ANNALES

DE

L'INSTITUT FOURIER

Jean-Pierre GAZEAU & Jean-Louis VERGER-GAUGRY

Diffraction spectra of weighted Delone sets on beta-lattices with beta a quadratic unitary Pisot number

DIFFRACTION SPECTRA OF WEIGHTED DELONE SETS ON BETA-LATTICES WITH BETA A QUADRATIC UNITARY PISOT NUMBER

by Jean-Pierre GAZEAU & Jean-Louis VERGER-GAUGRY (*)

————

ABSTRACT. — The Fourier transform of a weighted Dirac comb of beta-integers is characterized within the framework of the theory of Distributions, in particular its pure point part which corresponds to the Bragg part of the diffraction spectrum. The corresponding intensity function on this Bragg part is computed. We deduce the diffraction spectrum of weighted Delone sets on beta-lattices in the split case for the weight, when beta is the golden mean.

RÉSUMÉ. — On caractérise au moyen de la théorie des distributions la transformée de Fourier d'un peigne de Dirac avec poids, plus particulièrement la partie purement ponctuelle qui correspond aux pics de Bragg dans le spectre de diffraction. La fonction intensité de ces derniers est donnée d'une manière explicite. On en déduit le spectre de diffraction d'ensembles de Delaunay avec poids supportés par les beta-réseaux dans le cas où le poids est factorisable et où beta est le nombre d'or.

1. Introduction: quasicrystalline motivations

Mainly since the end of the 19th century, material scientists have been comprehending the crystalline order, owing to improvements in observational techniques, like $X-$ray or electron diffraction, and in quantum mechanics (e.g. Bloch waves) [10] [22]. The mathematical tools which have enabled them to classify and to improve the understanding of such structures are mainly lattices, finite groups (point and space groups) and their representations, and Fourier analysis. So to say, the structural role played

————

by the rational integers ($\mathbb{Z}$) was essential in that process of mathematical formalization.

A so-called quasicrystalline order has been discovered more than twenty years ago [38]. The observational techniques for this new state of matter are similar to those used for crystals. But the absence of periodicity (which does not mean that there is a random distribution of atomic sites) and the presence of self-similarities, which reveal to be algebraic integers [24] [42], as scaling factors demand new mathematical tools [2] [23] [25]. As a matter of fact, it became necessary to conceive adapted point sets and tilings as acceptable geometric supports of quasicrystals, and also to carry out a specific spectral analysis for quasicrystalline diffraction and electronic transport. Therefore an appealing mathematical program, combining number theory, free groups and semi-groups, measure theory and quasi-harmonic analysis, has been developing for the last two decades. The aim of this paper is first to recall the part of this program specifically devoted to the notions of sets of *beta-integers* ($\mathbb{Z}_\beta$), when β is a quadratic Pisot-Vijayaraghavan number, and associated *beta-lattices* (or *β-lattices*), and next to present some original results concerning the Fourier properties and diffraction spectra of Delone sets on beta-integers and on beta-lattices, and more generally of weighted Dirac combs supported by beta-lattices. This approach makes prominent the role played by nonclassical numerations [16] [26], associated with substitutive dynamical systems [34], and amounts to replace the traditional set of rational integers $\mathbb{Z}$ by $\mathbb{Z}_\beta$. This allows computations over this new set of numbers, where lattices are replaced by beta-lattices.

The organisation of this paper is as follows. Section 2 recalls the construction of the set of beta-integers $\mathbb{Z}_\beta$ [8] [17] [26] (introduced by Gazeau in [19]). We describe in Section 3 the relevance of the beta-integers in the description of quasicrystalline structures. More precisely, these numbers can be used as a sort of universal support for *model sets* or *cut-and-project sets*, *i.e.* those point sets paradigmatically supposed to support quasicrystalline atomic sites and their diffraction patterns. We then give in Section 4.1 their Fourier transform, in particular the support of the pure point part of the measure. We present in Section 4.2 the computation of diffraction formulae of weighted Delone sets on beta-integers, then on beta-lattices (Section 4.3), in the plane case with the golden mean for β, in the case where the weight is split. We indicate in particular how β-lattices can be viewed as the most natural indexing sets for the numbering of the spots (the" Bragg peaks") beyond a certain brightness in the diffraction pattern.

2. Numeration in base β a Pisot number and beta-integers $\mathbb{Z}_\beta$

2.1. Definitions and notations

We refer to [15] [16], Chapter 7 in [26], [33] [35] for the numeration in Pisot base, and to [20] [24] [28] [29] [30] [32] [41] [42] for an introduction to mathematical quasicrystals (to Delone sets, Meyer sets ...).

Notation 2.1. — For a real number $x \in \mathbb{R}$, the integer part of x will be denoted by $\lfloor x \rfloor$ and its fractional part by $\{x\} = x - \lfloor x \rfloor$.

DEFINITION 2.2. — *For $\beta > 1$ a real number and $z \in [0,1]$ we denote by $T_\beta(z) = \beta z \mod 1$ the β-transform on $[0,1]$ associated with β, and iteratively, for all integers $j \geqslant 0$, $T_\beta^{j+1}(z) := T_\beta(T_\beta^j(z))$, where by convention $T_\beta^0 = Id$.*

DEFINITION 2.3. — (i) *Given $\Lambda \subset \mathbb{R}$ a discrete set, we say that Λ is uniformly discrete if there exists $r > 0$ such that $\|x - y\| \geqslant r$ for all $x, y \in \Lambda$ with $x \neq y$. Therefore a uniformly discrete subset of $\mathbb{R}$ can be the "empty set", one point sets $\{x\}$, or discrete sets of cardinality $\geqslant 2$ having this property.*
   (ii) *A subset $\Lambda \subset \mathbb{R}$ is called relatively dense (after Besicovitch) if there exists $R > 0$ such that for all $x \in \mathbb{R}$, there exists $z \in \Lambda$ such that $\|x - z\| \leqslant R$. A relatively dense set is never empty.*
  (iii) *A Delone set of $\mathbb{R}$ is a subset of $\mathbb{R}$ which is uniformly discrete and relatively dense.*
  (iv) *A Meyer set Λ is a Delone set such that there exists a finite set F such that $\Lambda - \Lambda \subset \Lambda + F$.*
   (v) *A Pisot number (or Pisot-Vijayaraghavan number, or PV number) β is an algebraic integer > 1 such that all its Galois conjugates are strictly less than 1 in modulus.*

DEFINITION 2.4. — *Let $\beta > 1$ be a real number. A beta-representation (or β-representation, or representation in base β) of a real number $x \geqslant 0$ is given by an infinite sequence $(x_i)_{i \geqslant 0}$ and an integer $k \in \mathbb{Z}$ such that $x = \sum_{i=0}^{+\infty} x_i \beta^{-i+k}$, where the digits x_i belong to a given alphabet ($\subset \mathbb{N}$).*

Assume that $\beta > 1$ is a Pisot number of degree strictly greater than 1 in the sequel.

Among all the beta-representations of a real number $x \geqslant 0, x \neq 1$, there exists a particular one called Rényi β-expansion which is obtained through

the so-called *greedy algorithm*: in this case, k satisfies $\beta^k \leqslant x < \beta^{k+1}$ and the digits

$$(2.1) \qquad x_i := \left\lfloor \beta T_\beta^i \left(\frac{x}{\beta^{k+1}} \right) \right\rfloor \qquad i = 0, 1, 2, \ldots,$$

belong to the finite alphabet $\mathbb{A}_\beta := \{0, 1, 2, \ldots, \lfloor \beta \rfloor\}$.

Notation 2.5. — We denote by

$$(2.2) \qquad \langle x \rangle_\beta := x_0 x_1 x_2 \ldots x_k . x_{k+1} x_{k+2} \ldots$$

the couple formed by the string of digits $x_0 x_1 x_2 \ldots x_k x_{k+1} x_{k+2} \ldots$ and the position of the dot, which is at the kth position (between x_k and x_{k+1}).

DEFINITION 2.6. —   • *The integer part (in base β) of x is*

$$\sum_{i=0}^{k} x_i \beta^{-i+k}.$$

• *The fractional part (in base β) is*

$$\sum_{i=k+1}^{+\infty} x_i \beta^{-i+k}.$$

• *If a Rényi β-expansion ends in infinitely many zeros, it is said to be finite and the ending zeros are omitted.*
• *If it is periodic after a certain rank, it is said to be eventually periodic (the period is the smallest finite string of digits possible, assumed not to be a string of zeros).*

The particular Rényi β-expansion of 1 plays an important role in the theory. Denoted by $d_\beta(1)$ it is defined as follows: since $\beta^0 \leqslant 1 < \beta$, the value $T_\beta(1/\beta)$ is set equal to 1 by convention. Then using (2.1) for all $i \geqslant 1$ with $x = 1$, we have: $t_1 = \lfloor \beta \rfloor, t_2 = \lfloor \beta \{\beta\} \rfloor, t_3 = \lfloor \beta \{\beta \{\beta\}\} \rfloor$, etc. The equality $d_\beta(1) = 0.t_1 t_2 t_3 \ldots$ corresponds to $1 = \sum_{i=1}^{+\infty} t_i \beta^{-i}$.

