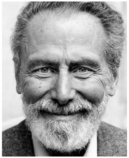
Aperiodic crystals: from quasicrystals to crystallines

Pavel Kurasov

OTAMP2026

In collaboration with



Yves Meyer Peter Sarnak

Plan of the talk

1. Ideal = periodic crystals
2. Quasicrystals in physics
3. Quasicrystals in mathematics
4. Crystalline measures and crystallines
5. Classification of crystallines
6. Arithmetic properties of crystallines
7. Crystallines and quasicrystals: mathematics
8. Crystallines and quasicrystals: physics

Freeman Dyson:
The one-dimensional quasi-crystals have a far richer structure since they are not tired to any rotational symmetry.

We focus on one-dimensional crystals, but figures will be multidimensional.

P.K., Yves Meyer, Peter Sarnak
Crystalline measures: ~~cinq~~ ans après (manuscript)
six

1. Periodic/ideal crystals

Point sets in $\mathbb{R}^d$: points = atoms.
Mathematician's view on **condensed matter**:

Def. *A set Λ in $\mathbb{R}^d$ is a* **Delaunay set** *(or Delone set) if it is*

1. **Uniformly Discrete:** *there is $r > 0$ such that every ball of (small) radius r contains at most one point of Λ.*
2. **Relatively Dense:** *there is $R > 0$ such that every ball of (large) radius R contains at least one point of Λ.*

Boris Delaunay: (r, R)-sets.

An **ideal crystal** is a point set $\Lambda \in \mathbb{R}^d$ of the form

$$L + F = \{x + f : x \in L, f \in F\},$$

where L is a full-rank lattice and F is a finite set.

Perfectly ordered system.
Example 1: **Poisson summation** formula:

$$\sum_{n \in \mathbb{Z}} f(x) = \sum_{m \in \mathbb{Z}} \hat{f}(k) \quad \Leftrightarrow \quad \mu = \sum_{n \in \mathbb{Z}} \delta_n, \hat{\mu} = \sum_{m \in \mathbb{Z}} \delta_m$$

1. Periodic/ideal crystals

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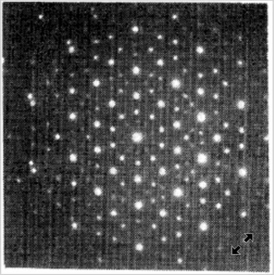
2. Quasicrystals in physics I

Dan Shechtman, Paul Steinhardt 1984



Phys. Rev. Lett. 53, 1951 (1984)

Ten-fold way. Quasiperiodic patterns have small repeating elements but on a larger scale do not exactly repeat (top). Daniel Schechtman's electron diffraction pattern from a metal alloy shows spots with a ten-fold rotational symmetry, which researchers in 1984 thought was impossible for a crystal (bottom). Today researchers call the material a quasicrystal because its structure is quasiperiodic.

Note: reflection points are in fact dense, but they are not seen in the picture if the corresponding intensity is low. One gets impression that the reflection is along a discrete set of directions, but this is not the case!

2. Quasicrystals in physics II

Properties of a set Λ that characterise it as a quasicrystal:

1. **crystal**
   only Delaunay sets can be considered;
2. **aperiodic**
   Λ is not invariant under any translation;
3. **long-range order**
   the set $\Lambda - \Lambda$ is well-structured, in particular reflected waves have clear peaks;
4. **finite number of cells or local rules**
   the set Λ can be obtained by repeating the same cells from a finite list, like Penrose tilling; Quasicrystal is obtained by adding layers.
5. **forbidden symmetries**
   ideal crystals in $\mathbb{R}^d$, or specifically in $\mathbb{R}^3$, may possess only specific rotational symmetries, while quasicrystals may exhibit other rotational symmetries. Can be used to distinguish quasicrystals from crystals.

