Quasicrystals from the point of view of Additive Combinatorics

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Crystals

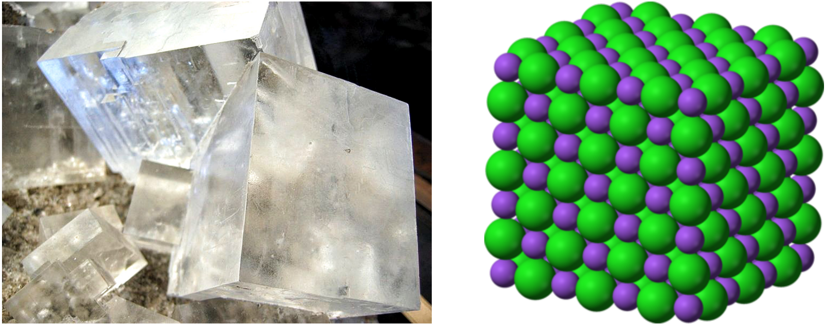

Figure: Salt crystal and the corresponding arrangement of molecules.

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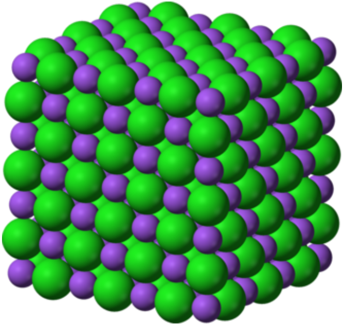
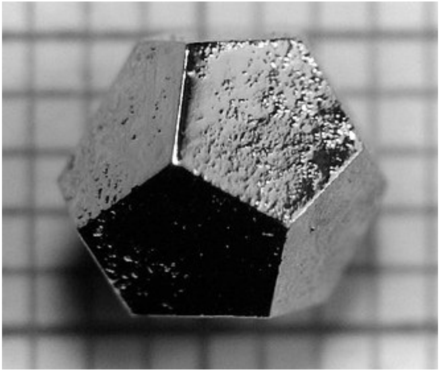


Figure: Salt crystal and the corresponding arrangement of molecules.

- Crystals are periodic arrangements of molecules.
- Possible symmetry groups are highly constrained.
- Mathematically, we are simply looking at lattices.

Quasicrystals



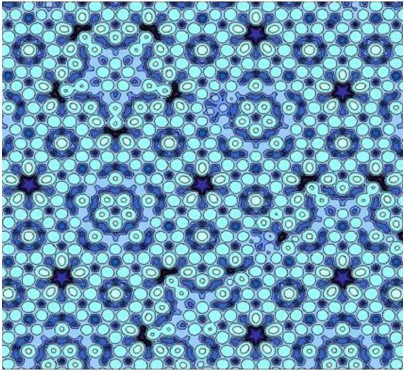


Figure: A photography of a piece of Ho-Mg-Zn, and surface potential for Al-Pd-Mn.

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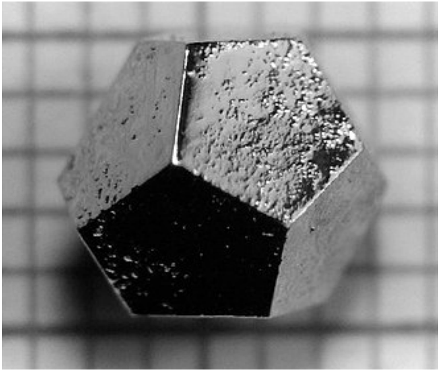


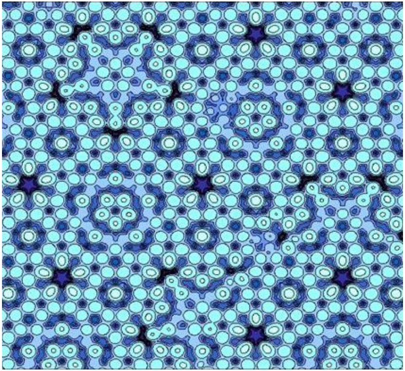
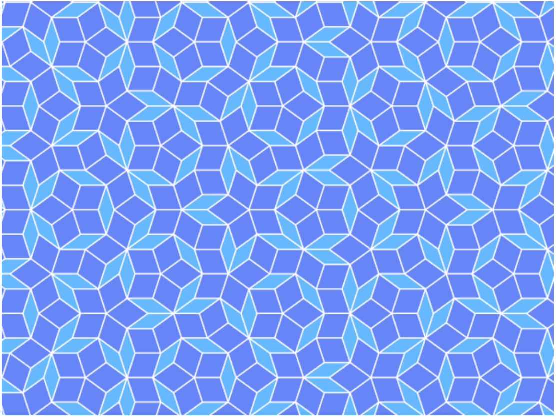


Figure: A photography of a piece of Ho-Mg-Zn, and surface potential for Al-Pd-Mn.