DEFINITION 2.7. — *The set*

$$\mathbb{Z}_\beta := \left\{ x \in \mathbb{R} \,\middle|\, |x| \text{ is equal to its integer part (in base β) } \sum_{i=0}^{k} x_i \beta^{-i+k} \right\}$$

is called set of beta-integers, or set of β-integers. The set of beta-integers is discrete and locally finite [41]. *It is usual to denote its elements by b_n so that $\mathbb{Z}_\beta = \{\ldots, b_{-n}, \ldots, b_{-1}, b_0, b_1, \ldots b_n, \ldots\}$ with $b_0 = 0, b_1 = +1, b_{-n} = -b_n$ for $n \geqslant 1$.*

A positive beta-integer is also defined [15] by a finite sum $\sum_{j=0}^{N} a_j \beta^j$ where the integers a_j satisfy $0 \leqslant a_j < \beta$, together with

$$\sum_{j=0}^{m} a_j \beta^j \; < \; \beta^{m+1}, \qquad m = 0, 1, \dots, N.$$

2.2. Beta-integers, Parry conditions and tilings

Let $\beta > 1$. The set $\mathbb{Z}_\beta$ is self-similar and symmetrical with respect to the origin:

$$\beta \mathbb{Z}_\beta \subset \mathbb{Z}_\beta, \qquad \mathbb{Z}_\beta = -\mathbb{Z}_\beta.$$

Denote $\mathbb{Z}_\beta^+ := \mathbb{Z}_\beta \cap \mathbb{R}^+$. The set $\mathbb{Z}_\beta^+$ contains $\{0, 1\}$ and all the positive polynomials in β for which the coefficients are given by the equations (2.1). Parry [33] has shown that the knowledge of $d_\beta(1)$ suffices to exhaust all the possibilities of such polynomials by the so-called "Conditions of Parry (CP$_\beta$)": let $(c_i)_{i \geqslant 1} \in \mathbb{A}_\beta^\mathbb{N}$ be the following sequence:

(2.3)

$$c_1 c_2 c_3 \cdots = \begin{cases} t_1 t_2 t_3 \cdots & \text{if } d_\beta(1) = 0.t_1 t_2 \cdots \text{ is infinite,} \\ (t_1 t_2 \cdots t_{m-1}(t_m - 1))^\omega & \text{if } d_\beta(1) \text{ is finite} \\ & \text{and equal to } 0.t_1 t_2 \cdots t_m, \end{cases}$$

where $()^\omega$ means that the word within $()$ is indefinitely repeated. We have $c_1 = t_1 = \lfloor \beta \rfloor$. Then the positive polynomial $\sum_{i=0}^{v} y_i \beta^{-i+v}$, with $v \geqslant 0$, $y_i \in \mathbb{N}$, belongs to $\mathbb{Z}_\beta^+$ if and only if $y_i \in \mathbb{A}_\beta$ and the following $v + 1$ inequalities, for all $j = 0, 1, 2, \dots, v$, are satisfied:

(2.4) (CP$_\beta$): $(y_j, y_{j+1}, y_{j+2}, \dots, y_{v-1}, y_v, 0, 0, 0, \dots) \prec (c_1, c_2, c_3, \dots)$

where "$\prec$" means lexicographical smaller. For a negative polynomial, we consider the above criterium applied to its opposite.

The set $\mathbb{Z}_\beta$ can be viewed as the set of vertices of the tiling $\mathcal{T}_\beta$ of the real line for which the tiles are the closed intervals whose extremities are two successive β-integers.

In the rest of Section 2 we assume that β is a quadratic unitary Pisot number. Such numbers are of two types [8]: if β is a quadratic unitary Pisot number, of minimal polynomial denoted by $P_\beta(X)$ and conjugate denoted by β', then it satisfies exclusively one of the two following relations ([18] Lemma 3 p. 721):

Case (i) β is the dominant root of $P_\beta(X) = X^2 - aX - 1$, with $a \geqslant 1$, or

Case (ii) β is the dominant root of $P_\beta(X) = X^2 - aX + 1$, with $a \geqslant 3$.

In **Case (i)**, $\beta' = -1/\beta$, the alphabet $\mathbb{A}_\beta$ is $\{0, 1, \ldots, a\}$ with $a = \lfloor \beta \rfloor$, and $d_\beta(1) = 0.a1$ is finite.

In **Case (ii)**, $\beta' = 1/\beta$, $\mathbb{A}_\beta = \{0, 1, \ldots, a-1\}$ with $a = \lfloor \beta \rfloor + 1$. The Rényi β-expansion of 1 is $d_\beta(1) = 0.(a-1)(a-2)^\omega$.

In both cases the tiling $\mathcal{T}_\beta$ can be obtained directly from a substitution system on a two-letter alphabet which is associated to β in a canonical way [14] [34] [40]. Hence, the number of (noncongruent) tiles of $\mathcal{T}_\beta$ is 2 in both cases, of respective lengths:

$$\textbf{Case (i)}: 1 \text{ and } 1/\beta, \qquad \textbf{Case (ii)}: 1 \text{ and } 1 - 1/\beta$$

and $\mathbb{Z}_\beta$ is a Meyer set [8] [20].

2.3. Averaging sequences of finite approximants of $\mathbb{Z}_\beta$

DEFINITION 2.8. — *An averaging sequence* $(U_l)_{l \geqslant 0}$ *of finite approximants of* $\mathbb{Z}_\beta$ *is given by a closed interval* J *whose interior contains the origin, and a real number* $t > 0$, *such that:*

$$U_l = t^l J \cap \mathbb{Z}_\beta, \qquad l = 0, 1, \ldots$$

A natural averaging sequence of such approximants for the beta-integers is yielded by the sequence $((-B_N) \cup B_N)_{N \geqslant 0}$, where

$$(2.5) \qquad B_N = \left\{ x \in \mathbb{Z}_\beta \,|\, 0 \leqslant x < \beta^N \right\}, \qquad N = 0, 1, \ldots$$

It is easy to check that $\mathrm{card}(B_N) = c_N$, a number in the Fibonacci-like sequence defined by the recurrence

$$(2.6) \qquad c_{N+2} = a\, c_{N+1} \pm c_N$$

with $c_0 = 1$, $c_1 = a$, and where "+" stands for **case (i)** whereas "−" is for **case (ii)**.

PROPOSITION 2.9. — *The cardinal* c_N *of the approximant set* B_N *asymptotically behaves as follows*

$$(2.7) \qquad c_N = \frac{\beta^N}{\gamma} + o(1) \qquad \text{for } N \text{ large}$$

where $\gamma = \begin{cases} 1 - \frac{1}{a}\left(\frac{1}{\beta} - 1\right)^2 = \frac{1+\beta^2}{\beta(1+\beta)} & \textbf{Case(i)}, \\ 1 - \frac{1}{\beta^2} & \textbf{Case(ii)}. \end{cases}$

Proof. — It suffices to observe

$$\beta^N \;=\; b_{c_N}, \qquad \text{for } N \geqslant 0,$$

and to apply Proposition 5 in [13]. □

3. Cut-and-project schemes and beta-integers

The most popular geometrical models for quasicrystals are the so-called *cut-and-project* sets. These sets actually were previously introduced by Meyer [28] [29] [31] [36] in the context of Harmonic Analysis and Number Theory and christened by him *model sets*. First, a *cut-and-projection scheme* is the following

$$\mathbb{R}^d \;\xleftarrow{\;\pi_1\;}\; \mathbb{R}^d \times G \;\xrightarrow{\;\pi_2\;}\; G$$
$$\cup$$
$$D$$

where π_1 and π_2 are the canonical projection mappings, G is a locally compact abelian group, called the *internal space*, $\mathbb{R}^d$ is called the *physical space* ($d \geqslant 1$), D is a lattice, *i.e.* a discrete subgroup of $\mathbb{R}^d \times G$ such that $(\mathbb{R}^d \times G)/D$ is compact. The projection $\pi_1|_D$ is 1-to-1, and $\pi_2(D)$ is dense in G.

Let $M = \pi_1(D)$ and set $* = \pi_2 \circ (\pi_1|_D)^{-1} : M \longrightarrow G$. The set $\Lambda \subset \mathbb{R}^d$ is a *model set* if there exist a cut-and-projection scheme and a relatively compact set $\Omega \subset G$ of non-empty interior such that $\Lambda = \{x \in M \mid x^* \in \Omega\}$. The set Ω is called a *window*.

The following was proved by Meyer (Theorem 9.1 in [30]): *A model set is a Meyer set. Conversely if Λ is a Meyer set, there exists a model set Λ_0 such that $\Lambda \subset \Lambda_0$.*

By decoration of a point set $\Lambda \subset \mathbb{R}^d, d \geqslant 1$, we mean the new point set $\Lambda + F$ where F is a finite point set containing 0 such that any element of $\Lambda + F$ has a unique writing in this sum decomposition; $\Lambda + F$ is a decoration of Λ with F.

In the rest of Section 3 β is a quadratic unitary Pisot number.

