

# From Quasicrystal to Crystallines

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The mathematical definitions of quasicrystals and crystallines are discussed within the framework of aperiodic crystals. It is shown that these are two different generalisations of ideal crystals, sharing long-range order and having completely different properties regarding short-range behaviour.

topics: quasicrystal, crystalline measure, Poisson summation formula, metric graphs

## 1. Introduction

The goal of this note is to sketch recent developments in the theory of aperiodic crystals, related to the discovery of crystallines — a new type of discrete sets that generalises the notion of classical periodic crystals. We restrict our discussion to one dimension, in which crystalline sets (more precisely, strong crystalline sets) have been completely classified as zero sets of trigonometric polynomials. We study these sets in relation to another family of aperiodic crystals, called quasicrystals, which have been studied by physicists over the last 40 years. Our goal is not to provide a rigorous treatment of the problem, but rather to present our results using physical language, hoping it will be useful for theoretical and experimental physicists. The mathematical details can be found in our upcoming paper with Yves Meyer and Peter Sarnak [1].

## 2. What is a crystal?

In mathematics, every crystal is associated with a discrete set of points, called atoms. It is natural to require that there is a minimal distance between the atoms and that there are no arbitrarily large holes in the structure. Such sets are called Delaunay (or Delone) sets.

**Definition 1.** A set  $\Lambda \subset \mathbb{R}^d$  is called Delaunay if it is

- uniformly discrete, i.e., there exists  $r > 0$  such that

$$\lambda_i, \lambda_j \in \Lambda, \lambda_i \neq \lambda_j \Rightarrow |\lambda_i - \lambda_j| > r, \quad (1)$$

and

- relatively dense, i.e., there exists  $R > 0$ , such that every ball  $\mathbb{B}_R(x)$  of radius  $R$  contains at least one point from the set,

$$\forall x \in \mathbb{R}^d \Rightarrow \mathbb{B}_R(x) \cap \Lambda \neq \emptyset. \quad (2)$$

These sets were originally named  $(r, R)$ -sets by Boris Delaunay. This definition introduces both local and global requirements on the set, but these are too weak to characterise crystals among all discrete sets.

For centuries, only perfectly periodic, or ideal, crystals were considered in crystallography. Any such discrete set is automatically a Delaunay set, because the configuration of atoms in the elementary cell is repeated periodically.

After the discovery of quasicrystals (discussed below), crystallographers changed the definition of a crystal to [2]

“A material is a crystal if it has essentially a sharp diffraction pattern...”

This new definition means that each crystal should have certain long-range order, leading to peaks in the diffraction pattern.

In discussing how such systems can be obtained in physical reality, it was suggested that they are created by repeating a finite number of local patterns, leading to an aperiodic structure. Probably the most well-known example is given by Penrose tiling [3], which covers the plane by rombs of two different shapes.

## 3. Quasicrystals

Quasicrystals were first observed by Dan Schechtman [4] and Dov Levine and Paul Steinhardt [5, 6], and were followed by the remarkable discovery of such structures in nature [7, 8]. One may trace the history of quasicrystals to medieval tilings in Central Asia or to the aperiodic tilings by Hao Wang and Robert Berger [9, 10]. It appears that Meyer sets and cut-and-project sets [11, 12], introduced at least ten years before the discovery of

quasicrystals by physicists, give one of mathematical interpretations for these sets [13]. It is clear that the experimental observation of quasicrystals inspired a rapid mathematical development of the theory. In particular, Galiulin proposed the concept of ‘zonohedral’ Delaunay sets, whose identity to Meyer sets are proven by Lagarias [14]. A Delaunay set  $\Lambda$  is called Meyer set if  $\Lambda - \Lambda \subset \Lambda + F$ , where  $F$  is a certain finite set. A Delaunay set  $\Lambda$  is zonohedral (or quasiregular, as Lagarias called it) if  $\Lambda - \Lambda$  is again a Delaunay set. For such sets, there exist finitely many local patterns; the neighbours to any atom in the set always belong to one of these patterns.

The most inclusive mathematical definition of a quasicrystal was proposed by Lagarias under the name of Delaunay sets of finite type [15].

**Definition 2.** A Delaunay set of finite type, is a Delaunay set  $\Lambda$  such that  $\Lambda - \Lambda$  is a discrete closed subset of  $\mathbb{R}^n$ , i.e., the intersection of  $\Lambda - \Lambda$  with any closed ball is a finite set.

These sets again have finitely many local patterns [16]. Nevertheless, the cut-and-project method remains the most common recipe to construct mathematical quasicrystals. In many examples, mathematicians removed the requirement on a set to be uniformly discrete and sometimes consider even sets that are dense in the space.

