaction laws, as an example of a Meyer set.

2. Mathematical Quasicrystals

We refer to [4], [5], [6], [10] and references herein in this section. Let Λ a Delone set in $\mathbb{R}^n$, $n \geqslant 1$ (real or physical space). Λ is a model set when there exists a cut-and-project scheme $(\mathbb{R}^n \times H, L)$ and a relatively compact set Ω (window) of H with non empty interior such that $\Lambda = \{\pi_1(l) | l \in L, \pi_2(l) \in \Omega\}$, where H is a locally compact Abelian group (internal space), π_1, π_2 the canonical projections, L a lattice in $\mathbb{R}^n \times H$, with $\pi_{1|_L}$ injective and $\pi_2(L)$ dense. Λ is a Meyer set if there exists a finite set F such that $\Lambda - \Lambda \subset \Lambda + F$. The class of model sets in $\mathbb{R}^n$ is strictly included in the class of Meyer sets since a Meyer set is always a subset of a certain model set (Theorem 9.1 in [6]). The construction of this latter model set is not effective and arises from the linear approximation property. When G is a finite group acting on $\mathbb{R}^k$, $k \leqslant n$, and X is a G-cluster of total length n or $2n$ (total number of points in the finite union of orbits of points which constitute X, viewed as a shellable discrete object), the construction of the cut-and-project scheme is effective from itself in $\mathbb{R}^n$ [10]. With a selection mode on L providing model sets or subsets, this allows to introduce naturally G-clustering in Meyer sets. Such Delone sets inherit local structures in G-clusters by partial repetition and translation. When $\partial\Omega$ is of Lebesgue measure zero, model sets have a pure point spectrum [2]. But, in general, Meyer sets have no reason to be *crystals*. As Meyer sets on the real line, cite the Thue-Morse quasicrystal $\Lambda_{a,b}$ formed from the $\pm$- Thue Morse sequence [9], G-cluster sets [10], $\mathbb{Z}_\beta$ when β is a Pisot number [11], sets of vertices of aperiodic tilings [7], [13], [14], constructions from algebraic numbers [12], etc. The Thue-Morse quasicrystal exhibit a singular continuous component since the spectral measure of the $\pm$- Thue Morse sequence is singular continuous [8], [15], hence it is not a *crystal*. It was shown that a cut-and-project scheme is canonically attached to a G-cluster [10], hence providing naturally model sets or model subsets according to the choice of windows and selection mode of points on the hyperlattice. This means that G-clustering is a notion naturally associated with the class of Meyer sets since these objects are always subsets of model sets [5], [6]. Now, Λ is said to be a finitely generated Delone set if

$[\Lambda - \Lambda]$, the Abelian group generated by $\Lambda - \Lambda$ (under +), is finitely generated [4]. And it is said to be a Delone set of finite type if $\Lambda - \Lambda$ is such that its intersection with any closed ball is finite. The class of finitely generated Delone sets is strictly larger than the class of Delone set of finite type. Obviously, the latter one contains the class of Meyer sets.

Hof [2] has developed the mathematics of diffraction for arbitrary Delone sets through the notion of autocorrelation measure. In particular, the Bombieri-Taylor argument ([16], p. 244 in [2]) states that the Fourier transform of Λ has a δ-peak at ξ when a certain limit $\lim_{L\to\infty} L^{-1}\hat{\nu}_L(\xi)$ exists. In [9], we show that, for all above-mentioned classes of Delone sets, the lattices which intersect Λ play a prominent role in the diffraction process by the rarefaction laws at infinity they exhibit. For 1D Delone sets having an average lattice, a δ-peak may exist without this limit exists. For the Thue-Morse quasicrystal, we reconsider the Bombieri-Taylor argument from the rarefaction laws viewpoint and the fact that the Thue-Morse sequence has a limit-periodic Fourier module [13], [17]. Ponctual scaling laws were already investigated in Kolař [14] to discriminate the atomic component of the spectrum from the singular continuous one.