- Quasicrystals exhibit approximate translation and rotation symmetries.
- Possible symmetry groups are much richer than for crystals.
- Mathematical description becomes considerably less trivial.

Penrose tiling



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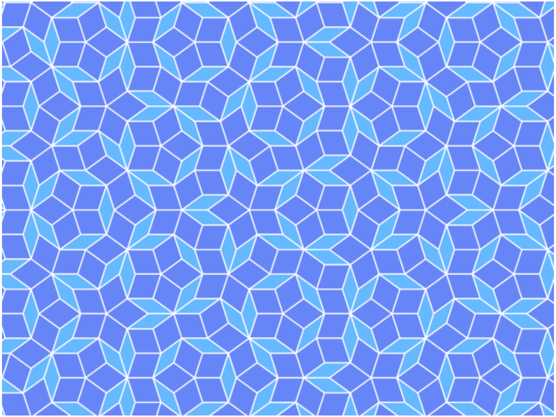

- Penrose constructed a quasiperiodic tiling of the plane with 2 tiles.
- Additionally there is a 5-fold approximate rotational symmetry.

Basic notation and terminology

Fix dimension $d \geq 1$. For $x = (x_i)_{i=1}^d \in \mathbb{R}^d$, $R > 0$, let

$$\mathcal{B}_\infty^d(x, R) = \prod_{i=1}^d (x_i - R, x_i + R)$$

denote the ℓ^∞ ball centred at x. Let λ denote the Lebesgue measure.

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Let $A \subset \mathbb{R}^d$ for some $d \geq 1$, and let $R, r > 0$. Then A is

- *R-relatively dense* if $\mathcal{B}_\infty^d(x, R) \cap A \neq \emptyset$ for each $x \in \mathbb{R}^d$;
- *r-uniformly discrete* if $\mathcal{B}_\infty^d(x, r) \cap A = \{x\}$ for each $x \in A$.

Accordingly, A is *relatively dense* if there exists $R > 0$ such that A is R-relatively dense. Likewise, A is *uniformly discrete* if there exists $r > 0$ such that A is r-uniformly discrete. If A is both relatively dense and uniformly discrete then A is a *Delone set*.

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We define the lower and upper uniform densities of A as

$$D^+(A) = \limsup_{R \to \infty} \sup_{x \in X} \frac{|A \cap \mathcal{B}_\infty^d(x, R)|}{\lambda(\mathcal{B}_\infty^d(x, R))}, \quad D^-(A) = \liminf_{R \to \infty} \inf_{x \in X} \frac{|A \cap \mathcal{B}_\infty^d(x, R)|}{\lambda(\mathcal{B}_\infty^d(x, R))},$$

If A is relatively dense then $D^-(A) > 0$. If A is uniformly discrete then $D^+(A) < \infty$.

Cut-and-project sets

Definition: Let $d, e \in \mathbb{N}_0$. For a discrete subgroup $\Gamma < \mathbb{R}^{d+e}$ and a "window" $\Omega \subset \mathbb{R}^e$, we define the corresponding *cut-and-project* set

$$\Lambda(\Gamma, \Omega) := \pi_1 \left(\Gamma \cap \pi_2^{-1}(\Omega)\right),$$

where $\pi_1 \colon \mathbb{R}^{d+e} \to \mathbb{R}^d$ and $\pi_2 \colon \mathbb{R}^{d+e} \to \mathbb{R}^e$ are the projections. The window Ω needs to be topologically "nice"; here, we require that Ω is compact and $\Omega = \operatorname{cl} \operatorname{int} \Omega$.

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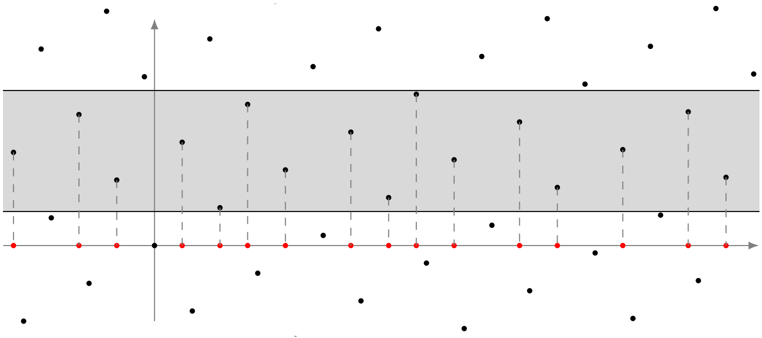

Figure: The red dots form a cut-and-project set.

