QUASICRYSTALS AND DISCRETE GEOMETRY

Jeff Lagarias
AT&T Labs- Research
Florham Park, NJ

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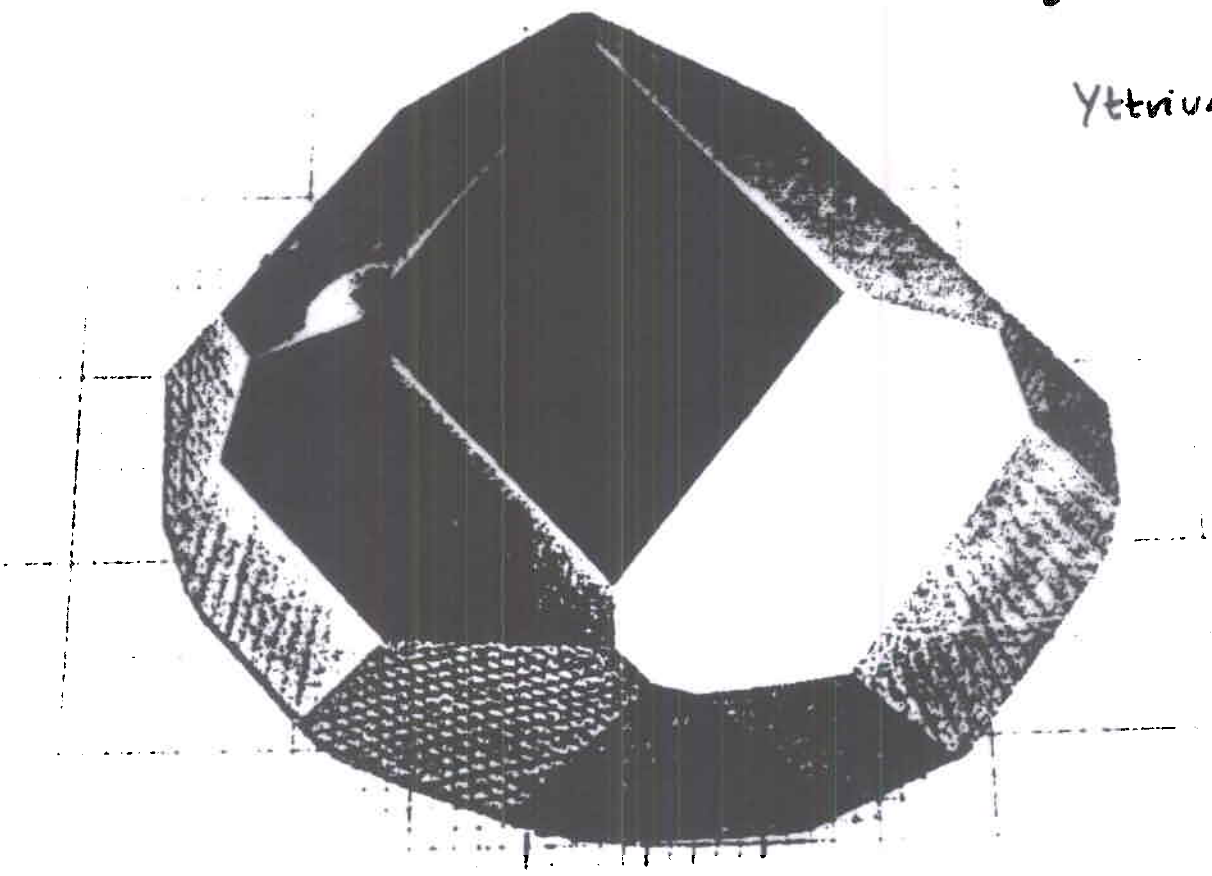
Topics

1. History: Crystals
2. Quasicrystals
3. Taxonomy of Delone Sets
4. Dynamical Systems Viewpoint
5. Characterizing Ideal Crystals
   (Periodicity vs. Aperiodicity)

1. CRYSTALS

$Y_3Fe_5O_{12}$

Yttrium Iron Garnet



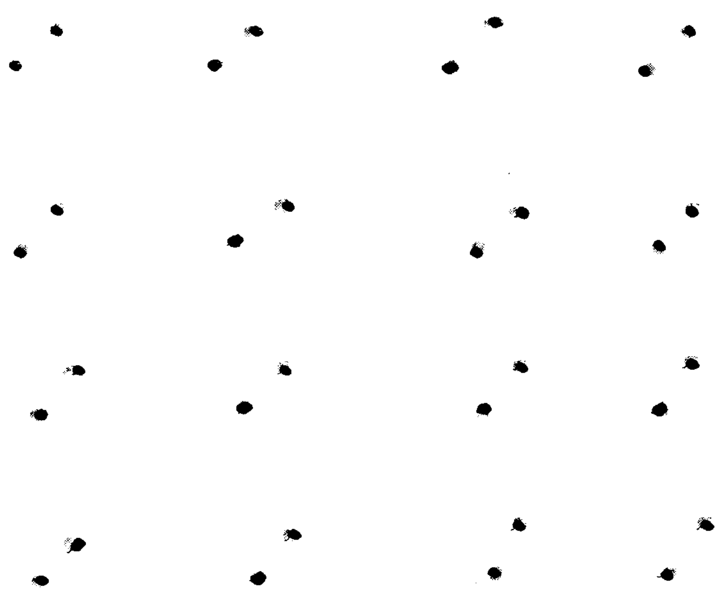
Greek = " ice "

κριστaλλοσ

__Defn.__ An __ideal crystal__ in $\mathbb{R}^n$ is a finite number of translates of a (full-dimensional) lattice L, i.e.

$$X = L + F$$

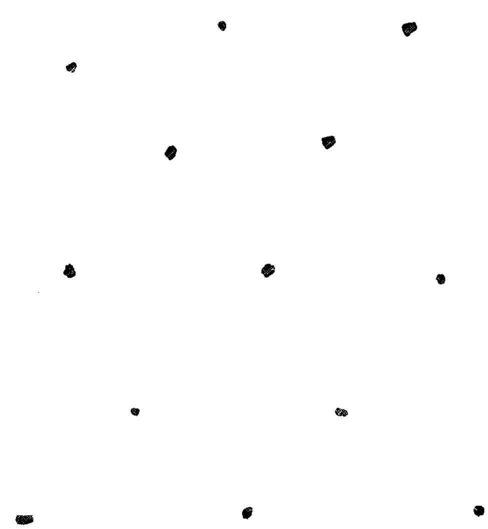
finite set



$$X = \mathbb{Z}^2 + \{(0,0), (\tfrac{1}{6}, \tfrac{1}{6})\}$$

Geometric Crystallography

Concerns infinite discrete sets of points X in $\mathbb{R}^n$.



Delone set = Delaunay set

= (r, R)-set

- relatively dense = finite covering radius by spheres, radius R

- uniformly discrete = finite packing radius by spheres, radius $r > 0$.