3. Cut and Congruence λ-Schemes

Definition 3.1. — *A cut and congruence λ-scheme consists of a direct product $\mathbb{R} \times \mathbb{R}/\lambda\mathbb{Z}$ of a real space and a torus, $\lambda > 0$, a real-valued function $\breve{g}(x)$ defined on $\mathbb{R}$, a lattice $D = \kappa\mathbb{Z}$ in $\mathbb{R}$, $\kappa > 0$, and a collection of vectors $\{ g_n \in \mathbb{R} \mid n \in \mathbb{Z}\}$ so that*

(i) the mapping $D \to \mathbb{R} : \kappa n \to \kappa n + g_n$ is injective.

(ii) $\breve{g}$ is an interpolating function of the set $\{(\kappa n, g_n) \mid n \in \mathbb{Z}\} : \forall n \in \mathbb{Z}, \quad \breve{g}(\kappa n) = g_n$

(iii) For all affine lattice $v \in \{ \overline{\kappa n + g_n} \mod (\lambda\mathbb{Z}) \mid n \in \mathbb{Z}\}$ of period λ, there exists real-valued functions $A_i(v,q)$ and exponents $\alpha_i(v)$, $i \in I(v)$ a finite or infinite set, such that, the $A_i(v,q)$ are uniformly bounded, $1 \geqslant \alpha_1(v) > \alpha_2(v) > \alpha_i(v) > \cdots \geqslant 0$ and, if q denotes the number of adjacent cells of this lattice counted from the origin towards $+\infty$ or $-\infty$, the number of points of $v \cap \Lambda$ within these q cells is given by, when q goes to infinity $A_1(v,q)q^{\alpha_1(v)} + A_2(v,q)q^{\alpha_2(v)} + A_3(v,q)q^{\alpha_3(v)} + \cdots$.

Assertion (i) means that the restriction of the first projection mapping $p_1 : \mathbb{R}\times\mathbb{R}/\lambda\mathbb{Z}$ to $\check{D}$ is 1-1, where D is identified with $\check{D} = \{(\kappa n, \overline{(\kappa n + g_n)} \bmod(\lambda\mathbb{Z})) \,/\, n \in \mathbb{Z}\} \subset D \times (\mathbb{R}/\mathbb{Z})$. Denote $\check{\Omega}_\lambda = \{\overline{(x + \breve{g}(x))} \mod (\lambda\mathbb{Z}) \mid x \in \mathbb{R}\}$. The second projection mapping $p_2 : \mathbb{R} \times \mathbb{R}/\lambda\mathbb{Z} \to \mathbb{R}/\lambda\mathbb{Z}$ is such that $p_2(\check{D}) \subset \check{\Omega}_\lambda$ is called the maximal window associated with $\breve{g}$. Identifying $\Lambda = \{\kappa n + g_n \mid n \in \mathbb{Z}\}$ with D, D with $\check{D}$ and using p_2, we obtain a $*$-operation $* : \Lambda \to \check{\Omega}_\lambda$. Note that $p_2(\check{D})$ is the space of all affine lattices of period λ which intersect Λ in a non-empty way. The distribution of points on v at infinity given by assertion (iii) is called a rarefaction law on v at infinity. When (iii) is valid, we say that assumption (F_λ) is satisfied. Denote $V = \{g_n \mid n \in \mathbb{Z}\}$.

Definition 3.2. — *A congruence model λ-set in $\mathbb{R}$ is a Delone set which can be written*

$$\Lambda_W = \{x \in (p_1 + \breve{g} \circ p_1)(\check{D}) \,/\, x^* \in W\}$$

for a certain window $W \subset p_2(\check{D}) \subset \mathbb{R}/\lambda\mathbb{Z}$.