Minimality assumptions: Γ is a lattice, π_1 is injective on Γ, $\pi_2(\Gamma)$ is dense.

Meyer sets

Cut-and-project sets have many properties that we would expect of a quasicrystal:

- They are Delone sets;
- They are approximately shift-invariant;
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Theorem (Meyer; Lagarias; Nir & Olevskii)

Let $A \subset \mathbb{R}^d$ be relatively dense. Then the following conditions are equivalent:

1. $D^+(A - A) < \infty$;
2. *$A - A$ is uniformly discrete;*
3. *A is uniformly discrete and $A - A \subset A + F$ for a finite set F;*
4. *$A \subset M + F$ for a cut-and-project set M and a finite set F.*

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Goal: We will show that this theorem follows from the Freiman–Ruzsa theorem.

Additive combinatorics

Setup: Let Z be an abelian group. Often, Z is one of $\mathbb{Z}$, $\mathbb{Z}/N\mathbb{Z}$, $\mathbb{F}_p^n$, etc.
Let $A, B \subset Z$ be finite sets. Then the sum-set and difference set of A and B are:

$$A + B = \{a + b \,:\, a \in A,\ b \in B\}\,,\ A - B = \{a - b \,:\, a \in A,\ b \in B\}\,.$$

More generally, for $k \in \mathbb{N}$, the k-fold sum-set of A is

$$kA = \{a_1 + a_2 + \cdots + a_k \,:\, a_1, a_2, \ldots, a_k \in A\}\,.$$

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- If $A, B \subset \mathbb{Z}$ then $|A + B| \geq |A| + |B| - 1$ (with equality for arithmetic progressions of equal step);
- Cauchy–Davenport: If $A, B \subset \mathbb{Z}/N\mathbb{Z}$ with N prime then $|A + B| \geq \min(|A| + |B| - 1, N)$;
- Freiman's "$3k - 4$": If $|A + A| \leq 3\,|A| - 4$ then A is contained in arithmetic progression of length $|A + A| - |A| + 1$;
- Plünnecke: If $|A + B| \leq K\,|A|$, then $|kB - lB| \leq K^{k+l}\,|A|$ for each $k, l \geq 0$.

Freiman–Ruzsa theorem

A *generalised arithmetic progression* (GAP) of rank d with steps $a_1, a_2, \ldots, a_d \in Z$ and side lengths $\ell_1, \ell_2, \ldots, \ell_d \in \mathbb{N}$ is

$$P = \{b + n_1 a_1 + n_2 a_2 + \cdots + n_d a_d \,:\, 0 \leq n_i \leq \ell_i \text{ for all } i = 1, 2, \ldots, d\},$$

As a special case, there are *symmetric generalised arithmetic progressions* which take the form

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Theorem (Freiman–Ruzsa)

Fix $K > 0$. Suppose that $|A| = |B| = n$ and $|A + B| \leq Kn$. Then there exists a generalised progression P of rank $O_K(1)$ and size $|P| = O_K(n)$ such that $A \subset P$.

More precisely: we can take $P = F + Q$ where F is a finite set of size $O_K(1)$ and Q is a symmetric generalised arithmetic progression with $Q \subset 2A - 2A$.

Continuous variants

Setup: Let G be a compact abelian group, such as $\mathbb{Z}/N\mathbb{Z}$ or $\mathbb{R}/\mathbb{Z}$. Let μ_G denote the Haar measure on G. Let $A, B \subset G$ be compact sets. Then $A + B$, $A - B$, kA ($k \in \mathbb{N}$) are defined the same way as before.

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Suppose that G is connected. Then $\mu_G(A + B) \geq \min(\mu_G(A) + \mu_G(B), 1)$.

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Corollary

Let $A \subset [0,1]^d$ be a measurable set with measure $\varepsilon > 0$. Then there exists $k = k(d,\varepsilon) \in \mathbb{N}$ with $k = O(d/\varepsilon^2)$ and $b \in \mathbb{R}^d$ such that $kA \supset [0,1]^d + b$.

Proof.

Without loss of generality, A is compact, $0 \in A$. We run induction with respect to d.