#### 4. Crystallines

An alternative approach to Delaunay sets, with long-range order, was proposed by Kahane and Mandelbrojt [17] following Hamburger’s studies of the functional equation satisfied by Riemann’s  $\zeta$ -function [18]. They introduced crystalline measures.

**Definition 3.** [19] An atomic measure  $\mu$  on  $\mathbb{R}^d$  is a crystalline measure if it is a tempered distribution and both  $\mu$  and its Fourier transform  $\hat{\mu}$  are supported by discrete subsets  $\Lambda$  and  $S$  of  $\mathbb{R}^d$ ,

$$\mu = \sum_{\lambda \in \Lambda} a_\lambda \delta_\lambda \quad \text{and} \quad \hat{\mu} = \sum_{s \in S} b_s \delta_s. \quad (3)$$

If, in addition, both  $|\mu|$  and  $|\hat{\mu}|$  are tempered, then  $\mu$  is called “strong crystalline measure”.

Strong crystalline measures defined above are usually called “Fourier quasicrystals”, but we prefer to distinguish them from usual quasicrystals and follow [20].

The formulae given in (3) naturally lead to the Poisson-type summation formula

$$\sum_{\lambda \in \Lambda} a_\lambda f(\lambda) = \sum_{s \in S} b_s \hat{f}(s). \quad (4)$$

When speaking about sets in  $\mathbb{R}^d$  we are going to identify these sets with the corresponding counting measure and call them a discrete set  $\Lambda$  crystalline and a strong crystalline set if the corresponding counting measure

$$\mu_\Lambda = \sum_{\lambda \in \Lambda} \delta_\lambda \quad (5)$$

is a crystalline measure and a strong crystalline measure, respectively. Our focus will be on strong crystalline sets, which are also Delaunay sets. We simply call such sets crystallines.

The Dirac comb  $\sum_{n \in \mathbb{Z}} \delta_n$  is a trivial example of a crystalline; the corresponding formula (4) is simply the classical Poisson summation formula. Other trivial examples of crystallines are given by finite linear combinations of scaled and shifted Dirac combs. Only periodic trivial crystalline sets are also Delaunay.

The first non-trivial crystallines were constructed by Kurasov and Sarnak [21] using the trace formula proven earlier for Laplacian functions on metric graphs [22–26]. Every strong crystalline multiset<sup>†1</sup> in  $\mathbb{R}^1$  is given by this construction [27, 28].

In this approach, every crystalline multiset is determined by

- a Lee-Yang multivariate polynomial  $P(\mathbf{z})$ :
  - no zeros inside the unit disk  $|z_j| < 1$  ( $j = 1, 2, \dots, n$ )  $\Rightarrow P(\mathbf{z}) \neq 0$ ;
  - no zeros inside the dual disk  $|z_j| > 1$  ( $j = 1, 2, \dots, n$ )  $\Rightarrow P(\mathbf{z}) \neq 0$ ;

and

- a positive vector  $\ell = (\ell_1, \ell_2, \dots, \ell_n) \in \mathbb{R}_+^n$ .

Then, to get a crystalline set, one considers the trigonometric polynomial

$$p(k) := P(e^{ik\ell}) = \sum_{1 \leq j \leq N} c_j e^{i\gamma_j k}, \quad (5)$$

where  $N \in \mathbb{N}$ ,  $c_j \in \mathbb{C}$ ,  $\gamma_j \in \mathbb{R}_+$ . All zeros of this trigonometric polynomial are real,

$$\begin{cases} \text{Im}(k) > 0 \Rightarrow |e^{ik\ell_j}| < 1, \\ \text{Im}(k) < 0 \Rightarrow |e^{ik\ell_j}| > 1, \end{cases} \Rightarrow P(e^{ik\ell}) \neq 0. \quad (6)$$

We denote by  $\Lambda$  the zero set of the trigonometric polynomial, thus

$$\Lambda(p) \equiv \Lambda(P, \ell) = \left\{ k_j : p(k_j) = 0 \right\} \subset \mathbb{R}. \quad (7)$$

It appears that every such  $\Lambda$  associated with a trigonometric polynomial  $p$  is a strong crystalline set. This set can be viewed as the intersection on the unit torus  $\mathbb{T}^n = \{z \in \mathbb{C}^n : |z_j| = 1\}$  between the

<sup>†1</sup>Multiset means that every point in it is equipped with a multiplicity indicating how many times this points is repeated.