3.1. One-dimensional model sets as subsets of beta-integers

Let us introduce the *algebraic model set*

(3.1) $$\Sigma^\Omega = \{x = m + n\beta \in \mathbb{Z}[\beta] \mid x' = m + n\beta' \in \Omega\},$$

where $\Omega \subset \mathbb{R}$ is such that the closure $\overline{\Omega}$ is compact and the interior $\overset{\circ}{\Omega}$ is not empty. Though $\mathbb{Z}_\beta$ is symmetrical, it is not a model set but a Meyer set, the positive and negative parts of $\mathbb{Z}_\beta$ can be interpreted in terms of model sets only.

PROPOSITION 3.1. — [8] *The algebraic characterizations of* $\mathbb{Z}_\beta^+$ *and* $\mathbb{Z}_\beta^-$ *are the following:*

Case (i):

$$(3.2) \qquad \mathbb{Z}_\beta^+ = \Sigma^{(-1,\beta)} \cap \mathbb{R}^+, \ \mathbb{Z}_\beta^- = -\mathbb{Z}_\beta^+ = \Sigma^{(-\beta,1)} \cap \mathbb{R}^-,$$

$$(3.3) \qquad \mathbb{Z}_\beta' \subset (-\beta, \beta) \ \text{ and } \ \mathbb{Z}_\beta' \cap (-1,1) = \mathbb{Z}[\beta] \cap (-1,1),$$

Case (ii):

$$(3.4) \qquad \mathbb{Z}_\beta^+ = \Sigma^{[0,\beta)} \cap \mathbb{R}^+ \ \text{ and } \ \mathbb{Z}_\beta^- = \Sigma^{(-\beta,0]} \cap \mathbb{R}^-,$$

$$(3.5) \qquad \mathbb{Z}_\beta \subset \Sigma^{(-\beta,\beta)} \subset \mathbb{Z}_\beta + \{0, \pm \tfrac{1}{\beta}\}.$$

Now, let us see how the set $\mathbb{Z}_\beta$ in Case (i) (resp. the decorated set $\widetilde{\mathbb{Z}}_\beta \overset{\text{def}}{=} \mathbb{Z}_\beta + \{0, \pm\frac{1}{\beta}\}$ in Case (ii)) can be considered as *universal* support of model sets like (3.1).

Let Ω be a bounded window in $\mathbb{R}$. It is always possible to find a λ in $\mathbb{Z}[\beta]$ and an integer j in $\mathbb{Z}$ such that $\Omega \subset (-\beta^j, \beta^j) + \lambda$. Let $\Delta = \beta^{-j}(\Omega - \lambda) \subset (-1,1)$. Then, one can easily prove that

$$\Sigma^\Omega = (-(\text{resp.} +1))^j \beta^{-j}\{x \in \mathbb{Z}_\beta (\text{resp.} \widetilde{\mathbb{Z}}_\beta) \mid x' \in \Delta\} + \lambda'.$$

Therefore $\mathbb{Z}_\beta$ (resp. $\widetilde{\mathbb{Z}}_\beta$) enumerates the model set Σ^Ω.

3.2. An alternate definition of beta-integers

PROPOSITION 3.2. — *The following characterization of* $\mathbb{Z}_\beta^+$ *holds :*

Case (i): *with* $\gamma = \dfrac{1 + \beta^2}{\beta(1+\beta)}$,

$$(3.6) \qquad \mathbb{Z}_\beta^+ = \left\{ b_n = \gamma n + \frac{1}{\beta}\frac{1-\beta}{1+\beta} - \frac{1-\beta}{\beta}\left\{\frac{n+1}{1+\beta}\right\}, \ n \in \mathbb{N} \right\};$$

Case (ii): *with* $\gamma = 1 - \dfrac{1}{\beta^2}$,

$$(3.7) \qquad \mathbb{Z}_\beta^+ = \left\{ b_n = \gamma n + \frac{1}{\beta}\left\{\frac{n}{\beta}\right\}, \ n \in \mathbb{N} \right\}.$$

Proof. — For each nonnegative n, let $\rho_L(n)$ (resp. $\rho_S(n) \equiv \rho(n)$) denote the number of long (resp. short) tiles between the nth beta-integer and the origin 0. The length of long tile is 1 whereas the length of short tile is $l_S = 1/\beta$ (**case (i)**) or $l_S = 1 - 1/\beta$ (**case (ii)**). From the two equalities

$$(3.8) \qquad\qquad n = \rho_L(n) + \rho(n),$$

$$(3.9) \qquad\qquad b_n = \rho_L(n) + l_S\rho(n),$$

we derive the expression for b_n in terms of n and β:

$$(3.10) \qquad\qquad b_n = n + (l_S - 1)\rho(n).$$

Now we know from Proposition 3.1 that the sets $\mathbb{Z}_\beta^+$ of nonnegative beta-integers are also defined through the following constraints on their Galois conjugates:

$$(3.11) \quad \mathbb{Z}_\beta^+ = \{x = r + s\beta \in \mathbb{Z}[\beta] \mid x \geq 0 \text{ and}$$
$$x' = r - s\frac{1}{\beta} \in (-1, \beta)\} \qquad \textbf{case (i)},$$

$$(3.12) \quad \mathbb{Z}_\beta^+ = \{x = r + s\beta \in \mathbb{Z}[\beta] \mid x \geq 0 \text{ and}$$
$$x' = r + s\frac{1}{\beta} \in [0, \beta)\} \qquad \textbf{case (ii)}.$$

There results for the conjugate of (3.10) the following inequalities obeyed by the nonnegative integer $\rho(n)$:

$$(3.13) \qquad \frac{n}{1+\beta} - \frac{\beta}{1+\beta} < \rho(n) < \frac{n}{1+\beta} + \frac{1}{1+\beta} \qquad \textbf{case (i)},$$

$$(3.14) \qquad \frac{n}{\beta} - 1 < \rho(n) \leq \frac{n}{\beta} \qquad\qquad \textbf{case (ii)}.$$

Since both intervals have length equal to 1, we conclude that

$$(3.15) \qquad \rho(n) = \left\lfloor \frac{n+1}{\beta+1} \right\rfloor \qquad\qquad \textbf{case (i)},$$

$$(3.16) \qquad \rho(n) = \left\lfloor \frac{n}{\beta} \right\rfloor \qquad\qquad \textbf{case (ii)}.$$

Combining (3.15), resp. (3.16) with (3.10) and using $\lfloor x \rfloor = x - \{x\}$ yield (3.6) and (3.7). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \square$

4. Diffraction spectra

Since the beta-integers or beta-lattices or some decorated version of them, besides their intrinsic rich arithmetic and algebraic properties, can be seen as a kind of universal support for quasicrystalline structures having five- or ten-fold or eight-fold or twelve-fold symmetries, we are naturally led to focus our attention on them, in particular to examine their diffractive properties when we assign to each point in such sets a weight describing to some extent its "degree" of occupation. We should insist here on the fact that this concept of degree of occupation of beta-integer sites encompasses the "Cut and Project" approach which has become like a paradigm for quasicrystal experimentalists. It is thus crucial to know in a comprehensive way the diffractive properties of "weighted" beta-integers by setting up explicit formulas, whereas the "constant weight" case is already mathematically well established [27].

4.1. Fourier transform of a weighted Dirac comb of beta-integers

Let us consider the following pure point complex Radon measure supported by the set of beta-integers $\mathbb{Z}_\beta = \{b_n \mid n \in \mathbb{Z}\}$:

$$(4.1) \qquad \mu = \sum_{n \in \mathbb{Z}} w(n) \delta_{b_n},$$

where $w(x)$ is a bounded complex-valued function, called *weight*. In a specific context, the latter will be given the meaning of a site occupation probability. In (4.1) δ_{b_n} denotes the normalized Dirac measure supported by the singleton $\{b_n\}$. Denote by δ the Dirac measure ($\delta(\{0\}) = 1$). Clearly, the measure (4.1) is translation bounded, *i.e.* for all compact $K \subset \mathbb{R}$ there exists α_K such that $\sup_{a \in \mathbb{R}} |\mu|(K + a) \leqslant \alpha_K$, and so is a tempered distribution. Its Fourier transform $\widehat{\mu}$ is also a tempered distribution defined by

$$(4.2) \qquad \widehat{\mu}(q) = \mu\left(e^{-iqx}\right) = \sum_{n \in \mathbb{Z}} w(n) e^{-iqb_n}.$$

It may or may not be a measure.