- $d = 1$: Let $A_1 = A \bmod \mathbb{Z}$. By Kneser, $k_1 A = \mathbb{R}/\mathbb{Z}$ for $k_1 = \lceil 1/\varepsilon \rceil$, so $k_1 A$ contains an integer $0 \neq m \leq k_1$. Let $A_2 = A \bmod m\mathbb{Z}$, so $k_2 A_2 = \mathbb{R}/m\mathbb{Z}$ for $k_2 = m\lceil 1/\varepsilon \rceil$.

  $$[0,m] \subset k_2 A - \{0, m, \ldots, k_2\} \subset k_2 A + k_1^2 A - k_2.$$

  Thus, we can take $k(1,\varepsilon) = k_2 + k_1^2 \leq 2\lceil 1/\varepsilon \rceil^2$.
- $d \geq 2$: The set $k(1,\varepsilon)A$ contains a unit segment in each of the d basic directions. Hence, we can take $k(d,\varepsilon) = dk(1,\varepsilon) \leq 2d\lceil 1/\varepsilon \rceil^2$. □

Characterisation of Meyer sets via the Freiman–Ruzsa Theorem

Theorem

Let $d \in \mathbb{N}$ and $A \subset \mathbb{R}^d$. Suppose that A is relatively dense and $D^+(A - A) < \infty$. Then there exists a finite set F and a cut-and-project set M such that $A \subset M + F$.

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Proof: Without loss of generality, A is 1-relatively dense. For $N \in \mathbb{N}$, let

$$A_N := A \cap \mathcal{B}^d_\infty(0, N)\,.$$

The sets A_N have bounded doubling:

$$\limsup_{N\to\infty} \frac{|A_N - A_N|}{|A_N|} \le \limsup_{N\to\infty} \frac{\left|(A-A) \cap \mathcal{B}^d_\infty(0, 2N)\right|}{|A \cap \mathcal{B}^d_\infty(0, N)|} \le \frac{2^d D^+(A-A)}{D^-(A)}.$$

Pick a constant $K > 0$ such that $|A_N - A_N| \le K\,|A_N|$ for all $N \in \mathbb{N}$.

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Pick a constant $K > 0$ such that $|A_N - A_N| \le K\,|A_N|$ for all $N \in \mathbb{N}$.
By Freiman–Ruzsa: there are symmetric generalised arithmetic progressions Q_N of rank $e = O_K(1)$ and finite sets F_N with cardinality $h = |F_N| = O_K(1)$ such that

$$Q_N \subset 2A_N - 2A_N \text{ and } A_N \subset F_N + Q_N.$$

We may write Q_N is the form

$$Q_N = \left\{ n_1 a_1^N + n_2 a_2^N + \cdots + n_e a_e^N \ : \ |n_i| < \ell_i^N \text{ for all } 1 \le i \le e \right\} \qquad (1)$$

for some $a_1^N, a_2^N, \ldots, a_e^N \in \mathbb{R}^d$ and $\ell_1^N, \ell_2^N, \ldots, \ell_e^N \in \mathbb{N}_0$.

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Claim 1. *There exist finite sets F'_N with $|F'_N| \leq h$ and $F'_N \subset \mathcal{B}^d_\infty(0, O_K(1))$ as well as a positive integer $k = O_{K,d}(1)$ such that $F_N + Q_N \subset F'_N + kQ_N$ for all $N \in \mathbb{N}$.*

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Proof: Without loss of generality, $F_N \subset \mathcal{B}^d_\infty(0, 5N)$. Since A is 1-relatively dense,

$$\mathcal{B}^d_\infty(0, N) \subset A_N + \mathcal{B}^d_\infty(0, 1) \subset F_N + Q_N + \mathcal{B}^d_\infty(0, 1).$$

Hence, by the union bound,

$$\lambda\Big(Q_N + \mathcal{B}^d_\infty(0, 1)\Big) \ge \lambda\Big(\mathcal{B}^d_\infty(0, N)\Big)/h.$$

From Macbeath's theorem, there exists $k_1 = O_{K,d}(1)$ and $b \in \mathbb{R}^d$ such that

$$k_1 Q_N + \mathcal{B}^d_\infty(0, k_1) + b \supset \mathcal{B}^d_\infty(0, 10N).$$

Using the symmetry of Q_N, we may remove the shift by b:

$$2k_1 Q_N + \mathcal{B}^d_\infty(0, 2k_1) \supset \mathcal{B}^d_\infty(0, 10N).$$

Hence, there exists a set $F'_N \subset \mathcal{B}^d_\infty(0, 2k_1)$ with $|F'_N| \le |F_N|$ such that

$$F_N \subset 2k_1 Q_N + F'_N.$$

Letting $k = 2k_1 + 1$ we find that $A_N \subset F_N + Q_N \subset F'_N + kQ_N$.