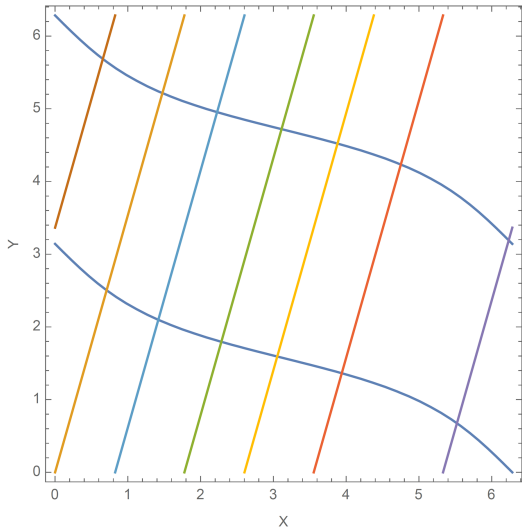


Fig. 1. The zero set of the trigonometric polynomial  $p(k)$  as the intersection between the zero set of  $P(z)$  and the line  $k\ell$ .

curve  $e^{ik\ell}$  ( $k \in \mathbb{R}$ ) and the zero set of the multivariate polynomial  $P(z)$  (see Fig. 1, where the real representation of the two-dimensional torus is used).

To prove that the counting measure

$$\mu(k) := \sum_{k_j: p(k_j) \equiv P(e^{ik\ell})=0} \delta_{k_j} \quad (8)$$

is crystalline, one may use the fact that it can be obtained by integrating the jump of the logarithmic derivative of  $p(k)$  on the real axis

$$\mu(k) = \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} dk \left[ \frac{p'(k+i\epsilon)}{p(k+i\epsilon)} - \frac{p'(k-i\epsilon)}{p(k-i\epsilon)} \right]. \quad (9)$$

The proof of the corresponding summation formula can be found in [21] and is similar to the proof of the trace formula for metric graphs.

Olevskii and Ulanovskii [28] showed that any strong crystalline set can be obtained as zeros of a real-rooted trigonometric polynomial. Alon, Cohen and Vinzant established that any real-rooted trigonometric polynomial comes from the Kurasov–Sarnak construction described above [27].

By choosing the trigonometric polynomial in a proper way, one obtains strong crystalline sets, which are in addition Delaunay and thus can be considered aperiodic crystals. It remains to be shown that reflection from such sets has a sharp diffraction pattern. A mathematically rigorous definition of the diffraction pattern is associated with the auto-correlation measures. The auto-correlation measure for strong crystallines was calculated in [29]. It is given by the sum of delta functions supported by the discrete set  $\mathcal{A}'$ . (Paper [29] is devoted to a multidimensional analog of the Kurasov–Sarnak construction, but the results hold even for one-dimensional crystalline measures.) This means that crystallines

have a very strong long-range order described by the trigonometric polynomial  $p(k)$ , while the only observed short-range order is uniform discreteness.

## 5. Comparison

Let us compare the two generalisations of ideal crystals described in this paper, namely quasicrystals and crystallines. As we already mentioned, quasicrystals are always characterized by short-range order in the sense that there are finitely many local patterns. In one dimension, this property implies that the distances between the atoms belong to a finite set, which in turn means that every quasicrystal  $\Lambda \subset \mathbb{R}$  is finitely generated over  $\mathbb{Z}$ . Thus every point  $\lambda \in \Lambda$  can be written as a finite sum of certain distances  $d_1, d_2, \dots, d_N \in \mathbb{R}_+$  with integer coefficients,

$$\lambda = \sum_{n=1}^N a_n(\lambda) d_n, \quad a_n(\lambda) \in \mathbb{Z}. \quad (10)$$

In contrast, strong crystalline sets are not finitely generated over  $\mathbb{Z}$ . This can be proven by generalising the results of [21] concerning the zeros of the trigonometric polynomial  $3 \sin(Ak) + \sin(k)$ ,  $A \in \mathbb{R} \setminus \mathbb{Q}$ . This proof uses Lang’s conjecture (a now-proven result) from diophantine analysis. It can be shown that if the strong crystalline set  $\Lambda$  is finitely generated on  $\mathbb{Z}$ , then  $\Lambda$  is a periodic (ideal) crystal [1].

Quasicrystals and crystallines (strong crystalline Delaunay sets) are two different generalisations of ideal crystals. Quasicrystals are formed according to local rules, which reminds the growth of usual crystals where layers are added one after the other. Crystallines are formed according to global law, with no observed local pattern.

In physical language, this means that quasicrystals can appear as a result of percolation, while crystallines require strong external forces applied to the system. It is interesting to note that the only two examples of physical quasicrystals observed in nature are connected with strong external forces [7, 8, 30]. The first case is connected with *carbonaceous chondritic meteorite* formed in the early solar system, while in the second case the material was formed as a result of an *electrical discharge event*. Therefore, it might happen that the observed natural quasicrystals are in fact crystallines, as classified by mathematicians.

## 6. Conclusions

Two competing mathematical definitions of aperiodic crystals (quasicrystals and crystallines) have been compared. Analyzing the arithmetic structure of these sets, we proved that they do not coincide,

unless the corresponding sets are periodic crystals. One should continue this research by determining whether other aperiodic crystals exist or not.

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