What is a Quasicrystal?

July 23, 2013

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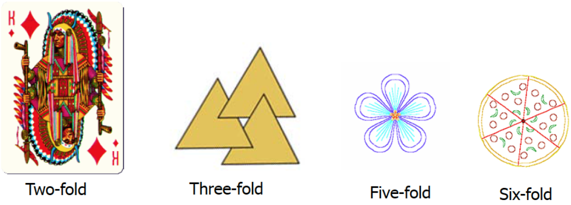
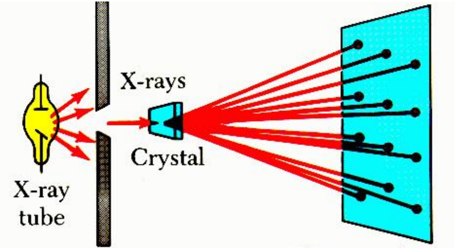
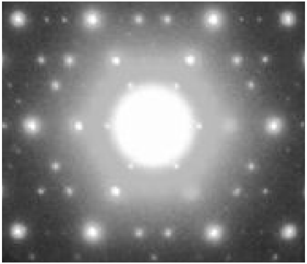


Figure : rotational symmetry

Crystallography: X-ray diffraction experiment.

The first x-ray diffraction experiment was performed by von Laue in 1912.





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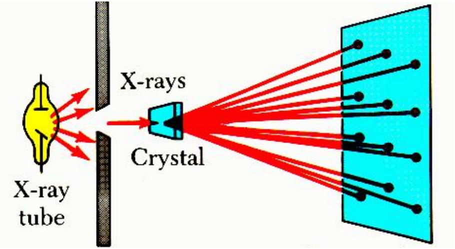

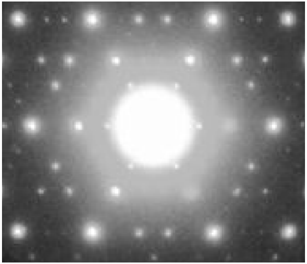

- Crystals are ordered
  $\Rightarrow$ a diffraction pattern with sharp bright spots, Bragg peaks.

A paradigm before 1982

- Crystallographic restriction:
  If atoms are arranged in a pattern periodic, then

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  for diffraction pattern of periodic crystals.
- All the crystals were found to be periodic from 1912 till 1982.
- Atoms in a solid are arranged in a periodic pattern.

Discovery of quasicrystals in 1982

- Dan Shechtman (2011 Nobel Prize winner in Chemistry)

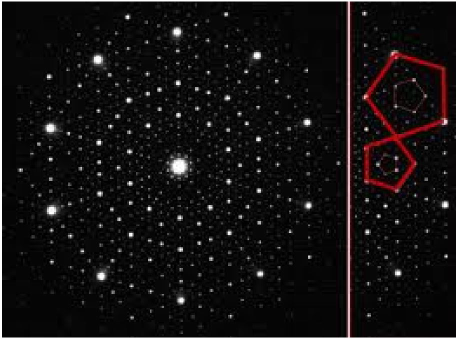

Figure : Al_6Mn

(Quasi)crystals

Definition for Crystal

- Till 1991: a solid composed of atoms arranged in a pattern periodic in three dimensions.
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Q. What are the appropriate mathematical models?

- A Delone set Λ in $\mathbb{R}^d$ is a set with the properties:
  - uniform discreteness: $\exists r > 0$ such that for any $y \in \mathbb{R}^d$

    $$B_r(y) \cap \Lambda \text{ contains at most one element.}$$

  - relative denseness: $\exists R > 0$ such that for any $y \in \mathbb{R}^d$

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Mathematical diffraction theory

Dirac Comb $\delta_\Lambda := \sum_{x\in\Lambda} \delta_x$ for $\Lambda \subset \mathbb{R}^d$.

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- a diffraction measure $\hat{\gamma}$ describes the mathematical diffraction.
  - $\hat{\gamma}$ is a positive measure: $\hat{\gamma} = \hat{\gamma}_d + \hat{\gamma}_c$.
- a quasicrystal: a Delone set Λ with $\hat{\gamma}_d \neq 0$.