Definition: Let $\Lambda_N < \mathbb{R}^{d+e}$ be the group spanned by

$$v_i^N = \left(a_i^N, \vec{e}_i/\ell_i\right), \qquad (1 \le i \le e), \tag{2}$$

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Proof: Pick any N and any $x \in kQ_N$. Then x can be written as

$$x = \sum_{i=1}^{e} n_i a_i^N,$$

where $|n_i| \le k\ell_i^N$ for all $1 \le i \le e$. Hence, x is the first coordinate of the point

$$\left(x,\ \sum_{i=1}^{e}(n_i/\ell_i^N)\vec{e}_i\right) \in \Lambda_N \cap \left(\mathbb{R}^d \times \bar{\mathcal{B}}^e_\infty(0,k)\right).$$

It follows that (3) holds:

$$A_N \subset F'_N + kQ_N \subset F'_N + \pi_1\left(\Lambda_N \cap \left(\mathbb{R}^d \times \bar{\mathcal{B}}^e_\infty(0,k)\right)\right).$$

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Proof: Suppose that Λ_N is not $1/M$-uniformly discrete. Pick a $u \in \Lambda_N$ with $\|u\|_\infty < 1/M$. Let integers n_i and vector c be defined by

$$u = \sum_{i=1}^{e} n_i v_i^N, \text{ and } c := \sum_{i=1}^{e} n_i a_i^N = \pi_1(u). \tag{4}$$

Combining (2) and (4), we see that

$$\|c\|_\infty < 1/M, \text{ and } |n_i| < \ell_i/M \text{ for } 1 \leq i \leq e. \tag{5}$$

Hence, $\pm c, \pm 2c, \ldots, \pm Mc \in Q_N \cap \mathcal{B}^d_\infty(0,1)$. Let $B \subset A$ be a maximal 2-separated subset and $B_N := B \cap \mathcal{B}^d_\infty(0,N)$. Since $Q_N \subset 2A_N - 2A_N$ and $B_N \subset A_N$,

$$mc + b \in 3A_N - 2A_N \text{ for all } -M \leq m \leq M \text{ and } b \in B_N.$$

Since all of these points are distinct,

$$|3A_N - 2A_N| \geq (2M+1)\,|B_N|$$

Conversely, by Plünnecke inequality,

$$|3A_N - 2A_N| \leq K^5\,|A_N|.$$

Consequently, $M \leq K^5\,|A_N|/|B_N|$, which leads to contradiction if M is large enough.

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Passing to a subsequence, we may assume:

- $\Lambda_N \to \Lambda$ as $N \to \infty$ for some set $\Lambda \subset \mathbb{R}^d$;
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Claim 4. *The set Λ is a discrete subgroup of $\mathbb{R}^d \times \mathbb{R}^e$, F' is finite and*

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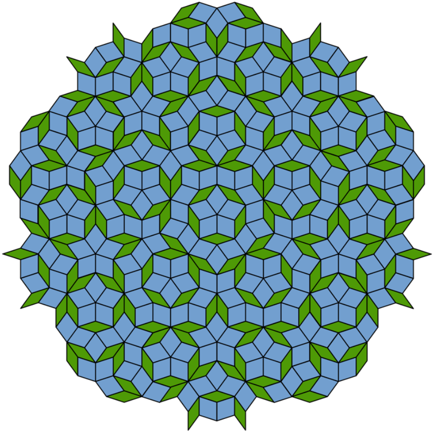
Proof: Because the relevant properties are preserved under limits:

- Λ is a r-uniformly discrete (with r from Claim 3);
- Λ is a subgroup of $\mathbb{R}^d$;
- $|F'| \leq h$ (where h is the cardinality of F_N).

Take any point $x \in A$. Then $x \in A_N$ for all large N. By Claim 2, there are $y_N \in F'_N$ and $z_N \in \Lambda_N \cap \left(\mathbb{R}^d \times \bar{\mathcal{B}}^e_\infty(0, k)\right)$ such that

$$x = y_N + \pi_1(z_N)$$

By Claim 1, y_N are bounded as $N \to \infty$, and hence so are z_N. We may assume that $y_N \to y \in F'$ and $z_N \to z \in \Lambda$ as $N \to \infty$. Notice that $z \in \mathbb{R}^d \times \bar{\mathcal{B}}^e_\infty(0, k)$ and $x = y + \pi_1(z)$. Hence, (6) follows.



Thank You for Your attention!