2. Quasicrystals in physics III

Aperiodic crystals

New definition of a crystal adopted by crystallographers:

Def. *A material is a* **crystal** *if it has essentially a sharp diffraction pattern ...*

NB! *This broader definition allows for possible discoveries of other kinds of crystals.*

Sharp diffraction pattern means that the material has certain **long-range order**.

3. Quasicrystals in mathematics

Discovered at least decade earlier: Mathematicians were ahead of physicists!

- Meyer sets $\Lambda - \Lambda \subset \Lambda + F$, Λ – Delaunay, F - finite
- cut-and-project sets (Meyer)
- quasiregular sets (zonohedral Delone sets) $\Lambda - \Lambda$ – Delaunay (Galiulin)

Def (Lagarias). *A* **Delaunay set of finite type** *is a Delaunay set Λ 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.*

Arithmetic properties:

Theorem (Lagarias). *Every Delaunay set of finite type is finitely generated over $\mathbb{Q}$, i.e. the Abelian group*

$$[\Lambda - \Lambda] := \mathbb{Z}\,[\boldsymbol{x} - \boldsymbol{y} : \boldsymbol{x}, \boldsymbol{y} \in \Lambda]$$

is finitely generated.

This factl in one dimension:
there are finitely many possible distances between neighbouring points.

4. Crystalline measures and crystallines

Def. *Crystalline measure (after Meyer):*

- *atomic measure supported by a locally finite set,*
- *tempered distribution*
- *the Fourier transform is an atomic measure supported by a locally finite set.*

$$\mu = \sum_{\lambda \in \Lambda} a_\lambda \delta_\lambda, \qquad \hat{\mu} = \sum_{s \in S} b_s \delta_s.$$

The sets Λ (the support) and S (the spectrum) need to be very well structured.

Def. *Crystalline (set) (Instead of Fourier quasicrystals):*

- *the crystalline measure μ is a counting measure $\mu = \sum_{\lambda \in \Lambda} \delta_\lambda$.*
- *$|\hat{\mu}|$ in addition is tempered*

$$|\hat{\mu}| = \sum_{s \in S} |b_s| \delta_s.$$

Example 1: (again) **Poisson summation formula**

$$\sum_{n \in \mathbb{Z}} f(n) = \sum_{m \in \mathbb{Z}} \hat{f}(m) \quad \Leftrightarrow \quad \mu = \sum_{n \in \mathbb{Z}} \delta_n, \hat{\mu} = \sum_{m \in \mathbb{Z}} \delta_m.$$

5. Classification of crystallines I

K.-Sarnak construction; One-dimensional Fourier Quasicrystals via Lee-Yang polynomials

Mathematical generalization of the trace formula connecting spectra of Laplacians on metric graphs to periodic orbits.
Gutkin-Kottos-K.-Nowaczyk-Roth-Smilansky trace formula

Multivariate polynomial $P(\mathbf{z})$ is stable iff $P(\mathbf{z}) \neq 0$ for $\mathbf{z} = (z_1, \dots, z_n) : |z_j| < 1$.

Def. *Lee-Yang polynomial*

1. *P is stable – no zeroes inside the unit disc;*
2. *invariant under involution*

$$P(\mathbf{z}) = \; z_1^{m_1} z_2^{m_2} \dots z_n^{m_n} P(1/\mathbf{z}); \quad \mathbf{m} = (m_1, m_2, \dots, m_n) \in \mathbb{N}^n;$$

3. *normalisation condition*

$$P(\vec{0}) = 1.$$

5. Classification of crystallines II

Trigonometric polynomial

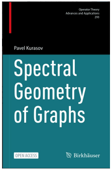
Consider any vector $\boldsymbol{\ell} = (\ell_1, \ell_2, \dots, \ell_n) \in \mathbb{R}^n_+$. Build trigonometric polynomial:

$$p(k) := P(e^{ik\ell}) = \sum_{1 \le j \le N} c_j e^{i\gamma_j k}, \quad N \in \mathbb{N}, c_j \in \mathbb{C}, \gamma_j \in \mathbb{R}_+.$$

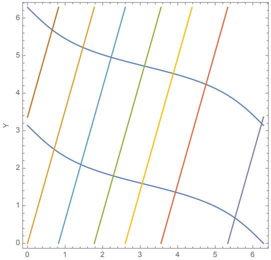
It is enough to consider $\boldsymbol{\ell}$ with rationally independent entries.