We know from Proposition 3.2 that b_n has the general form $b_n = \gamma n + \alpha_0 + \alpha\{x(n)\}$, where $\alpha_0 = \frac{1-\beta}{\beta(1+\beta)}$, $\alpha = 1/\beta$ in **case (i)**, $\alpha_0 = 0$, $\alpha = 1 - 1/\beta$ in **case(ii)**. It contains a fractional part. Now, for any $x \in \mathbb{R}$, the "fractional

part" function $x \mapsto \{x\} = x - \lfloor x \rfloor \in [0,1)$ is periodic of period 1 and so is the piecewise continuous function $e^{-iq\alpha\{x\}}$. Let

$$c_m(q) = \int_0^1 e^{-iq\alpha\{x\}} e^{-2\pi imx}\, dx$$

(4.3)
$$= i\frac{e^{-iq\alpha} - 1}{2\pi m + q\alpha} \;=\; (-1)^m e^{-i\frac{\alpha}{2}q} \operatorname{sinc}\left(\frac{\alpha}{2}q + m\pi\right)$$

be the coefficients of the expansion of $e^{-iq\alpha\{x\}}$ in Fourier series. In (4.3), sinc denotes the cardinal sine function, $\operatorname{sinc}(x) = \dfrac{\sin x}{x}$. Thus

(4.4)
$$e^{-iq\alpha\{x\}} = \sum_{m-\infty}^{+\infty} c_m(q) e^{2\pi imx}$$

where the convergence is punctual in the usual sense of Fourier series for piecewise continuous functions.

Given $T > 0$ and the set of Fourier coefficients $\{c_m(q) \mid m \in \mathbb{Z}\}$ in (4.3), let J_T be the space of complex-valued functions $q \mapsto g(q)$ such that the series

(4.5)
$$\sum_{m \in \mathbb{Z}} c_m(q) g(q - \frac{2\pi}{T}m) e^{2\pi imx}$$

converges (in the punctual sense) to a function $G_x(q)$ which is slowly increasing and locally integrable in q uniformly with respect to $x : \sup_x |G_x(q)|$ is locally integrable and there exists $A > 0$ and $\nu > 0$ such that $\sup_x |G_x(q)| < A|q|^{\nu}$ for $|q| \to \infty$. As a matter of fact, for any $T > 0$, all Fourier exponentials $e^{i\omega q}$ are in J_T for all $\omega \in \mathbb{R}$, by (4.4). With these definitions, we can enunciate the main result of this section.

THEOREM 4.1. — *Suppose that the Fourier series*

(4.6)
$$\sum_{n \in \mathbb{Z}\setminus\{0\}} \frac{w(n)}{(-2\pi in)} e^{-2\pi inx}$$

*converges in the punctual sense to a periodic piecewise continuous function $f_w(x)$, of period 1, which has a derivative $f'_w(x)$ continuous bounded on the open set $\mathbb{R} - \bigcup_p \{a_p\}$, where the a_p's are the discontinuity points of $f_w(x)$. Let $\sigma_p = f_w(a_p + 0) - f_w(a_p - 0)$ be the jump of f_w at the singularity a_p. Suppose further that, for **case (i)**, the function $q \mapsto e^{-iq\frac{1-\beta}{\beta(\beta+1)}q} f'_w\left(\frac{\gamma}{2\pi}q\right)$ is in J_T with $T = \beta + 1/\beta$ and, for **case (ii)**, the function $q \mapsto f'_w\left(\frac{\gamma}{2\pi}q\right)$ is in J_T with $T = \beta - 1/\beta$. Then,*

(i) the Fourier transform $\widehat{\mu}$ of μ is the sum of a pure point tempered distribution $\widehat{\mu}_{pp}$ and a regular tempered distribution $\widehat{\mu}_r$ as follows:

$$\widehat{\mu} = \widehat{\mu}_{pp} + \widehat{\mu}_r$$

with :

(4.7) $$\widehat{\mu}_r(q) = \sum_{m\in\mathbb{Z}} d_m(q)\left(w(0) + f'_w\left(\frac{\gamma}{2\pi}q - \frac{m}{\kappa}\right)\right),$$

(4.8) $$\widehat{\mu}_{pp}(q) = \frac{2\pi}{\gamma} \sum_{m,p\in\mathbb{Z}} d_m(q)\,\sigma_p\,\delta\left(q - \frac{2\pi}{\gamma}\left(\frac{m}{\kappa} + a_p\right)\right),$$

where $\kappa = 1 + \beta$ in **case (i)** or $\kappa = \beta$ in **case (ii)**, and

$$d_m(q) = \begin{cases} c_m(q)e^{\frac{2i\pi}{\beta(1+\beta)}\left(m\beta - \frac{q(1-\beta)}{2\pi}\right)} & \textbf{case(i)}, \\ c_m(q) & \textbf{case(ii)}, \end{cases}$$

(ii) the pure point part $\widehat{\mu_{pp}}$ is supported by the scaled finite union of translates of $\mathbb{Z}[\beta]$:

(4.9) $$\frac{2\pi}{\gamma}\left(\{a_1, a_2, \ldots, a_N\} + \mathbb{Z}[\beta]\right)$$

where $a_1, a_2, \ldots, a_N$ are the discontinuities of f_w in $[0, 1)$.

Proof. — By Proposition 3.2, for $n \geqslant 0$, we express the Fourier exponential in (4.2) as follows

(4.10) $$e^{-iqb_n} = e^{-iq\frac{1-\beta}{\beta(1+\beta)}}\,e^{-in\gamma q}\,e^{-iq\frac{\beta-1}{\beta}\left\{\frac{n+1}{1+\beta}\right\}} \qquad \textbf{case (i)},$$

(4.11) $$e^{-iqb_n} = e^{-in\gamma q}\,e^{-iq\frac{1}{\beta}\left\{\frac{n}{\beta}\right\}} \qquad \textbf{case (ii)}.$$

Due to the periodicity of the "fractional part" function $x \to \{x\}$, of period 1, we expand the last factor in (4.10) and (4.11) in Fourier series :

(4.12) $$e^{-iqb_n} = e^{-iq\frac{1-\beta}{\beta(1+\beta)}}\,e^{-in\gamma q}\sum_{m\in\mathbb{Z}} c_m(q)\,e^{2\pi im\left\{\frac{n+1}{1+\beta}\right\}} \qquad \textbf{case (i)},$$

(4.13) $$e^{-iqb_n} = e^{-in\gamma q}\sum_{m\in\mathbb{Z}} c_m(q)\,e^{2\pi im\left\{\frac{n}{\beta}\right\}} \qquad \textbf{case (ii)}.$$

Since

$$e^{2\pi im\{x\}} = e^{2\pi imx}\,e^{-2\pi im\lfloor x\rfloor} = e^{2\pi imx},$$

we get the following Fourier expansions :

Case (i).

$$e^{-iqb_n} = \sum_{m\in\mathbb{Z}} c_m(q)\,e^{-iq\frac{1-\beta}{\beta(1+\beta)}}\,e^{2\pi im\frac{1}{1+\beta}}\,e^{-2\pi in\left(\frac{\gamma}{2\pi}q - \frac{m}{1+\beta}\right)}$$

Case (ii).

$$(4.14) \qquad e^{-iqb_n} = \sum_{m \in \mathbb{Z}} c_m(q) \, e^{-2\pi i n \left(\frac{\gamma}{2\pi} q - \frac{m}{\beta} \right)},$$

For both cases we adopt the generic expansion

$$(4.15) \qquad e^{-iqb_n} = \sum_{m \in \mathbb{Z}} d_m(q) \, e^{-2\pi i n \left(\frac{\gamma}{2\pi} q - \frac{m}{\kappa} \right)},$$

where $\kappa = 1 + \beta$ (**case (i)**) or $\kappa = \beta$ (**case (ii)**). These expansions can be extended to all $n \in \mathbb{Z}$. Thus, the Fourier transform of the measure can be written as the double sum:

$$(4.16) \qquad \widehat{\mu}(q) = \sum_{m \in \mathbb{Z}} d_m(q) \sum_{n \in \mathbb{Z}} w(n) \, e^{-2\pi i n \left(\frac{\gamma}{2\pi} q - \frac{m}{\kappa} \right)}.$$

With our hypothesis on $w(n)$ we know that

$$(4.17) \qquad \sum_{n \in \mathbb{Z} \setminus \{0\}} w(n) \, e^{-2\pi i n x}$$

is the derivative, in the distribution sense ([37], Chap. II, §4) of the piece-wise continuous periodic function $f_w(x)$, of period 1. From a classical result ([37], Chap. II, §2) we have the equality

$$
\sum_{n \in \mathbb{Z}} w(n) \, e^{-2\pi i n \left(\frac{\gamma}{2\pi} q - \frac{m}{\kappa} \right)}
$$

$$(4.18) \qquad = w(0) + f'_w \left(\frac{\gamma}{2\pi} q - \frac{m}{\kappa} \right) + \sum_{p \in \mathbb{Z}} \sigma_p \, \delta \left(\frac{\gamma}{2\pi} q - \frac{m}{\kappa} - a_p \right),$$

where f'_w has to be taken in a distributional sense.