"Solid state"

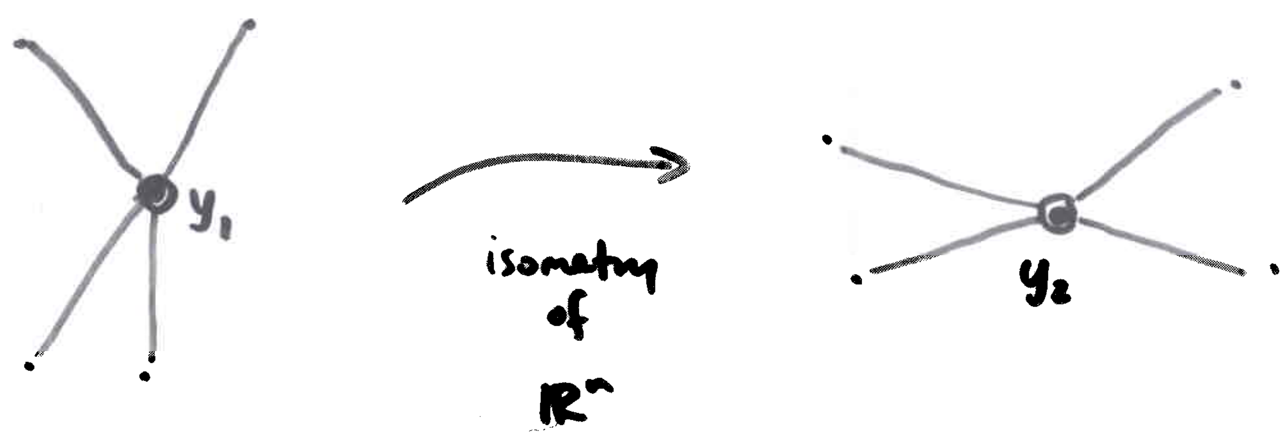
Basic Concept of Geometric Crystallography

C. Wiener 1863
L. Sohnke 1874

A **regular point system** in $\mathbb{R}^n$ is any set Y such that

① Y is a Delone set.

② Y "looks the same" from each point of Y



global star of Y at y_1

global star of Y at y_2

CRYSTALLOGRAPIC GROUPS

Definition. A crystallographic group is a symmetry group Sym(Y) of some regular point system Y.

Problem: Characterize crystallographic groups.

1874 (Sohncke) 17 2-dimensional crystallographic groups

1879 (Sohncke) 65 3-dimensional (proper) crystallographic groups

1890 Fedorov
1891 Schoenflies
1894 Barlow

230 3-dimensional crystallographic groups

Mathematical count: 54 proper 3-d groups
219 3-d groups

!!

Hilbert's 18th Problem (1900)

(1) In n-dimensional Euclidean space are there finitely many essentially different groups of motions with a fundamental region?

(2) Whether polyhedra exist which are not fundamental regions for groups of motions, yet tile space by congruent copies?

(3) How can one pack most densely in space <u>spheres</u> or <u>regular tetrahedra</u>?

Hilbert's 18th Problem

Answers

(1) Yes (Bieberbach 1910
1912)

(2) Yes (Reinhardt 1928
Heesch 1935
Conway - Danzer 1994)
- Schmitt

(3) (i) Solved Kepler's Conjecture

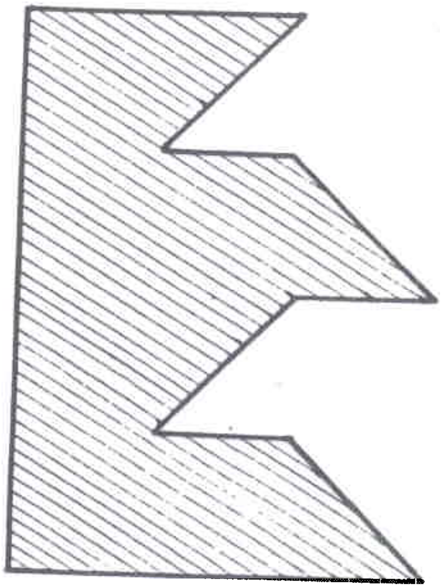
Hales - 1998++ Densest = "Cannonball packing" in $\mathbb{R}^3$
Ferguson

n-dimensional sphere-packing density:

$$2^{-n} \leq \delta(B_n) \leq 2^{-(0.599 + o(1))n}$$

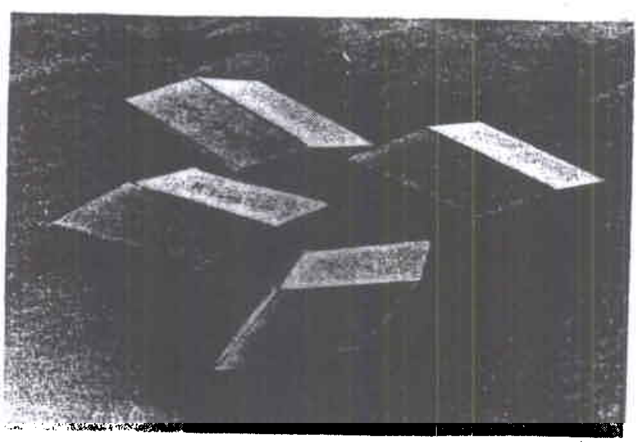
(3) (ii) Unsolved

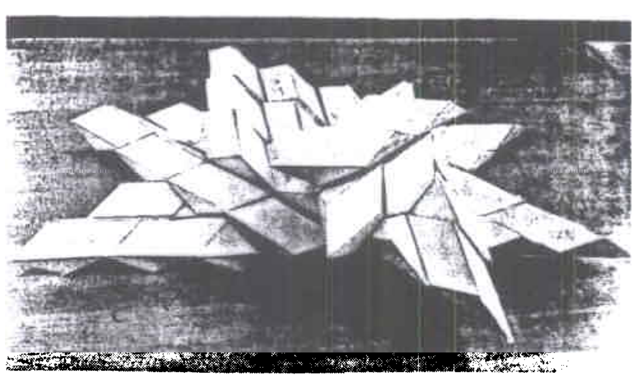
TILING SPACE BY POLYTOPES – I



Heesch polygonal tile

([redacted] periodic)
/not fundamental domain





~~Schmitt~~-
Conway – Danzer biprism

(8 faces) convex polyhedron

- all tilings $\mathbb{R}^3$ are aperiodic
- uncountably many different tilings

Bieberbach's First Theorem

(1) Every discrete subgroup Γ of isometries of $\mathbb{R}^n$ with compact fundamental domain contains a full rank lattice T of translations. Also T is of finite index in Γ.

$\Rightarrow$ Every regular point system is a periodic crystal.

(Not vice-versa)

Crystallographic Restriction :

Any motion fixing a point of X must leave lattice invariant.

$\Rightarrow$

(Point Group conjugate to [finite] subgroup of $GL(n, \mathbb{Z})$)

Dimension 3 :

Only rotations of order $1, 2, 3, 4$ or 6 can occur.

2. QUASICRYSTALS

In 1982 Schechtman et al. prepared a material ($Al_{86}Mn_{14}$) whose electron diffraction image indicated:

(1) Long Range Order (Discrete Spots)

(2) Icosahedral Symmetry.

This is impossible for crystal: 5-fold symmetry violates crystallographic restriction.