All zeroes of this trigonometric polynomial are real:

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



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



$\Lambda(p)$ appears as the intersection between

- the curve $e^{ik\boldsymbol{\ell}}, k \in \mathbb{R}$

  and

- the zero set $\mathcal{Z}_P$ of $P(\mathbf{z})$

on the unit torus $\mathbb{T}^n = \left\{ \mathbf{z} \in \mathbb{C}^n : |z_j| = 1 \right\}.$

5. Classification of crystallines III skip

Summation formula

Consider the measure:

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

It can be obtained by integrating the jump of the logarithmic derivative of $p(k)$ on the real axis:

$$\mu(k) = \lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} \left(\frac{p'(k+i\epsilon)}{p(k+i\epsilon)} - \frac{p'(k-i\epsilon)}{p(k-i\epsilon)} \right) dk$$

Expanding the logarithm around $k = 0 \Leftrightarrow \mathbf{z} = \mathbf{1}$ one gets summation formula

$$\sum_{k \in \Lambda} h(k_j) = \sum_{s_j \in S} b_j \hat{h}(s_j), \quad \text{where} \quad S = \pm \Big\{ \mathbf{n} \cdot \boldsymbol{\ell} \Big\}_{\mathbf{n} \in \mathbb{Z}_+^n}$$

The set S is discrete because both $\mathbf{n}$ and $\boldsymbol{\ell}$ have positive coordinates!

General references:

- P.K., P. Sarnak, *Stable polynomials and crystalline measures*, *J.Math.Phys.*, 2020.
- P.K., P. Sarnak, *The arithmetic structure of the spectraum of a Laplacian on a metric graph, to appear soon*.

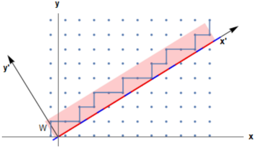
5. Classification of crystallines IV

Cut-and-project sets vs crystallines following Yves Meyer

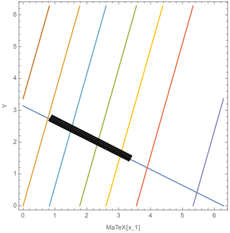
Cut-and-project model

$\mathbb{L}$ - regular lattice in a higher dimensional space

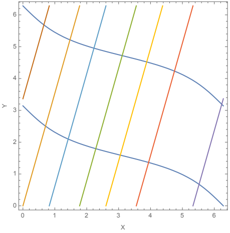
Λ is obtained by projecting all points form a strip to a lower-dimensional subspace



Classical cut-and-project.



Modified cut-and-project.



Curved model set.

Classical cut-and-project set:

- The support of $\hat{\mu}$ is dense, **not discrete** – Gibbs phenomenon.

Curved model set:

- The support of $\hat{\mu}$ is **discrete**.

5. Classification of crystallines IV

We have K.-Sarnak construction of crystallines

- **Olevskii-Ulanovskii**: trigonometric polynomials
  Every crystalline in $\mathbb{R}^1$ is given by a **real rooted** exponential polynomial

$$p(k) = \sum_{1 \le j \le N} c_j e^{2\pi i \gamma_j k}, \quad N \in \mathbb{N}, c_j \in \mathbb{C}, \gamma_j \in \mathbb{R}.$$

- **Alon-Cohen-Vinzant**: using amoebas
  Every **real rooted** trigonometric polynomial comes from K.-Sarnak construction.

Conclusion:
Every crystalline in $\mathbb{R}^1$ is given by K.-Sarnak construction via stable polynomials.