Finally, we are led to the following formula for the Fourier transform of μ:

$$
\widehat{\mu}(q) = \sum_{m \in \mathbb{Z}} d_m(q) \left(w(0) + f'_w \left(\frac{\gamma}{2\pi} q - \frac{m}{\kappa} \right) \right) +
$$

$$(4.19) \qquad + \frac{2\pi}{\gamma} \sum_{m, p \in \mathbb{Z}} d_m(q) \, \sigma_p \, \delta \left(q - \frac{2\pi}{\gamma} \left(\frac{m}{\kappa} + a_p \right) \right)$$

within the framework of the distribution theory. With our hypothesis on f_w the first term of the right-hand side defines a regular tempered distribution. We infer from (4.19) that if the Fourier transform of the measure μ can be interpreted as a measure too, then the first term of the rhs of (4.19) may be interpreted as a "continuous part" of that measure. On the other hand, there is in (4.19) a pure point part which is supported by the dense set given by (4.9). $\qquad \square$

Note that the support of the pure point part $\widehat{\mu}_{pp}$ given by (4.9) is also equal to

$$(4.20) \qquad \frac{2\pi}{\gamma} \times \Big(\bigcup_{i \in \mathcal{N}_\beta} (a_i + \mathbb{Z}[\beta]) \Big)$$

where $\mathcal{N}_\beta$ is a subset of $\{a_1, a_2, \ldots, a_N\}$ such that $a_i, a_j \in \mathcal{N}_\beta, a_i - a_j \notin \mathbb{Z}[\beta]$ as long as $i \neq j$. There is no major problem to consider that $\{a_1, a_2, \ldots, a_N\}$ is already composed of discontinuities a_j algebraically independent over $\mathbb{Z}[\beta]$.

If all the singularities a_j are in $\mathbb{Z}[\beta]$, then this support is included in

$$\frac{2\pi}{\beta^2 \pm 1} \mathbb{Z}[\beta]$$

where "+" stands for **case (i)** whereas "−" is for **case (ii)** (see Proposition 2.9).

4.2. Diffraction spectrum of a set of weighted beta-integers

For the last two decades it has becoming traditional to define the *Bragg spectrum*, *i.e.* the more or less bright spots we see in a diffraction experiment on a long range order material, as the pure-point component of the measure defined by the Fourier transform $\widehat{\gamma}$ of the so-called autocorrelation γ of the measure μ (for the definition of γ, see [23]).

On the other hand, the function giving the intensity per diffracting site of $\mathbb{Z}_\beta$ is defined as [10] [22] [23] [25] [36]:

$$(4.21) \qquad I_w(q) = \limsup_{l \to \infty} \left| \frac{1}{\mathrm{card}(U_l)} \sum_{b_n \in U_l} w(n) e^{-iqb_n} \right|^2,$$

where $(U_l)_l$ is an averaging sequence of finite approximants to the set $\mathbb{Z}_\beta$ (Section 2.3). Under some assumptions on

  (i) the point set of diffractive sites, *e.g.* model sets, set $\mathbb{Z}_\beta$ etc.,
  (ii) the uniqueness of γ (see Theorem 3.4 in [23]),
  (iii) the existence of a limit in the sense of Bohr-Besicovich for the averaged Fourier transform of finite approximants of the measure μ (see Theorems 5.1 and 5.4 in [23]),

it can be shown that the values of (4.21) at the points of the pure-point spectrum of $\widehat{\mu}$ are the intensities of the Bragg peaks; see for instance Definition 3.1 in Strungaru [39]. This statement originates in the so-called

Bombieri-Taylor conjecture [6, 7]. Under such assumptions, the autocorrelation is even the sum of two pure point measures (Proposition 3.3 in [39]), the two parts being called strongly and null-weakly almost periodic after Argabright and Gil de Lamadrid [1] [21]. Though the general methodology for computing the diffraction spectrum of μ was provided earlier (by Meyer in Proposition 1 in [27] p 32), recent investigations on weighted Dirac combs [2] [9] [23] [39] show a need for introducing new theories to describe the structure of this spectrum.

By Section 3 the elements in $\mathbb{Z}_\beta$ are in one-to-one correspondence with elements of $(-\beta, \beta)$ (Proposition 3.1) by the $*$-operation. Let us denote by w^* the conjugate weight defined on the dense subset $\left(\mathbb{Z}_\beta^+\right)' \subset (-1, \beta)$ or $\left(\mathbb{Z}_\beta^+\right)' \subset [0, \beta)$ by

(4.22) $$w^*(b_n') = w(n), \qquad n \in \mathbb{N}.$$

We assume in the sequel that the function w^* can be extended to a continuous function in the interior of its support $\text{supp}(w^*) \subset (-1, \beta)$ or $\subset [0, \beta)$, and that it is integrable over the window $\text{supp}(w^*)$.

Let $\mathcal{L}$ be the space of complex-valued functions on $\mathbb{Z}_\beta$ (or equivalently on $\mathbb{Z}$ through $n \to b_n$). For $w \in \mathcal{L}$, we denote by $\|w\|$ the pseudo-norm ("norm 1") of Marcinkiewicz of w defined as

$$\|w\| = \limsup_{l \to +\infty} \frac{1}{\text{Card}(U_l)} \sum_{n \in \mathbb{Z}} |w(n)|$$

where $(U_l)_l$ is an averaging sequence of finite approximants of $\mathbb{Z}_\beta$. The Marcinkiewicz space $\mathcal{M}$ is the quotient space of the subspace

$$\{g \in \mathcal{L} \mid \|g\| < +\infty\}$$

of $\mathcal{L}$ by the equivalence relation $\mathcal{R}$ defined by

(4.23) $$h \, \mathcal{R} \, g \iff \|h - g\| = 0$$

(Bertrandias [4] [5], Vo Khac [43]). The class of w is denoted by $\overline{w}$ in $\mathcal{M}$. Though the definition of $\|\cdot\|$ depends upon the chosen averaging sequence $(U_l)_l$ the space $\mathcal{M}$ obviously does not. This equivalence relation is called Marcinkiewicz equivalence relation. The vector space $\mathcal{M}$ is normed with $\|\overline{g}\| = \|g\|$, and is complete (Bertrandias [4] [5], Vo Khac [43]). By $\mathcal{L}^\infty$ we will mean the subspace of $\mathcal{L}$ of bounded weights endowed with the $\mathcal{M}$-topology in the sequel.

PROPOSITION 4.2. — *Let $h, g \in \mathcal{L}$ such that $\overline{h}, \overline{g} \in \mathcal{M}$. Then, for $q \in \mathbb{R}$,*

(4.24) $$I_h(q) \leqslant \|h\|^2,$$

(4.25) $h \,\mathcal{R}\, g \implies I_h(q) = I_g(q).$

   Proof. — Immediate.   □

   The relation (4.25) means that the set of weighted Dirac combs on beta-integers is classified by the Marcinkiewicz relation. The intensity function I_w is a class function on $\mathcal{M}$. We now express the diffracting intensity $I_w(q)$ by taking the sequence $((-B_N) \cup B_N)_N$ as averaging sequence of finite approximants to $\mathbb{Z}_\beta$, in order to compute it. The following formulae are important in the sense that $I_w(q)$ is what we observe in diffraction experiment.

   THEOREM 4.3. — *Let $w \in \mathcal{L}^\infty$ be a weight on $\mathbb{Z}_\beta$. Assume that the singularities a_j are all in $\mathbb{Z}[\beta]$. Then the pure point part (Bragg part) of the intensity $I_w(q)$ is equal to*

$$I_w(q) =$$

(4.26) $\left| \dfrac{1}{|\mathrm{supp}(w^\star)|} \displaystyle\int_{-1}^{\beta} \left[w^\star(x) e^{iq'x} + w^\star(-x) e^{-iq'x} \right] dx \right|^2$ **case (i),**

(4.27) $\left| \dfrac{1}{|\mathrm{supp}(w^\star)|} \displaystyle\int_{0}^{\beta} \left[w^\star(x) e^{iq'x} + w^\star(-x) e^{-iq'x} \right] dx \right|^2$ **case (ii).**

*where $q = \frac{2\pi}{\beta^2 \pm 1}\kappa$ and $q' = \frac{2\pi\beta^2}{\beta^2 \pm 1}\kappa'$, with $\kappa \in \mathbb{Z}[\beta]$, and where "+" stands for **case (i)** whereas "−" is for **case (ii)**.*

   Proof. — The intensity function is equal to :
(4.28)

$$I_w(q) = \limsup_{N \to \infty} \left| \frac{1}{2c_N - 1} \sum_{b_n \in B_N} \left[w(n) e^{-iqb_n} + w(-n) e^{iqb_n} - w(o) \right] \right|^2.$$

Note that the term $w(o)$ can be dropped for obvious reasons. The Galois conjugation $\kappa = r + s\beta \to \kappa' = r \mp s\frac{1}{\beta}$, $r, s \in \mathbb{Z}$ (**case (i)** or **case (ii)**) in the ring $\mathbb{Z}[\beta]$ leads to:

(4.29) $\dfrac{\kappa}{\beta^2 \pm 1} \pm \dfrac{\beta^2 \kappa'}{\beta^2 \pm 1} \in \mathbb{Z}.$

So we can write, for any $q \in \frac{2\pi}{\beta^2 \pm 1}\mathbb{Z}[\beta]$,

(4.30) $qb_n \equiv -q'b'_n \mod (2\pi\mathbb{Z}),$

where we have denoted by q' the number $\pm\frac{2\pi\beta^2}{\beta^2 \pm 1}\kappa'$ if $q = \frac{2\pi}{\beta^2 \pm 1}\kappa$ for $\kappa \in \mathbb{Z}[\beta]$ ("+" stands for **case (i)** whereas "−" is for **case (ii)**). Hence, the intensity