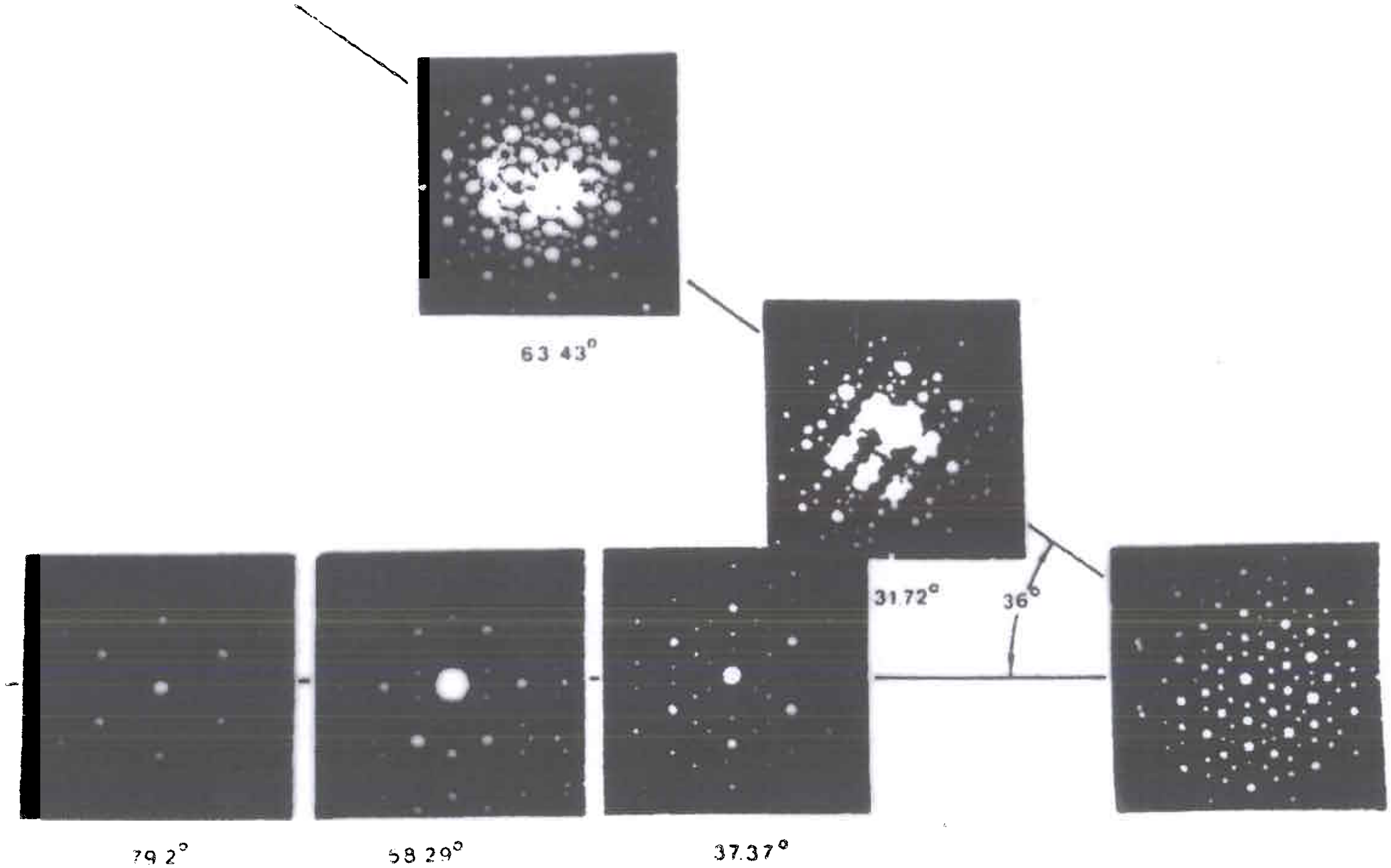


Figure 7.1. Diffraction patterns exhibiting icosahedral symmetry.

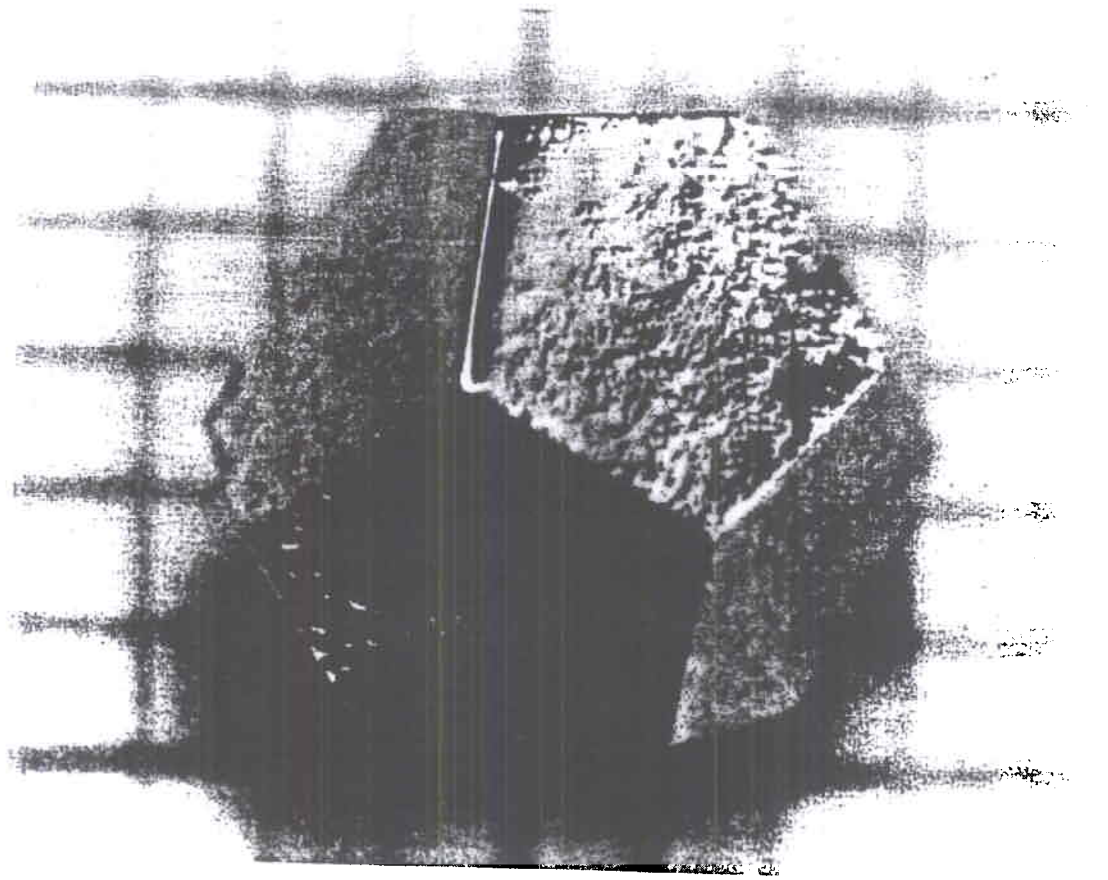


Fig. 1. Photograph of an icosahedral Ho–Mg–Zn quasicrystal grown from the ternary melt, shown over a millimetre scale (after Ref. [1]).