Example: a lattice

- $L \subset \mathbb{R}^d$ a lattice, i.e., $L = A(\mathbb{Z}^d)$,
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- Poisson summation formula says that

$$\hat{\gamma} = \frac{1}{|\det A|} \sum_{x \in L^*} \delta_x$$

Meyer sets

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Theorem If Λ is a Delone set, then the above three conditions are equivalent.

Cut and Project method

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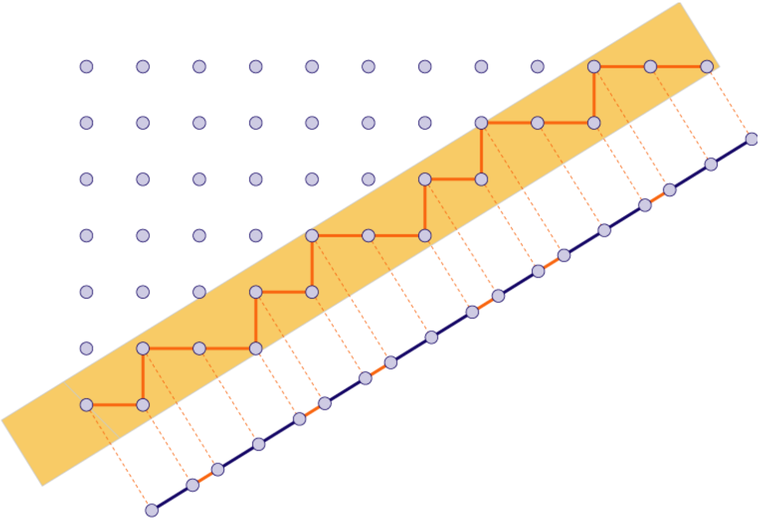

Model Sets

a model set (or cut and project set) is the translation of

$$\Lambda = \Lambda(W) = \{\pi_1(x) : x \in L, \pi_2(x) \in W\}.$$

- $\mathbb{R}^d$: a real euclidean space
- G: a locally compact abelian group
- projection maps

$$\pi_1 : \mathbb{R}^d \times G \to \mathbb{R}^d, \pi_2 : \mathbb{R}^d \times G \to G$$

- L: a lattice in $\mathbb{R}^d \times G$ with
    - $\pi_1|_L$ is injective and $\pi_2(L)$ is dense.
- $W \subset G$ is non-empty and $W = \overline{W^0}$ is compact.

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  A Meyer is a subset of some model sets.
- Strungaru, 2005
  A Meyer set has a discrete diffraction spectrum. $(\hat{\gamma}_d \neq 0)$.

Pisot and Salem numbers

Definition

- A Pisot number is a real algebraic integer $\theta > 1$ whose conjugates all lie inside the unit circle.
- A Salem number is a real algebraic integer $\theta > 1$ whose conjugates all lie inside or on the unit circle, at least one being on the circle.

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Remark

- The set S of all Pisot numbers is infinite and has a remarkable structure: the sequence of derived sets

$$S, S', S'', \ldots$$

does not terminate.

Example

- $\theta = \frac{1+\sqrt{5}}{2}$ and $\theta' = \frac{1-\sqrt{5}}{2}$.
- $L = \{(a + b\theta, a + b\theta') : a, b \in \mathbb{Z}\}$ is a Lattice in $\mathbb{R}^2$.
- $\Lambda = \{a + b\theta : |a + b\theta'| < 1\}$ is a model set with

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Theorem

- Given a Pisot or Salem number θ, there exists a model set Λ such that

$$\theta\Lambda \subset \Lambda.$$

- Given a model set Λ, if θ is a positive real number with $\theta\Lambda \subset \Lambda$, then θ is a Pisot or Salem number.

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- Riemann hypothesis: the non-trivial zeros should lie on the critical line $1/2 + it$.
- Z: the set of imaginary parts of the complex zeros.
  - Z is not uniformly discrete.
  - Truth of hypothesis implies that the Fourier transform of Z is

$$\sum c_{m,p} \delta_{\pm \log p^m},$$

where p is a prime and m is a positive integer.

A generalized quasicrystal

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Exercise for students. Classify all one-dimensional generalized quasicrystals. After you have done this, look at the list and see whether Z is there. If Z is there, you have proved RH.

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