(4.28) can be rewritten as

$$(4.31) \quad I_w(q) =$$

$$\limsup_{N \to \infty} \left| \frac{1}{2c_N - 1} \sum_{b_n \in B_N} \left[w(n)e^{iq'b'_n} + w(-n)e^{-iq'b'_n} - w(o) \right] \right|^2.$$

Let us now use the "algebraic cut-and-project" properties (3.11) and (3.12) of the positive beta-integers and the fact that the sets $\mathbb{Z}_\beta^+$ arise from model sets. The conjugate sets $\left(\mathbb{Z}_\beta^+ \right)' = \{ x \in \mathbb{Z}[\beta] \cap (-1, \beta) \mid x' \geqslant 0 \}$ (**case (i)**) and $\left(\mathbb{Z}_\beta^+ \right)' = \{ x \in \mathbb{Z}[\beta] \cap [0, \beta) \mid x' \geqslant 0 \}$ (**case (ii)**) densely fill the intervals $(-1, \beta)$ (of length $1 + \beta$) and $[0, \beta)$ (of length β) respectively with uniform distribution modulo 1. Hence we can assert that the finite sum

$$\frac{1}{2c_N} \sum_{b_n \in B_N} \left[w(n)e^{iq'b'_n} + w(-n)e^{-iq'b'_n} \right]$$

is just a Riemann sum approximating, for large N and for "reasonable" weight w, the integral :

$$\frac{1}{2c_N} \sum_{b_n \in B_N} \left[w(n)e^{iq'b'_n} + w(-n)e^{-iq'b'_n} \right]$$

$$(4.32) \quad \approx \frac{1}{|\mathrm{supp}(w^\star)|} \int_{-1}^{\beta} \left[w^\star(x)e^{iq'x} + w^\star(-x)e^{-iq'x} \right] dx, \quad \textbf{case (i)}$$

$$(4.33) \quad \approx \frac{1}{|\mathrm{supp}(w^\star)|} \int_{0}^{\beta} \left[w^\star(x)e^{iq'x} + w^\star(-x)e^{-iq'x} \right] dx, \quad \textbf{case (ii)}.$$

At the limit, using Proposition 2.9, we obtain (4.26) and (4.27).   □

The proof of Theorem 4.3 shows that the limsup (4.21) becomes a true limit because we have used the formalism of cut-and-project schemes and that the positive and negative parts of the beta-integers can be interpreted in terms of model sets.

Let us now consider discontinuities a_j not in $\mathbb{Z}[\beta]$. Theorem 4.3 gives an expression of $I_w(q)$ as a continuous function of the variable q'. Since $q' \in \frac{2\pi\beta^2}{\beta^2 \pm 1} \mathbb{Z}[\beta]$ and that $\mathbb{Z}[\beta]$ is dense in $\mathbb{R}$, we can prolongate by continuity the intensity function $I_w(q)$ given by (4.26) or (4.27): if $q \in \frac{2\pi}{\gamma} \left(\bigcup_{j=1}^{N} (a_j + \mathbb{Z}[\beta]) \right)$, there exist $j \in \{1, 2, \ldots, N\}$ and $\kappa \in \mathbb{Z}[\beta]$ such that

$$q = \frac{2\pi}{\beta^2 \pm 1} (a_j + \kappa), \qquad \kappa \in \mathbb{Z}[\beta].$$

It suffices to take any sequence $(a_{j,l})_{l \geqslant 0}$ of elements of $\mathbb{Z}[\beta]$ which converges to the discontinuity a_j:

$$a_j = \lim_{l \to \infty} a_{j,l}$$

and to compute the associated numbers

$$q_l = \frac{2\pi}{\beta^2 \pm 1}(a_{j,l} + \kappa), \qquad q_l' = \pm \frac{2\pi\beta^2}{\beta^2 \pm 1}(a_{j,l}' + \kappa').$$

Then the intensity $I_w(q)$ is given by

$$I_w(q) = I_w(\lim_{l \to \infty} q_l) = \lim_{l \to \infty} I_w(q_l)$$

where $I_w(q_l)$ is computed by (4.26) or (4.27) using q_l' and passing to the limit $q' = \lim_{l \to \infty} q_l'$.

Let us now give simple or standard examples. For a uniform distribution $w(n) = 1$, Formula (4.26) reduces to

$$(4.34) \qquad I_w(q) = 4 \left(\cos \frac{q'(\beta - 1)}{2} \right)^2 \left(\operatorname{sinc} \frac{q'(\beta + 1)}{2} \right)^2,$$

where $\operatorname{sinc}(x) = \dfrac{\sin x}{x}$ designates the sinus cardinal. On the other hand, Formula (4.27) becomes

$$(4.35) \qquad I_w(q) = 4 \left(\operatorname{sinc} \frac{q'\beta}{2} \right)^2,$$

In **Case (i)**, for a model set Σ^Ω, determined algebraically by a window $\Omega \subset [-1, 1]$ through the sieving procedure

$$(4.36) \qquad \Sigma^\Omega = \{x \in \mathbb{Z}[\beta] \mid x' \in \Omega\} = \{x \in \mathbb{Z}_\beta \mid x' \in \Omega\},$$

where the corresponding weight is given by $w^\star(x) = \chi_\Omega(x)$ the characteristic function of Ω: then the diffraction intensity of such a model set is given by

$$(4.37) \qquad I_w(q) = 4 \left| \frac{1}{|\Omega|} \int_\Omega e^{iq'x} \, dx \right|^2.$$

In **Case (ii)**, dealing with model sets for the computation of the intensity function forces us to consider the decorated version (Section 3) of $\mathbb{Z}_\beta$. A slight adaptation of the above formalism becomes then necessary.

Our aim is to reconstruct to a certain extent (the phase problem!) the weight function $n \to w(n)$ through its "Galois conjugate" $(-1, \beta)$ or $[0, \beta) \ni x \to w^\star(x)$. This reconstruction should take into account the partitioning of the Marcinkiewicz classes, and what we may expect is probably the reconstruction of a peculiar representant for each class. This reconstruction

can be partially implemented through a sort of multiresolution analysis of the intensity function $I_w(q)$, a method developed in [12] and [11]. There are alternative expressions for $I_w(q)$ which could reveal themselves useful for this so-called homometry problem.

4.3. Diffraction spectrum of a weighted beta-lattice

Theorem 4.1 and Theorem 4.3 give the pure point part of the diffraction spectra of weighted beta-integers. We are now ready to deduce the Bragg part of diffraction spectra of weighted Delone sets on beta-lattices in general (see Figure 4.3 for an illustration).

Let us briefly recall what is a beta-lattice. We report to [13] for the full description of symmetry groups on beta-lattices.

Beta-lattices are aimed to replace lattices in the context of quasicrystals. They are based on beta-integers, like lattices are based on integers:

$$(4.38) \qquad \Gamma = \sum_{i=1}^{d} \mathbb{Z}_\beta \mathbf{e}_i \,,$$

with $(\mathbf{e}_i)_{1 \leqslant i \leqslant d}$ a base of $\mathbb{R}^d, d \geqslant 1$. Figure 4.1 gives the example of the tau-lattice (or tau-grid) $\Gamma_1(\tau) = \mathbb{Z}_\tau + e^{\frac{i\pi}{5}} \mathbb{Z}_\tau$ in $\mathbb{R}^2$.
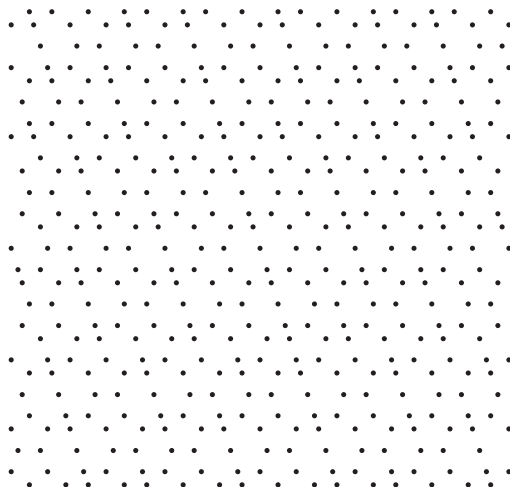

Figure 4.1. τ-lattice $\Gamma_1(\tau) = \mathbb{Z}_\tau + e^{\frac{i\pi}{5}} \mathbb{Z}_\tau$ in $\mathbb{R}^2$.

Beta-lattices are eligible frames in which one could think of the properties of quasiperiodic point-sets and tilings, thus generalizing the notion of lattice in periodic cases.