6. Arithmetic properties of crystallines I

Factorisation of trigonometric polynomials

Every exponential polynomial p can be factorized as (Ritt 1927)

$$p = \underbrace{\left(s_1 \; s_2 \; \dots \; s_I \right)}_{\substack{\text{simple factors,} \\ \text{each depending} \\ \text{on one frequency}}} \; \underbrace{\left(p_1 \; p_2 \; \dots \; p_J \right)}_{\text{irreducible factors}} .$$

The frequencies in s_i are pairwise rationally independent.

Structure of the zeroes

- **Arithmetic part**
  simple factors $s_i(k)$ are periodic in $k \Rightarrow$ finitely many full size arithmetic progressions $\Rightarrow$ ideal crystals
- **Non-arithmetic part**
  irreducible factors $\Rightarrow$ aperiodic sequences not containing full size arithmetic progressions

We need to study zeroes of irreducible trigonometric polynomials only.

6. Arithmetic properties of crystallines II

Lang's conjecture

Theorem 1. *(P. Sarnak, P. Liardet, W. Schmidt, M. Laurent, J-H. Evertse ...)*

- $V \subset (\mathbb{C}^*)^N$ *- an algebraic subvariety – zero set of Laurent polynomial;*
- Γ *- finitely generated subgroup of the torus* $T \subset (\mathbb{C}^*)^N$*, considered as a group under coordinatewise product;*
- $\overline{\Gamma}$ *- the division group of* Γ

$$\overline{\Gamma} = \left\{ z \in T : z^m \in \Gamma \textit{ for some } m \geq 1 \right\}.$$

Then there exists finitely many translates of (may be low dimensional) subtori $T_1, T_2, \dots, T_\nu$ **contained** *in* V *such that*

$$\overline{\Gamma} \cap V = \overline{\Gamma} \cap (T_1 \cup T_2 \cup \cdots \cup T_\nu).$$

The number of tori can be effectively estimated: $\nu \leq \Big(C(V) \Big)^r$.

6. Arithmetic properties of crystallines III Skip!!!

We apply this theorem to an **irreducible** trigonometric polynomial $p(k)$.

We want to prove that: $\boxed{\dim_{\mathbb{Q}} \mathcal{L}_{\mathbb{Q}}\{k_n\} = \infty}$ Ex: $3\sin k + \sin Ak = 0, A \notin \mathbb{Q}$

Assume the opposite $\dim_{\mathbb{Q}} \mathcal{L}_{\mathbb{Q}}\{k_n\} < \infty$, *i.e.*

$$k_n = \alpha_1^n k_1 + \alpha_2^n k_2 + \cdots + \alpha_{n_0}^n k_{n_0}, \quad \alpha_j^n \in \mathbb{Q}$$

for a certain n_0 and arbitrary n.

It follows that

$$e^{ik_n\ell_j} = \left(e^{ik_1\ell_j}\right)^{\alpha_1^n} \left(e^{ik_2\ell_j}\right)^{\alpha_2^n} \dots \left(e^{ik_{n_0}\ell_j}\right)^{\alpha_{n_0}^n}$$

in other words, all $(e^{ik_n\ell_1}, \dots, e^{ik_n\ell_N})$ belong to the division group for the multiplicative group Γ generated by

$$(e^{ik_i\ell_1}, e^{ik_i\ell_2}, \dots, e^{ik_i\ell_N}), \quad i = 1, 2, \dots, n_0.$$

Multiplication is carried coordinate-wise.

It feels like Liardet's theorem was proven especially to serve our purposes!

6. Arithmetic properties of crystallines IV **Skip!!!**

Hypertori in the zero set

$$z_1^{\alpha_1} z_2^{\alpha_2} \dots z_N^{\alpha_N} = q z_1^{\beta_1} z_2^{\beta_2} \dots z_N^{\beta_N}$$

$$\alpha_j \beta_j = 0 \quad \text{and} \quad |q| = 1.$$

Each hypertori corresponds to a simple trigonometric polynomial s in Ritt's factorization.