"Perfect" Quasicrystal

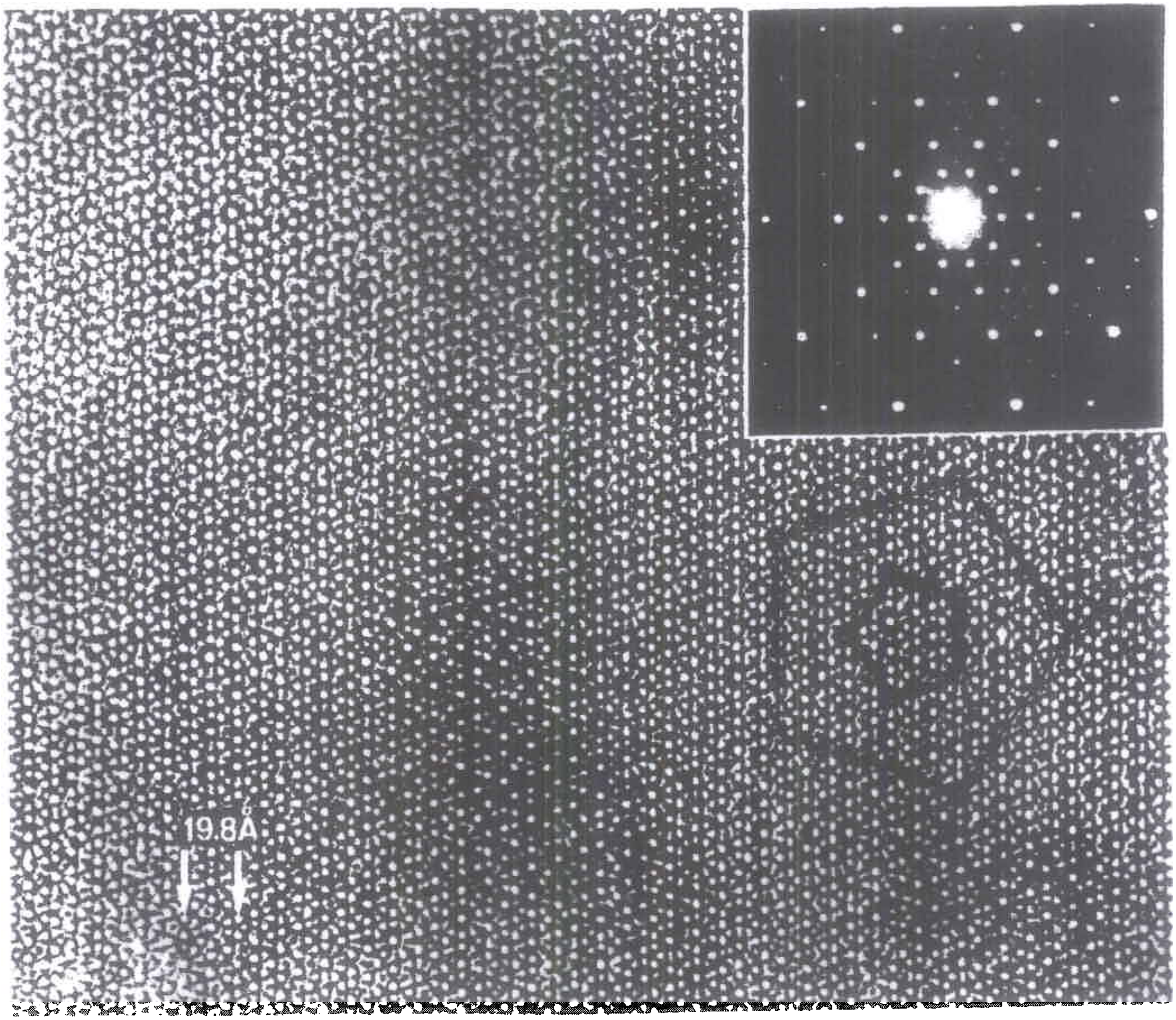


FIG. 2.18 HREM of the icosahedral AlCuFe sample corresponding to a 5-fold zone axis. Pentagonal arrangements are outlined. The succession of lattice planes, when looked at from a grazing angle, is not periodic: the mean distances betweem planes are related by τ, the golden mean. (Courtesy of M. Audier).

High Resolution Electron Microscope Image

Types of Quasicrystals

- Over 100 quasicrystalline materials are known

- "Perfect Quasicrystals"

  Thermodynamically Stable

  "As perfect as crystals."

- Entropically Stabilized Phases

  Exist at certain temperature/pressure

  "Positive Entropy"

  (Most materials of this type)

Motivating Problems

(1) Explain pure point diffraction with "extra symmetries."

- Classify allowed symmetries

(2) Where are the atoms?

(Aperiodic order)

- Discrete Geometry models
- Dynamical System ($\mathbb{R}^n$-action)

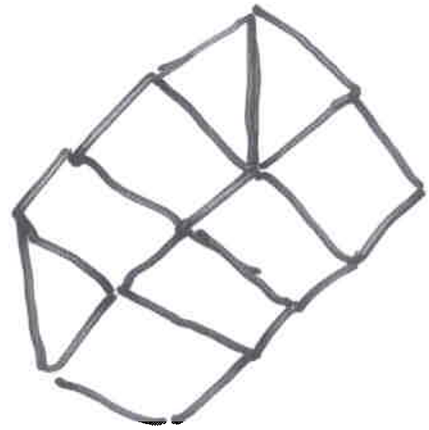
(3) What is formation mechanism?

- "Local Rules."

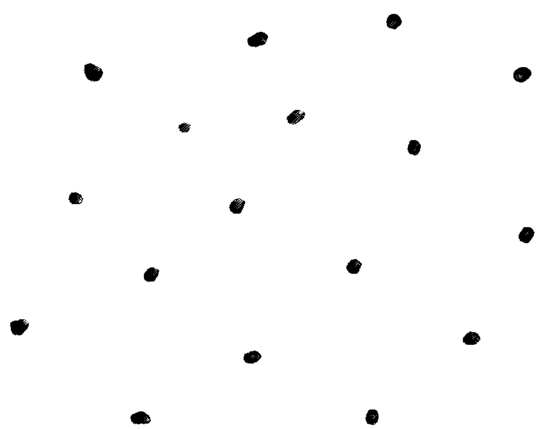
(4) What is boundary between crystals and quasicrystals?

Geometric Models

Tilings :



Delone Sets:



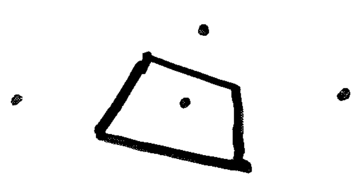
Conversions:

- Tiling ⇒ Delone Set

  add marks to tiles

- Delone Set ⇒ Tiling

  Voronoi regions



MATHEMATICS OF QUASICRYSTALS

- <u>Group Theory</u>

  Classify Quasicrystallographic Groups (Mermin; Piunikhin)

  Strange Symmetry Groups (Radin, Sadun; Conway) [Pinwheel Tiling]

- <u>Harmonic Analysis</u>

  Mathematical Diffraction (A. Hof) [Y. Meyer]

  * Wavelets, Fractals, Tilings

- <u>Discrete Geometry</u>

  Taxonomy of Delone Sets

  "Local Rules" (R. Robinson; Solomyak)

- <u>Dynamical Systems</u>

  Tiling Dynamical Systems — Ergodic Theory; C^* - Algebras

- <u>C^* - Algebras</u>

  Model Conductivity / Resistivity Properties (Bellissard)

Structures Constructed by "Local Rules"

- Finite List $\mathcal{L}$ of "allowed" local patches (up to translation)

Perfect Local Rules

- Local rules $\mathcal{L}$ such that all structures satisfying them look "the same". (locally isomorphic) [cannot be told apart on any finite-size region.]

Motivation : "Local Rules"

Minimize $\sum_{\text{atoms}} V(x_i)$

potential

Assume:

Potential has finitely many local minima up to isometries.

Geometric Analogue

Configurations that achieve local minimum at every atom

$\Rightarrow$ "local rules" under isometries.

$\Rightarrow$ finite # of local neighborhoods (radius $2R$) under isometries.

LATTICES & QUASILATTICES

- A *lattice* L in $\mathbb{R}^n$ is a discrete additive subgroup that spans $\mathbb{R}^n$

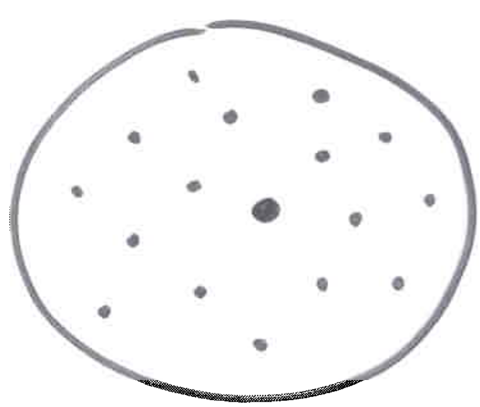
- A *quasilattice* Λ in $\mathbb{R}^n$ is a finitely generated additive subgroup that spans $\mathbb{R}^n$, [rank = minimum # generators]

  If $\mathrm{rank}(\Lambda) = r > n$, it is *dense*.

  If $\mathrm{rank}(\Lambda) = n$, it is a *lattice*

PATCHES

A T-patch is all points in a Delone set X within T of center point $x \in X$



Diffractivity

- Rigorous mathematical version of parallel-beam diffraction developed by A. Hof ("Fourier transform")

- Form autocorrelation measure = two-point correlation measure μ_X for Delone set X. If it is unique, diffraction measure is

$$\gamma_X := \hat{\mu}_X ,$$

It is a Positive Measure

Fourier transform of μ_X.