As a matter of fact, it has become like a paradigm that geometrical supports of quasi-crystalline structures should be Delone sets obtained through "cut and projection" from higher-dimensional lattices. Now, it is easily understood from Section 3 that most of such cut-and-project sets are subsets of suitably rescaled beta-lattices. We show in Figure 4.2 a cut-and-project 2D decagonal set and its embedding into the tau-lattice of Figure 4.1 is shown in Figure 4.3.
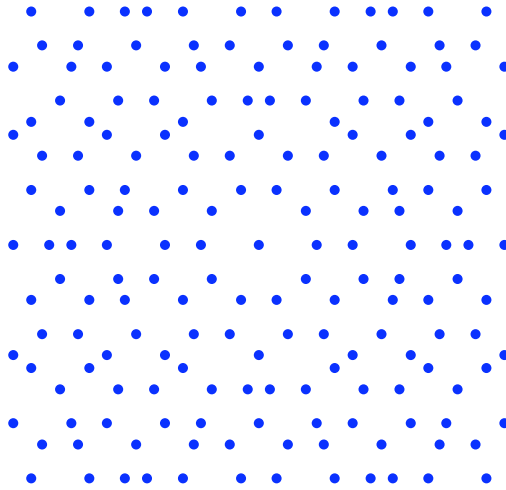

Figure 4.2. *A decagonal cut-and-project set*

It is well known that the condition $2\cos(2\pi/N) \in \mathbb{Z}$, *i.e.* $N = 1, 2, 3, 4$ and 6, characterizes N-fold Bravais lattices in $\mathbb{R}^2$ (and in $\mathbb{R}^3$) (see also [3] for Pisot-Cyclotomic numbers). Now, what can we do when N is quasicrystallographic *i.e.* $N = 5, 10, 8$ and 12, respectively associated with one of the cyclotomic Pisot units $\tau = 2\cos(2\pi/10)$, $\delta = 1 + 2\cos(2\pi/8)$ and $\theta = 2 + 2\cos(2\pi/12)$? Possible answers are provided by beta-lattices in the plane. These point sets are defined as

$$(4.39) \qquad\qquad \Gamma_q(\beta) = \mathbb{Z}_\beta + \mathbb{Z}_\beta \zeta^q \,,$$

with $\zeta = e^{i\frac{2\pi}{N}}$, for $1 \leqslant q \leqslant N-1$. Besides the example of tau-lattice shown in Figure 4.1, beta-lattices for $\beta = \tau, \delta$, and θ are given in [13]. Note the following important features:
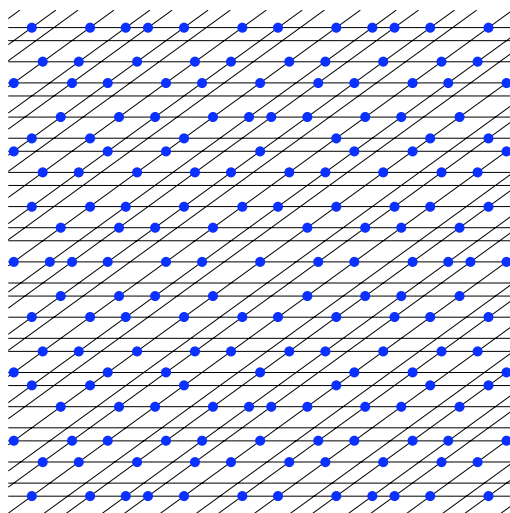
Figure 4.3. *Embedding of the cut-and-project set of Figure 4.2 into the τ-lattice of Figure 4.1. The τ-lattice is here the set of the intersection points of the lines.*

- they are lattices for a new internal law $\oplus$: $\Gamma_q(\beta) \oplus \Gamma_q(\beta) = \Gamma_q(\beta)$,
- they are self-similar: $\beta\Gamma_q(\beta) \subset \Gamma_q(\beta)$,
- they satisfy a more general "quasi" self-similarity (with new external law): $\mathbb{Z}_\beta \otimes \Gamma \subset \Gamma$,
- however, they are neither rotationally invariant nor translationally invariant,
- as already pointed out [8] [13], a large class of aperiodic sets like model sets (or "cut-and-project" sets), currently used by physicists as geometric models supporting atomic sites in quasicrystals, can be embedded in these beta-lattices $\Gamma_q(\beta)$ or in some "decorated" version of them.

Let us extend to higher dimensional cases the formulae (4.26) and (4.27) for the Bragg part of the diffraction intensity. It is more or less straightforward, depending on the chosen weight and geometry. For the sake of simplicity, the general case being similar, we consider here the plane $(d = 2)$ case $\beta = \tau$ only and its corresponding tau-grid, actually the simplest one among several possible ones :

$$(4.40) \qquad \Gamma_1 = \left\{ z \in \mathbb{C} \mid z_{m,n} = b_m + b_n e^{i\frac{\pi}{5}}, \ b_m, b_n \in \mathbb{Z}_\tau \right\}.$$

This discrete set is a subset of the dense cyclotomic ring $\mathbb{Z}[e^{i\frac{\pi}{5}}] = \mathbb{Z}[\tau] + \mathbb{Z}[\tau]e^{i\frac{\pi}{5}}$.

We now consider the pure point measure supported by Γ_1 :

$$(4.41) \qquad \mu = \sum_{m,n\in\mathbb{Z}} w(m,n)\delta_{z_{m,n}}$$

where $(x,y) \to w(x,y)$ is a generally complex-valued weight, assumed split as follows:

$$w(m,n) \;=\; w_1(m)w_2(n), \qquad \text{with } w_1, w_2 \in \mathcal{L}^\infty.$$

The Fourier transform of the measure (4.41) is defined (in a distributional sense), by

$$(4.42) \qquad \widehat{\mu}(\mathbf{k}) = \mu\left(e^{-i\mathbf{k}\cdot\mathbf{z}_{m,n}}\right) = \sum_{m,n\in\mathbb{Z}} w(m,n)e^{-i\mathbf{k}\cdot\mathbf{z}_{m,n}},$$

where $\mathbf{z}_{m,n}$ denotes the vector defined by the complex $z_{m,n}$.

We choose to study the diffraction pattern in the plane with "oblique" components (k_1, k_2) of the wavevector $\mathbf{k}$, namely components defined through the Euclidean scalar product $\mathbf{k} \cdot \mathbf{z}_{m,n}$, with $\mathbf{k} = \left(k_1 + k_2 \cos\left(\frac{\pi}{5}\right)\right)\mathbf{e}_1 + k_2\sin\left(\frac{\pi}{5}\right)\mathbf{e}_2$, $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$ in the plane reads as :

$$(4.43) \qquad \mathbf{k} \cdot \mathbf{z}_{m,n} = b_m\left(k_1 + k_2 \cos\left(\frac{\pi}{5}\right)\right) + b_n\left(k_2 + k_1 \cos\left(\frac{\pi}{5}\right)\right).$$

Hence, the Fourier transform (4.42) of the measure factorizes as the product of two one-dimensional Fourier transform of the type (4.2) :

$$(4.44) \qquad \widehat{\mu}(\mathbf{k}) = \left(\sum_{m\in\mathbb{Z}} w_1(m)e^{-iq_1 b_m}\right)\left(\sum_{n\in\mathbb{Z}} w_2(n)e^{-iq_2 b_n}\right),$$

with $q_1 = \left(k_1 + k_2\cos\left(\frac{\pi}{5}\right)\right)$, $q_2 = \left(k_2 + k_1\cos\left(\frac{\pi}{5}\right)\right)$, i.e.

$$k_1 = \frac{q_1 - q_2\cos\left(\frac{\pi}{5}\right)}{\sin^2\left(\frac{\pi}{5}\right)} = \frac{1}{\tau^2+1}\left(4\tau^2 q_1 - 2\tau^3 q_2\right),$$

$$k_2 = \frac{q_2 - q_1\cos\left(\frac{\pi}{5}\right)}{\sin^2\left(\frac{\pi}{5}\right)} = \frac{1}{\tau^2+1}\left(4\tau^2 q_2 - 2\tau^3 q_1\right)$$

Since we know from Section 4.1 that the pure-point support of each factor in the rhs of (4.44) is $\frac{2\pi}{\tau^2+1}\mathbb{Z}[\tau]$, we conclude that the pure-point part of the diffraction is supported by the cyclotomic ring up to a scale factor :

$$(4.45) \qquad \mathbf{k} = k_1 + k_2 e^{i\frac{\pi}{5}} \in \frac{2\pi}{(\tau^2+1)^2}\,\mathbb{Z}[e^{i\frac{\pi}{5}}],$$

in (abusive) complex notations.

The computation of the corresponding intensity function is just a repetition of the computation for the one-dimensional case :

$$I_w(\mathbf{k}) = \left| \left[\frac{1}{|\operatorname{supp}(w_1^\star)|} \int_{-1}^{\tau} \left[w_1^\star(x)e^{iq_1'x} + w_1^\star(-x)e^{-iq_1'x} \right] dx \right] \times \right.$$

$$\left. (4.46) \qquad \times \left[\frac{1}{|\operatorname{supp}(w_2^\star)|} \int_{-1}^{\tau} \left[w_2^\star(x)e^{iq_2'x} + w_2^\star(-x)e^{-iq_2'x} \right] dx \right] \right|^2 .$$

For instance, for the tau-grid itself with a uniform distribution :

$$(4.47) \qquad I(\mathbf{k}) = 16 \left(\cos\frac{q_1'}{2\tau} \cos\frac{q_2'}{2\tau} \right)^2 \left(\operatorname{sinc}\frac{q_1'\tau^2}{2} \operatorname{sinc}\frac{q_2'\tau^2}{2} \right)^2 .$$

For a non-split weight $w(m,n) \neq w_1(m)w_2(n)$, it is clear that we have to resume the approach we have followed in the one-dimensional case within the theory of distributions. However, we expect that the result concerning the pure-point support of the Fourier transform will not appear different of (4.45).