Hilbert's Nullstellensatz implies that s is a factor in $p(k)$ — contradiction.

Lower dimensional tori

– are not "dangerous", since entries in ℓ are rationally independent.
Hence there are just finitely many intersections $\Rightarrow$ contradiction, since there are infinitely many zeroes.

Conclusion:

$$p(k) \text{ is irreducible} \Rightarrow \begin{cases} \dim_{\mathbb{Q}} \{k_n\} = \infty \\ \Lambda \text{ contains no full arithmetic progression.} \end{cases}$$

6. Arithmetic properties of crystallines V

Theorem.

- *$p(k)$ – real rooted trigonometric polynomial,*
- *$\Lambda_p = \left\{ z \in \mathbb{C} : p(k) = 0 \right\}$ – its zero set;*

then it holds

i)
$$\Lambda_p = \underbrace{L_1 \sqcup L_2 \sqcup \cdots \sqcup L_D}_{\text{arithmetic part}} \sqcup \mathcal{N},$$

with

- *$L_1, \dots, L_D$ full size arithmetic progressions,*
- *$\mathcal{N}$, if not empty, is infinite dimensional over $\mathbb{Q}$.*

ii) *there is $C = C(P) < \infty$ such that any arithmetic progression in $\mathbb{R}_+$ meets $\mathcal{N}$ in at most C points.*

6. Arithmetic properties of crystallines VI

Reformulation for crystallines.

Theorem.

- Λ – *crystalline;*

then it holds

i)
$$\Lambda = \underbrace{L_1 \sqcup L_2 \sqcup \cdots \sqcup L_D}_{\text{arithmetic part}} \sqcup \mathcal{N},$$

with

- $L_1, \ldots, L_D$ *full size arithmetic progressions,*
- $\mathcal{N}$*, if not empty, is infinite dimensional over* $\mathbb{Q}$*,*

ii) *there is* $C = C(\Lambda) < \infty$ *such that any arithmetic progression in* $\mathbb{R}_+$ *meets* $\mathcal{N}$ *in at most* C *points.*

7. Crystallines and quasicrystals I Mathematics
Looking at the physical space

Theorem. *Let $\Lambda \in \mathbb{R}$ be a crystalline and a Delaunay set of finite type, then Λ is an ideal crystal, i.e. a finite periodic sum of Dirac combs.*

> Mathematical quasicrystals and crystallines
> are two different generalizations of ideal (periodic) crystals.

Proof.

Every quasicrystal Λ is finitely generated over $\mathbb{Q}$.

Crystalline set Λ is finitely generated over $\mathbb{Q}$ iff it corresponds to a product of simple trigonometric polynomials, *i.e.* the non-arithmetic part $\mathcal{N}$ is absent.

Every such Delaunay set is an ideal (periodic) crystal.

□

Quasicrystals and crystallines have completely different arithmetic properties.

7. Crystallines and quasicrystals II Mathematics Looking on the Fourier side

Theorem. *Let $\Lambda \in \mathbb{R}$ be a crystalline and a Meyer set simultaneously, then Λ is an ideal crystal, i.e. a finite periodic sum of Dirac combs.*

> Meyer sets and crystallines are two different generalizations of ideal (periodic) crystals.

Proof

Theorem (Lev-Olevskii, 2015, Theorem 1)**.** *Let μ be a crystalline measure on $\mathbb{R}$. Assume in addition that both Λ and S are uniformly discrete. Then the support Λ is contained in a finite union of translates of a certain lattice. The same is true for S (with the dual lattice).*

Conclusion: if a crystalline is uniformly discrete and not periodic, then its Fourier transform is supported by a **not** uniformly discrete set.