- $$\gamma_X = \gamma_{pp} + \gamma_{ac} + \gamma_{sc}$$

Lebesgue decomposition.

pure point / absolutely continuous / singular continuous

TWO KINDS OF ~~DIFFRACTIVE MODEL~~ STRUCTURES:

(1) Cut-and-Project Sets $X \subseteq \mathbb{R}^{r}$

[Yves Meyer 1972]

"model sets"

$$
\begin{tikzcd}
 & \text{lattice } L \subseteq \mathbb{R}^{r} \arrow[dl, "\pi_{\parallel}"'] \arrow[dr, "\pi_{\perp}"] & \\
X \subseteq \mathbb{R}^{n} & & W \subseteq \mathbb{R}^{r-n}
\end{tikzcd}
$$

one-to-one

dense image

Compact set "window"

(Locally Compact Abelian Group)

"Always"

- pure point diffractive

V. Elser; de Bruijn; Meyer; Hof; Schlottmann

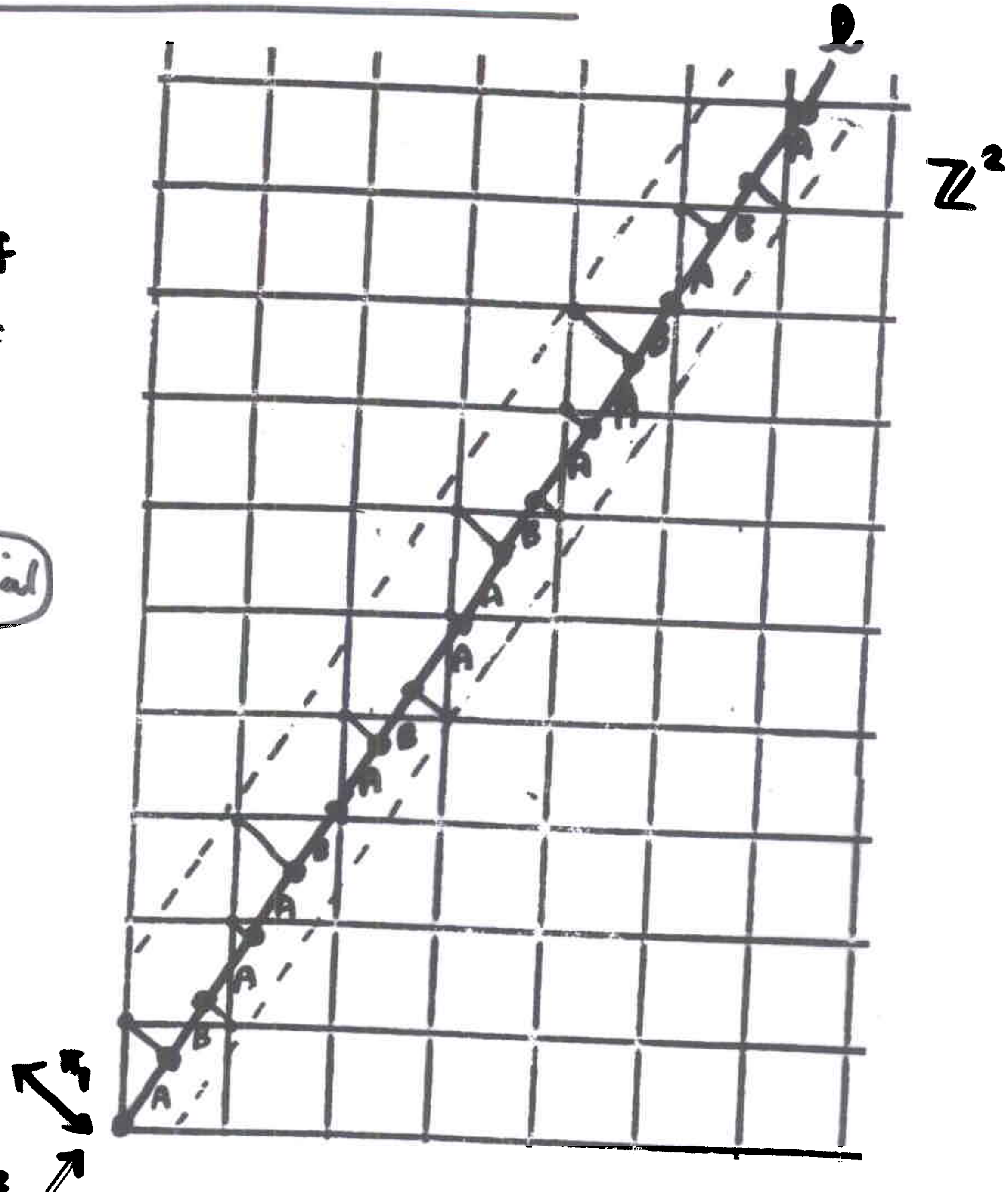
"Sometimes perfect

- "local rules" Known, only in special cases.

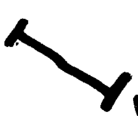
Fibonacci Quasicrystal (1-dimensional)

slope of line = $\frac{1+\sqrt{5}}{2}$

irrational



Fibonacci quasicrystal.



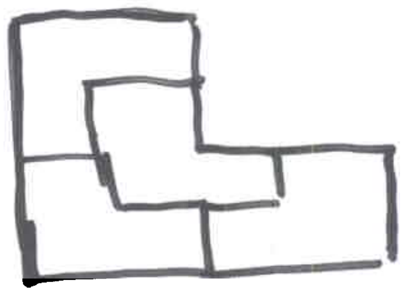
mask/window

$$\begin{cases} r = 2 \\ n = 1 \text{ dim.} \end{cases}$$

Two Kinds of diffractive structures:

(2) <u>Self-similar / Hierarchical</u>
<u>Sets / Tilings</u>

(Inflation / Deflation Rules)



"chair tiling"

- <u>Sometimes</u> pure point diffractive, sometimes not. (Solomyak 1997)

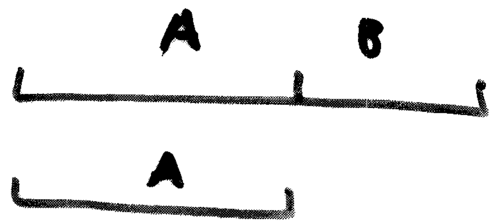
- "Always" have perfect local rules.
  (Goodman-Strauss 1998)

FIBONACCI QUASICRYSTAL

- inflation rule (applies very special cases only)

blow up tiles by $\frac{1+\sqrt{5}}{2}$ →

$$\begin{cases} A \longrightarrow AB \\ B \longrightarrow A \end{cases}$$



A

A B

A B A

A B A A B

A B A A B A B A

. . .

inflate by

$\tau = \frac{1+\sqrt{5}}{2} = 1.6180\ldots$

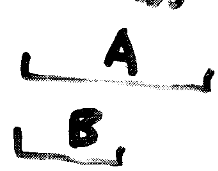
inflation matrix

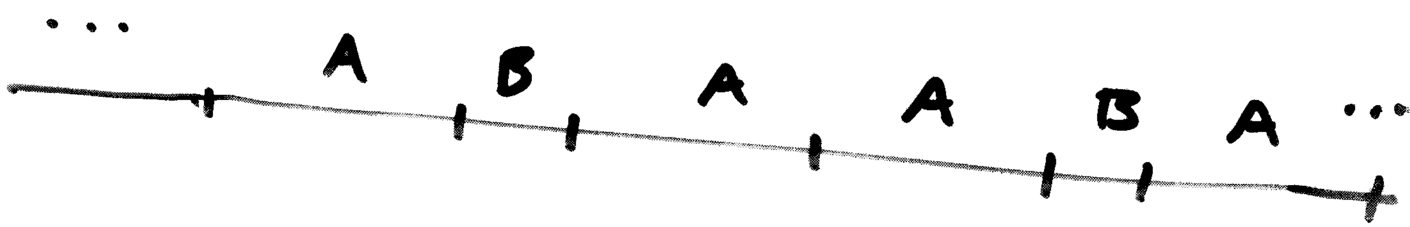
$A = \left[\frac{1+\sqrt{5}}{2} \right]$