Acknowledgements

BIBLIOGRAPHY

[1] L. ARGABRIGHT & J. GIL DE LAMADRID, *Fourier Analysis of Unbounded Measures on Locally Compact Abelian Groups*, Memoirs of the American Mathematical Society, vol. 145, American Mathematical Society, Providence, RI, 1974.

[2] M. BAAKE & R. V. MOODY, "Weighted Dirac combs with pure point diffraction", *J. Reine Angew. Math.* **573** (2004), p. 61-94.

[3] J. P. BELL & K. G. HARE, "A Classification of (some) Pisot-Cyclotomic Numbers", *J. Number Theory* **115** (2005), p. 215-229.

[4] J.-P. BERTRANDIAS, "Espaces de fonctions continues et bornées en moyenne asymptotique d'ordre p", *Mémoire Soc. Math. France* (1966), no. 5, p. 3-106.

[5] J.-P. BERTRANDIAS, J. COUOT, J. DHOMBRES, M. MENDÈS-FRANCE, P. PHU HIEN & K. VO KHAC, *Espaces de Marcinkiewicz, corrélations, mesures, systèmes dynamiques*, Masson, Paris, 1987.

[6] E. BOMBIERI & J. E. TAYLOR, "Which distributions diffract? An initial investigation", *J. Phys. Colloque* **47** (1986), no. C3, p. 19-28.

[7] ———, "Quasicrystal, tilings, and algebraic number theory: Some preliminary connections", in *The legacy of S. Kovalevskaya*, Contemporary Mathematics, vol. 64, American Mathematical Society, Providence, RI, 1987, p. 241-264.

[8] Č. Burdík, C. Frougny, J.-P. Gazeau & R. Krejčar, "Beta-integers as natural counting systems for quasicrystals", *J. of Physics A: Math. Gen.* **31** (1998), p. 6449-6472.

[9] A. Cordoba, "Dirac combs", *Lett. Math. Phys.* **17** (1989), p. 191-196.

[10] J.-M. Cowley, *Diffraction Physics*, North-Holland, Amsterdam, 1986, 2nd edition.

[11] F. Denoyer, A. Elkharrat & J.-P. Gazeau, "Beta-lattice multiresolution of quasicrystalline Bragg peaks", submitted, 2006.

[12] A. Elkharrat, "Scale dependent partitioning of one-dimensional aperiodic set diffraction", *Europ. Phys. J.* **B39** (2004), p. 287-294, and Thèse de l'Université Paris 7 - Denis Diderot (2004).

[13] A. Elkharrat, C. Frougny, J.-P. Gazeau & J.-L. Verger-Gaugry, "Symmetry groups for beta-lattices", *Theor. Comp. Sci.* **319** (2004), no. 1-3, p. 281-305.

[14] S. Fabre, "Substitutions et β-systèmes de numération", *Theor. Comp. Sci.* **137** (1995), p. 219-236.

[15] A. S. Fraenkel, "Systems of numeration", *Amer. Math. Monthly* **92** (1985), no. 2, p. 105-114.

[16] C. Frougny, "Number Representation and Finite Automata", *London Math. Soc. Lecture Note Ser.;* **279** (2000), p. 207-228.

[17] C. Frougny, J.-P. Gazeau & R. Krejčar, "Additive and multiplicative properties of point-sets based on beta-integers", *Theor. Comp. Sci.* **303** (2003), p. 491-516.

[18] C. Frougny & B. Solomyak, "Finite beta-expansions", *Ergod. Theor. Dynam. Syst.* **12** (1992), p. 713-723.

[19] J.-P. Gazeau, "Pisot-cyclotomic integers for quasilattices", in *The Mathematics of Long-Range Aperiodic Order* (R. Moody, ed.), NATO advances Science Institutes, Series C: Mathematical and Physical Sciences 489, Kluwer Academic Publishers, Dordrecht, 1997, p. 175-198.

[20] J.-P. Gazeau & J.-L. Verger-Gaugry, "Geometric study of the beta-integers for a Perron number and mathematical quasicrystals", *J. Théorie Nombres Bordeaux* **16** (2004), p. 125-149.

[21] J. Gil de Lamadrid & L. Argabright, "Almost Periodic Measures", *Memoirs of the American Mathematical Society, American Mathematical Society, Providence, RI* **85** (1990), no. 428, p. vi+219.

[22] A. Guinier, *Theory and Techniques for X-Ray Crystallography*, Dunod, Paris, 1964.

[23] A. Hof, "On diffraction by aperiodic structures", *Commun. Math. Phys.* **169** (1995), p. 25-43.

[24] J. C. Lagarias, "Geometric Models for Quasicrystals I. Delone Sets of Finite Type", *Discr. Comput. Geom.* **21** (1999), p. 161-191.

[25] ———, "Mathematical Quasicrystals and the problem of diffraction", in *Directions in Mathematical Quasicrystals* (M. Baake & R. V. Moody, eds.), CRM Monograph Series, Amer. Math. Soc., Providence, RI, 2000, p. 61-93.

[26] M. Lothaire, *Algebraic Combinatorics on Words*, Cambridge University Press, 2002.

[27] Y. Meyer, "Nombres de Pisot, Nombres de Salem et Analyse Harmonique", in *Lect. Notes Math.*, vol. 117, Springer, 1969, p. 63.

[28] ———, *Algebraic Numbers and Harmonic Analysis*, North-Holland, 1972.

[29] ———, "Quasicrystals, Diophantine approximation and algebraic numbers", in *Beyond Quasicrystals* (F. Axel & D. Gratias, eds.), Springer-Verlag & Les Editions de Physique, 1995, p. 3-16.

[30] R. V. Moody, "Meyer sets and their duals", in *The Mathematics of Long-Range Aperiodic Order* (R. V. Moody, ed.), Kluwer, 1997, p. 403-442.

[31] ———, "From quasicrystals to more complex systems", in *Model Sets: A Survey* (F. Axel, F. Denoyer & J.-P. Gazeau, eds.), Springer & Les Editions de Physique, 2000, p. 145-166.

[32] G. Muraz & J.-L. Verger-Gaugry, "On lower bounds of the density of Delone sets and holes in sequences of sphere packings", *Exp. Math.* **14** (2005), no. 1, p. 47-57.

[33] W. Parry, "On the β-expansions of real numbers", *Acta Math. Acad. Sci. Hungar.* **11** (1960), p. 401-416.

[34] N. Pythéas Fogg, "Substitutions in dynamics, arithmetics and combinatorics", in *Lecture Notes in Math.*, vol. 1794, Springer, 2003.

[35] A. Rényi, "Representations for real numbers and their ergodic properties", *Acta Math. Acad. Sci. Hung.* **8** (1957), p. 477-493.

[36] M. Schlottmann, "Cut-and-Project sets in locally compact Abelian groups", in *Quasicrystals and Discrete Geometry* (J. Patera, ed.), Fields Institute Monograph Series, vol. 10, Amer. Math. Soc., Providence, RI, 1998, p. 247-264.

[37] L. Schwartz, *Théorie des distributions*, Hermann, Paris, 1973.

[38] D. Shechtman, I. Blech, D. Gratias & J. Cahn, "Metallic phase with long-range orientational order and no translational symmetry", *Phys. Rev. Lett.* **53** (1984), p. 1951-1953, 1951.

[39] N. Strungaru, "Almost Periodic Measures and Long-Range Order in Meyer Sets", *Discr. Comput. Geom.* **33** (2005), p. 483-505.

[40] W. P. Thurston, "Groups, tilings, and finite state automata", A.M.S. Colloquium Lectures, Boulder, Summer 1989.

[41] J.-L. Verger-Gaugry, "On gaps in Rényi β-expansions of unity for $\beta > 1$ an algebraic number", Annales Institut Fourier, 2006.

[42] ———, "On self-similar finitely generated uniformly discrete (SFU-) sets and sphere packings", in *Number Theory and Physics* (L. Nyssen, ed.), IRMA Lectures in Mathematics and Theoretical Physics, E.M.S. Publishing House, 2006.

[43] K. Vo Khac, "Fonctions et distributions stationnaires. Application à l'étude des solutions stationnaires d'équations aux dérivées partielles", in *Espaces de Marcinkiewicz, corrélations, mesures, systèmes dynamiques*, Masson, Paris, 1987, p. 11-57.

Jean-Pierre GAZEAU
Université Paris 7-Denis Diderot
APC - UMR CNRS 7164
Boite 7020
75251 Paris cedex 05 (France)
gazeau@ccr.jussieu.fr

Jean-Louis VERGER-GAUGRY
Université Grenoble I
Institut Fourier - UMR CNRS 5582
BP 74
38402 Saint-Martin d'Hères (France)
jlverger@ujf-grenoble.fr