7. Crystallines and quasicrystals II Mathematics Looking on the Fourier side

Theorem (Lev-Olevski 2017, Theorem 7.1). *Let μ be a crystalline measure on $\mathbb{R}^n$, and assume that the support of Λ is a Meyer set. Then, either*

- (i) *S is also uniformly discrete, or*
- (ii) *S has a relatively dense set of accumulation points.*

Conclusion: the Fourier transform of a non-periodic Meyer set is not uniformly discrete due to finite accumulation points.
Fourier transform of a crystalline is supported by

$$\pm \left\{ s = \mathbf{n} \cdot \boldsymbol{\ell}, \mathbf{n} \in \mathbb{Z}_+^n \right\}.$$

This set is discrete and closed $\Rightarrow$ does not contain any (finite) accumulation point.
Conclusion: the Fourier transform of a non-periodic crystalline is not uniformly discrete due to arbitrarily close points at infinity.
Hence only periodic sets are simultaneously Meyer and crystalline.

8. Crystallines and quasicrystals I Physics

Just two examples of quasicrystals in nature
(both connected with Paul Steinhardt):

- the icosahedrite found in Koryak mountains is an icosahedral quasicrystalline phase with composition $\mathrm{Al}_{63}\mathrm{Cu}_{24}\mathrm{Fe}_{13}$ and is *likely formed in the early solar system about* $4.5\mathrm{Gya}$;
- dodecagonal composition $\mathrm{Mn}_{72.3}\mathrm{Si}_{15.6}\mathrm{Cr}_{9.7}\mathrm{Al}_{1.8}\mathrm{Ni}_{0.6}$ was formed during *an electrical discharge event in 2008 in the eolian dunes of the Sand Hills in the High Plains of north central Nebraska*.

Presence of extreme exernal forces is obvious in both events. Is it possible that the systems observed in nature are crystallines, not quasicrystals?

8. Crystallines and quasicrystals II Physics
Looking at the physical space

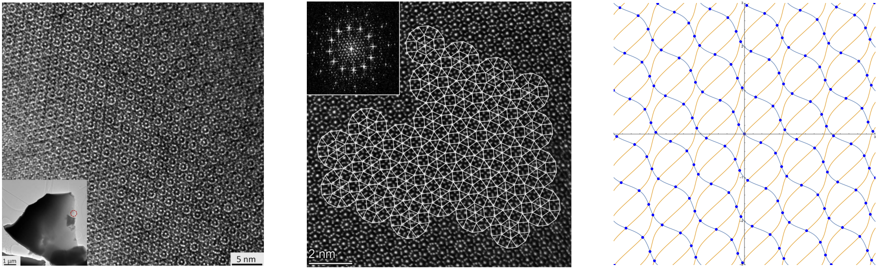


Figure: Images of experimental samples (the first two figures) and simulations for crystallines (blue points in the third figure).

It is hard to see any difference.

8. Crystallines and quasicrystals III Physics
Looking on the Fourier side

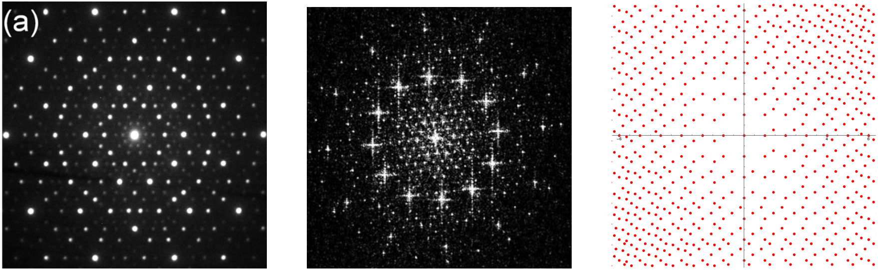


Figure: Diffraction patterns from experimental samples (the first two figures) and from crystallines (the third figure).

Clear difference:

- Experimental samples have finite accumulation points
- Crystallines have arbitrarily close points at infinity

THANK YOU!