substitution matrix

$S = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$

two tiles

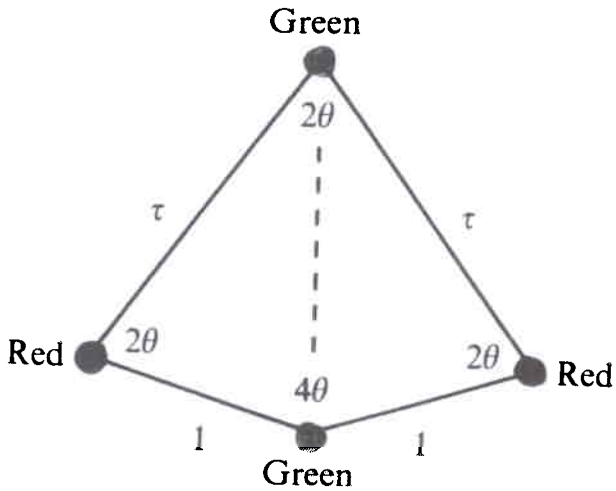




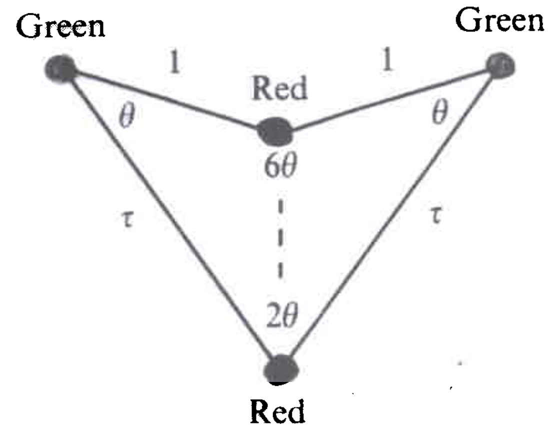
" inflation symmetry " = self-similarity (kind of)

Penrose Tiles

$\theta = \frac{\pi}{5} = 36°$

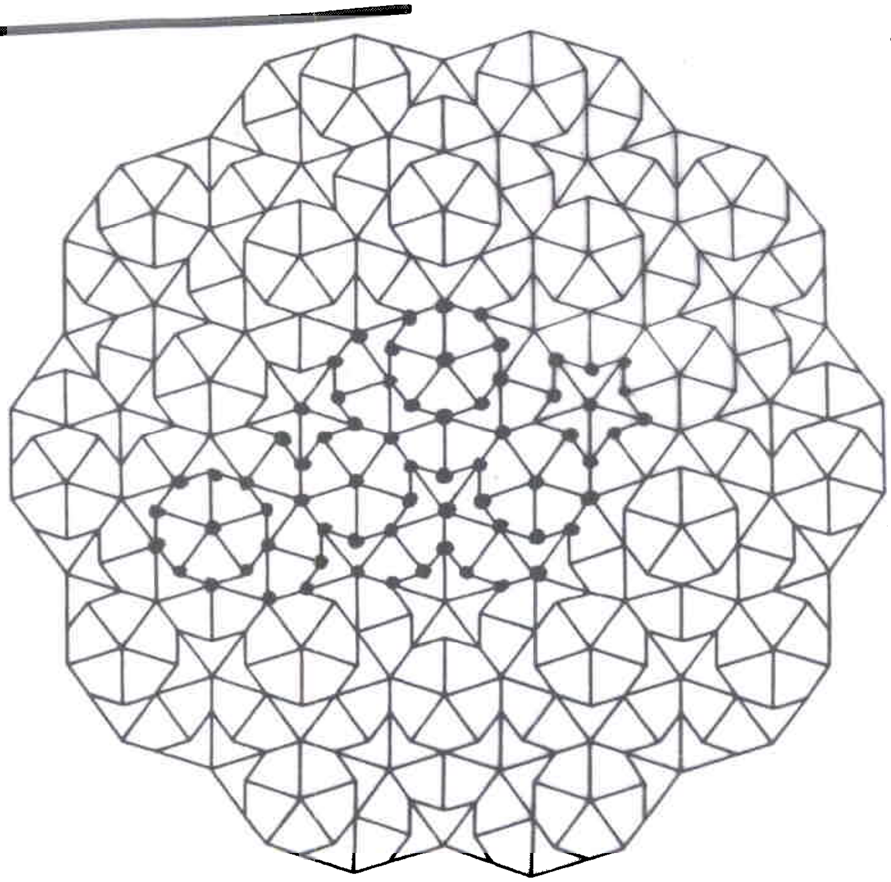


"Kite"



"Dart"

Penrose Tiling



Part of Tiling

- Uncountably many different Penrose tilings

Pure Point Diffraction: Constructions

[Features]

- Delone set X has points contained in a quasilattice L of rank r. in $\mathbb{R}^n$.

- Pure point diffraction spectrum is supported in a quasilattice L^* of equal rank r in "Fourier space."

- Spectrum is dense set if $r > n$. (Only discrete set of "brightest spots" visible in actual measurements.)

3. Taxonomy: Delone Set Models

for Quasicrystals

Finitely Generated Delone Sets

$\cup|$

Delone sets of Finite Type ("Finite Local Complexity" = FLC Sets)

$\cup|$

Meyer Sets

$\cup|$

Model Sets (Cut & Project Sets)

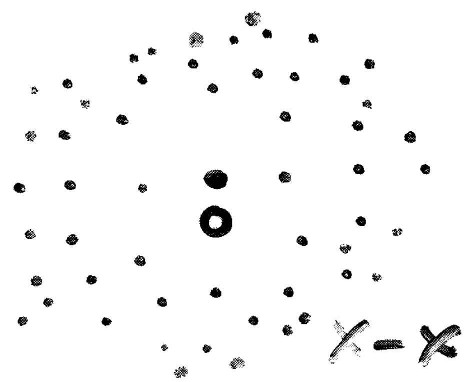
$\cup|$

Ideal Crystals

DEFINITIONS

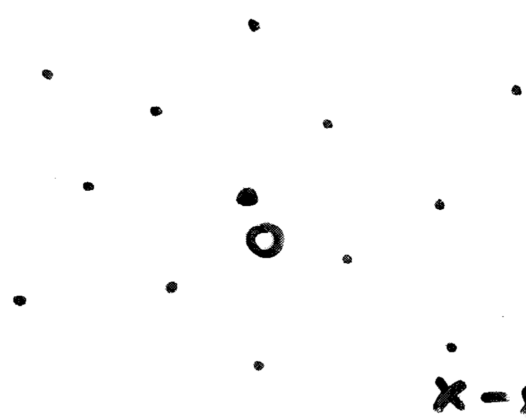
① A Delone set X is **finitely generated** if $\mathbb{Z}[X-X]$ is a quasilattice.

② A Delone set X is **of finite type** if $X-X$ is a discrete closed set.



③ A Delone set X is a **Meyer set** if $X-X$ is a Delone set.

NOT ORIGINAL DEFN. OF MEYER. PROVED EQUIVALENT LATER.



Characterizing Delone Sets of Finite Type

THEOREM

X is a Delone set of finite type

$\Longleftrightarrow$ ("Local Rules")

X has finitely many types of patches of radius $2R$, under translations

$$N_X(2R) < \infty$$

$\Longleftrightarrow$ (Finite Local Complexity)

X has finitely many types of patches of radius T, all $T > 0$.

$$N_X(T) < \infty$$

$\Longleftrightarrow$ (Finite Tile Types)

The Voronoi cells of X are of finitely many types (with centers marked)

[Tiling with finite # of polyhedral prototiles.]