Congruence model λ-sets are obtained similarly as model sets that is by a formal unique $*$-operation which detects the points to be selected [6]. Given $\lambda > 0$, the class of congruence model λ-sets is not included in the class of model sets and intersects a priori all the classes of mathematical quasicrystals which are mentioned above. Varying now λ allows to study them. If V is finite or if $[V-V]$ is discrete with $\mathbb{Q}\otimes_{\mathbb{Z}}[V-V] = \mathbb{Q}\otimes_{\mathbb{Z}}\kappa\mathbb{Z}$, and $\Lambda = \Lambda_{p_2(\check{D})}$ is relatively dense, any congruence model set Λ_W, $W\subset p_2(\check{D})$, is a Meyer set whose intersections with each affine lattice $\{x \bmod (\lambda\mathbb{Z}) \mid x\in\Lambda_W\}$ behave regularly at infinity according to assumption (F_λ). Set $k = 2\pi/\lambda$ and denote $d_W \geqslant 1$, the ratio of the point densities of $\Lambda_{p_2(\check{D})}$ and Λ_W. Let $I_N(k) = \frac{d_W}{2N}\left|\sum_{n=-N+1}^{+N-1} e^{ik(\kappa n+g_n)}\right|^2$, the sum being taken such that $p_2(\overline{(\kappa n+g_n)} \bmod \lambda\mathbb{Z}) \in W$. It gives the Fourier transform of the autocorrelation measure of Λ_W. By the following result, we obtain a limit in the sense of Bombieri-Taylor [16].

THEOREM 3.3. — *Assume $p_2(\check{D})$ is finite and the $A_i(v,q)$'s are independant of q. If $\mathcal{M}_W$ denotes $\{v\in W\subset p_2(\check{D}) \mid \alpha_1(v)$ is maximal$\}$ and if $\sum_{v\in\mathcal{M}_W} e^{ikv}A_1(v,q)\left(\frac{\kappa}{\lambda}\right)^{\max_v\{\alpha_1(v)\}} \neq 0$, the scaling behaviour of the diffracting intensity of the congruence model set Λ_W is given by*

$$\lim_{N\to\infty}\frac{I_N(k)}{N^{2\max_v\{\alpha_1(v)\}-1}} = \left|\sum_{v\in\mathcal{M}_W} e^{ikv}A_1(v,q)\left(\frac{\kappa}{\lambda}\right)^{\max_v\{\alpha_1(v)\}}\right|^2$$

In particular, under these assumptions, there is a δ-peak at k if and only if $\max\{\alpha_1(v) \mid v\in \mathcal{M}_W\} = 1$.

This theorem contains implicitly the fact that the type of a peak (δ or singular continuous) can be determined by a scaling law with N at the point q. This approach was already discussed in [9], Kolar et al [14] and [16].

4. Thue-Morse Quasicrystal, *p*-Rarefaction and Diffraction

The $\pm$-Thue-Morse sequence [8] is defined by $\eta_n = (-1)^{S_2(n)}$ where $S_2(n)$ is the sum of the 2-digits in the binary expansion of $n\in\mathbb{N}$. From it [9], given two real numbers $a, b, a > b > 0$, we build the aperiodic discrete point set $\Lambda_{a,b}$ on the real line as in Section 3 by: $\kappa = (a+b)/2$, $g_n = \sum_{0\leqslant m\leqslant n-1}\left(\frac{1}{2}(a-b)\eta_n\right)$, $g_{-n} = -g_n$ It is called the Thue-Morse quasicrystal associated with a and b. Since it is Delone and $\Lambda_{a,b}-\Lambda_{a,b}\subset\Lambda_{a,b}+\frac{a-b}{2}\{\pm3,\pm2,\pm1,0\}$, it is a Meyer set. It is the set of vertices of the aperiodic tiling obtained iteratively by the substitution rule $a\to ab, b\to ba$. The pure point component of the spectrum is described in [13]. In [9], it is proved that rarefaction laws on $\pm b+\lambda\mathbb{Z}$, for $\lambda = a+b$, are: $q/2$, and that of $\lambda\mathbb{Z}$ is: q. A consequence is that we have δ-peaks at $2\pi m/(a+b)$, $m\in\mathbb{Z}$. We will show in [19] that rarefaction laws of the affine lattices of period $(p/s)(a+b)$, where p and s are positive integers, are given by p-rarefaction laws. They are basically of the type $A_1(v)q + A_2(v,q)q^{\alpha_2(v)}$ where $A_2(v,q)$ is a bounded fractal function depending upon $\log q/\log 4$ and the $\alpha_2(v)'s$ are closely related to $\log p/(p-1)\log 2$. For instance, take $s=1$ and $p=3$. Denote, for all integer $n\geqslant 1$, any odd prime p and $i = 0,1,\ldots,p-1$