Address Map

If $X \subseteq$ quasilattice L of rank r

can coordinatize X in higher-dim'l.

space $\mathbb{R}^r$:

$$
\begin{tikzcd}
 & \mathbb{R}^r \arrow[dl, "\pi_\parallel"'] \arrow[d, phantom, "\cup"] \arrow[drr, "\pi_\perp"] & & \\
\mathbb{R}^n \arrow[d, phantom, "\cup"] & \underset{\text{lattice}}{Y \subseteq \mathbb{Z}^r} \arrow[drr, dashed] & & \mathbb{R}^{r-n} \\
X \arrow[ur, "\phi"] & & & ?
\end{tikzcd}
$$

"internal space"

$X \subseteq$ quasilattice

$$L = \mathbb{Z}[v_1, v_2, \dots, v_r]$$

$$\underline{x} = \sum_{i=1}^{r} n_i v_i \rightsquigarrow (n_1, \dots, n_r) \in \mathbb{Z}^r$$

"address" map $\phi(\underline{x})$

Structure of X reflected in "wildness" of Y under address map ϕ

X Delone of finite type

$\iff$ address map is Lipschitz-like

$$\|\phi(x_1) - \phi(x_2)\|_{\mathbb{R}^r} \leq C \, \|x_1 - x_2\|_{\mathbb{R}^n}$$

X is Meyer set

$\iff$ address map is almost linear

$$\|\phi(x) - L(x)\| \leq C$$

$L : \mathbb{R}^n \hookrightarrow \mathbb{R}^r$, linear.

[Meyer, Moody]

THEOREM. Let X be a Delone set, and suppose τ is an "inflation factor" with

$$\tau X \subseteq X \qquad \tau > 1.$$

① X finitely generated $\Longrightarrow$ τ is algebraic integer.

② X of finite type $\Longrightarrow$ τ is algebraic integer and all algebraic conjugates $|\tau'| \leq \tau$.

③ X Meyer set $\Longrightarrow$ τ is algebraic integer and all algebraic conjugates $|\tau'| \leq 1$.

---

③ Yves Meyer 1972 ①,② JCL 1998.

4. Dynamical System Viewpoint

Two Delone sets X and X' are "the same" (**locally isomorphic**) if they cannot be told apart locally in any finite piece:

$$\left\{ \begin{array}{l} \text{each } T\text{-patch of } X \text{ occurs in } X' \\ \text{and vice-versa.} \end{array} \right\}$$

for all $T > 0$.

C. Radin

M. Baake R. Moody

B. Solomyak

etc.

Delone Dynamical System

$\mathcal{X}_X = [[X]]$

= closure of all translates

$X + \underline{y}$ of Delone set X

[X, X' <u>close</u> if all points are within ε in large ball, radius $1/\varepsilon$, centered at origin.]

<u>BASIC FACT</u>. If X has Finite Local Complexity then $\mathcal{X}_X$ is compact topological space with $\underbrace{\mathbb{R}^n\text{-action}}$ by translation.

"dynamics"

"Ground States"

- A dynamical system $\mathfrak{X}_X$ is <u>minimal</u> if every orbit is dense.

$$\Updownarrow$$

- A Delone set X is <u>repetitive</u> if for every T-patch $\mathcal{P}$ there is a radius $r(\mathcal{P})$ such that each ball of radius $r(\mathcal{P})$ contains a copy of $\mathcal{P}$ in X.

[The centers of copies of $\mathcal{P}$ form a Delone set.]

<u>Example.</u> Penrose tiling is linearly repetitive ; $r = 14\,T$.

DYNAMICAL SYSTEM $[[X]]$

ENCODES ALL STATISTICAL PROPERTIES AND 'STATISTICAL SYMMETRIES' OF X.

- RECOGNIZES "GROUND STATE" X — { MINIMAL ; UNIQUELY ERGODIC

- RECOGNIZES DIFFRACTION SPECTRUM (PURE POINT PART) — { Dworkin 1983; Lee, Moody, Solomyak 2002

- RECOGNIZES EXTRA SYMMETRIES (HIERARCHICAL STRUCTURE) — { "INFLATION" SYMMETRY & ROTATIONAL SYMMETRIES

DYNAMICAL SPECTRUM $\cong$ DIFFRACTION SPECTRUM

[Radin-Wolff, Solomyak et al]

(1) TOPOLOGICAL DYNAMICS $[[X]]$

A continuous eigenfunction is

continuous map $f : [[X]] \to \mathbb{C}$

with

$$f(T_{\underline{t}}(P)) = e^{2\pi i \langle \underline{t}, \underline{x} \rangle} f(P)$$

Here

$\underline{x} \in \mathbb{R}^n$ is (joint) "eigenvalue"

$T_{\underline{t}}(P) = P + \underline{t}$ ($\mathbb{R}^n$-action)