$$\mathcal{R}_{p,i}(n) = \sum_{\substack{0\leqslant j<n\\ j\equiv i(\bmod p)}} (-1)^{S_2(j)} \tag{1}$$

Goldstein et al [18] (previously Coquet for $i=0$; see ref. therein) proved a general expression for the 3-rarefied partial Thue-Morse sums, with $\alpha = \log 3/(2\log 2)$, $t_3(n) = 0$ if n is even and $t_3(n) = \eta_{3n-3}$ if n is odd,

$$\mathscr{R}_{3,i}(n) \;=\; n^{\alpha}\psi_{3,i}\left(\frac{\log n}{\log 4}\right) - \frac{t_3(n)}{3} \tag{2}$$

where for all $i = 0, 1, 2$, the (fractal) functions $\psi_{3,i}$ are continuous, nowhere derivable, periodic of period 1. Rarefaction laws on the 9 affine lattices of period $3(a+b)$ intersecting $\Lambda_{a,b}$ are of the type: $q, q+1$ or $q/2 \pm \mathscr{R}_{3,i}(3q)$, making a link between the functions $\psi_{3,i}$ and the coefficients $A_1(v,q), A_2(v,q)$.

THEOREM 4.1 ([9]). — *The spectrum of the Thue-Morse quasicrystal $\Lambda_{a,b}$ exhibits a singular continuous peak at $k = 2\pi/(3(a+b))$. The Fourier transform of the autocorrelation measure I_N satisfies*

$$\forall \epsilon, \exists N_0 \text{ such that } \forall N \geqslant N_0, \quad \frac{I_N}{N^{2\alpha-1}} \in \frac{1}{18}\,|\mathscr{F}(k)|^2 +]-\epsilon; +\epsilon[$$

where $\mathscr{F}(k)$ is the closed interval obtained as the image of $[0;1]$ by the continuous mapping

$$x \to \frac{1}{2}(\psi_{3,2}(x) - \psi_{3,0}(x)) \sin\left(\frac{\pi(a-b)}{3(a+b)}\right).$$

$\mathscr{F}(k)$ is a fractal compact curve lying on the real line described fractally as the image of $\mathbb{N}^*$ by the mapping

$$q \to \frac{1}{2}\sin\left(\frac{\pi(a-b)}{3(a+b)}\right)\left(\psi_{3,0}\left(\frac{\log(3q)}{\log 4}\right) - \psi_{3,2}\left(\frac{\log(3q)}{\log 4}\right)\right)$$

$\mathscr{F}(k)$ does not contain the origin leading to no extinction of this singular continuous peak.

The asymptotic growth of $\mathscr{R}_{3,i}$ is of the order of $n^{\frac{\log 3}{\log 4}}$ in the sense

$$-\infty \;<\; \liminf_{n\to+\infty} \frac{\mathscr{R}_{3,i}(n)}{n^{\alpha}} \;<\; \limsup_{n\to+\infty} \frac{\mathscr{R}_{3,i}(n)}{n^{\alpha}} \;<\; +\infty$$

with fractal undulations between the bounds. These bounds are reached. This has led us to reconsider the Thue-Morse quasicrystal as an incommensurate crystal with a fractal decoration within the average cell. The Thue-Morse quasicrystal is a congruence model λ-set for $\lambda = a+b$ and $\lambda = 3(a+b)$.

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