(2) METRICAL DYNAMICS $([[X]], d\mu)$

invariant measure $\circlearrowleft$ $\mathbb{R}^n$-action

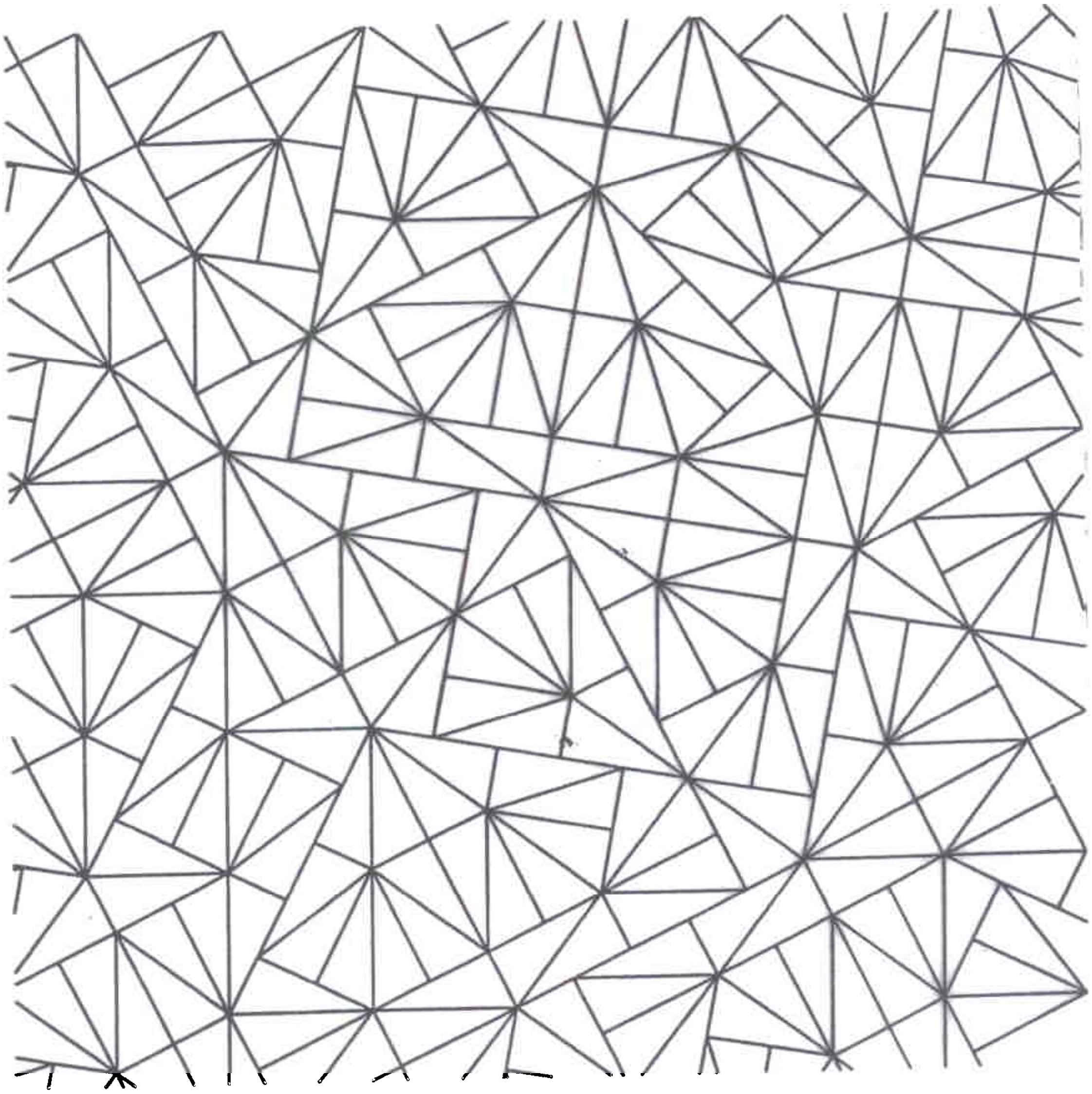
A measurable eigenfunction is

$$f \in L^2([[X]], d\mu)$$

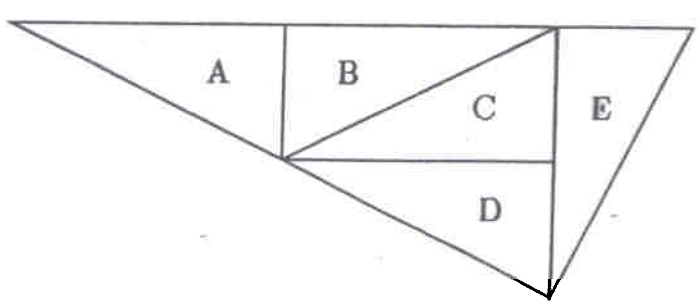
with

$$f(T_{\underline{t}}(P)) = e^{2\pi i \langle \underline{t}, \underline{x} \rangle} f(P) \quad \text{almost everywhere } [d\mu]$$

PINWHEEL TILING (Conway – Radin)



INFLATION RULE:



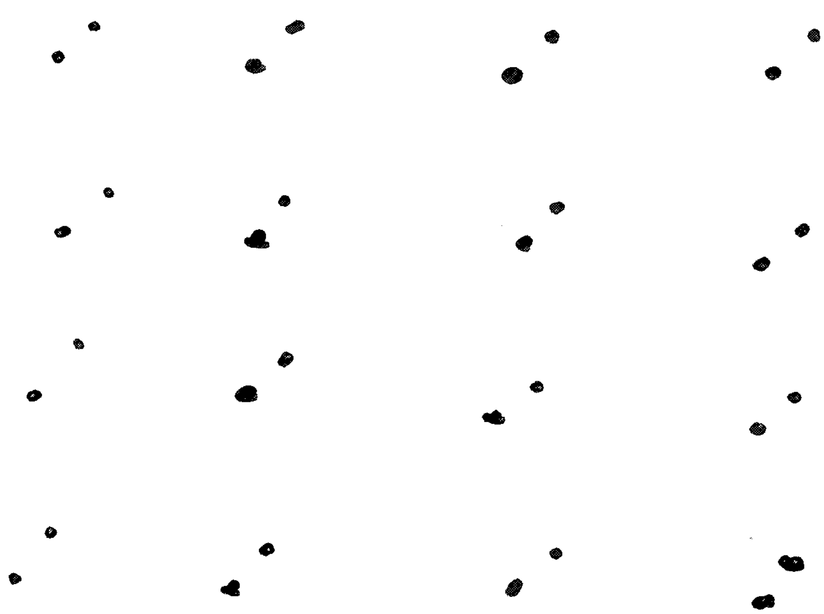
- Has "irrational rotation" symmetry.
- "Point group" = O(2) continuous symmetry.

§. Characterizing Properties of Ideal Crystals

Defn. An ideal crystal in $\mathbb{R}^n$ is a finite number of translates of a (full-dimensional) lattice L, i.e.

$$X = L + F$$

finite set



$$X = \mathbb{Z}^2 + \left\{ (0,0), \left(\tfrac{1}{6}, \tfrac{1}{6}\right) \right\}$$

Property 1. (Bounded Patch - Counting Function)

ⓐ Let $N_X(T)$ denote the number of different patches of radius T in X, up to translations. Then

$$N_X(T) \leq c,$$

for all T.

ⓑ Let $N_X^*(T)$ denote the number of different patches, up to isometry. Then

$$N_X^*(T) \leq c^*,$$

for all T.

- These properties characterize ideal crystals
  Delone et al. 1976
  Dolbilin, JCL, Senechal 1998

Property 1'. (Linear-Volume Patch-Counting Function)

Let $N_X(T)$ count the number of different patches of radius T in X in $\mathbb{R}^n$ up to translations. Then

$$N_X(T) \leq c\,T^n$$

for all T.

- (marked) Penrose tilings have this property.

Property 2. (Bounded Repetitivity)

There is a constant C such that any ball of radius $T+C$ contains a translated copy of every type of patch of radius T in X.

- This property characterizes ideal crystals: easy proof.

Property 2′. (Linear Repetitivity)

There is a constant c such that each ball of radius cT in $\mathbb{R}^n$ contains a translated copy of each type of patch of radius T in X.

- (marked) Penrose tilings have this property. with $c \cong 13$ (tiles of side ≤ 1.618)

Property 3. (Delone set diffractivity)

The set X has a (mathematical) diffraction measure that is pure point and is supported on a Delone set.

- This property holds for ideal crystals, but also for other sets, since removing a density zero set of points doesn't change diffraction measure.

Conjecture. If X is repetitive, spans a quasilattice & is Delone set diffractive, then it is an ideal crystal.

Property 3′ (Pure Point Diffractivity)

The Delone set X in $\mathbb{R}^n$ has a (mathematical) diffraction measure which is pure point and supported on a quasilattice.

- (marked) Penrose tilings have this property, and are repetitive & span a quasilattice.

Property 4. (Self-Similarity on Multiple Scales)

There is a finite partition

$$X = \bigcup_{i=1}^{k} X_i$$

such that for all $m \geq 2$,

$$X_i = \bigcup_{i=1}^{k} (m X_j + F_{ij})$$

for certain finite sets F_{ij}.

[Here m = inflation factor.]

- It is not known if this property characterizes ideal crystals.

(I think it probably does.)

- There are Analogous self-similar tiling properties.

Property 4′. (Self-similar on one scale)

The set X has a finite partition

$$X = \bigcup_{i=1}^{K} X_i$$

such that there is a real constant $\lambda > 1$ and finite sets F_{ij} with

$$X_i = \bigcup_{j=1}^{K} (\lambda X_j + F_{ij})$$

- There exists a (special) marked Penrose tiling with this property, and $\lambda = \frac{3+\sqrt{5}}{2}$.

CONCLUSION: Study of quasicrystal problems leads to:

- Boundary between periodic/aperiodic structures better understood.

- Dynamical systems, Harmonic Analysis viewpoint ($\mathbb{R}^n$-action) usefully applied in discrete geometry & diffraction.

- Construction of some "perfect" aperiodic sets.

- Find/Understand "new" kinds of statistical symmetries. (C. Radin et al.)

Hilbert Problems (Paris 1900)

23 problems

Research programs:

Problem 6. Axiomatize Physics

(Rigorous derivations of results.)

Specific problems: Three Remaining unsolved:

- **Problem 8.** Riemann hypothesis
- **Problem 16.(ii).** Limit cycles for polynomial vector fields in $\mathbb{R}^2$.
- **Problem 18 (iii-b).** Densest packing of regular tetrahedra in $\mathbb{R}^3$.

Unsolved Hilbert Problems:

- Each problem Apparently has associated dynamical system!

Problem 8: Riemann hypothesis

appears to have "Unknown" dynamical system.

[M. Berry - J. Keating, C. Deninger, N. Katz - P. Sarnak]
random matrix

Problem 16 (ii): Limit Cycles — polynomial vector fields in $\mathbb{R}^2$

is dynamical problem from Poincaré.

Problem 18 (iii-b): Densest Packing of Regular Tetrahedra.

Dynamical system X_P with $\mathbb{R}^3$-action associated to densest packing may have interesting properties.