What is a Quasicrystal?

July 23, 2013
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An object with **rotational symmetry** is an object that looks the same after a certain amount of rotation.

Figure: rotational symmetry

- **Two-fold**
- **Three-fold**
- **Five-fold**
- **Six-fold**

Figure: rotational symmetry
Crystallography: X-ray diffraction experiment.

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- Crystals are ordered
  ⇒ a diffraction pattern with sharp bright spots, Bragg peaks.
A paradigm before 1982

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

∃ only 2,3,4 and 6-fold rotational symmetries

for diffraction pattern of periodic crystals.

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- Crystallographic restriction:
  If atoms are arranged in a pattern periodic, then
  \[ \exists \text{ only } 2, 3, 4 \text{ and } 6\text{-fold rotational symmetries} \]
  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: $Al_6Mn$
Definition for Crystal

- Till 1991: a solid composed of atoms arranged in a pattern periodic in three dimensions.
(Quasi)crystals

Definition for Crystal

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Q. What are the appropriate mathematical models?
A Delone set $\Lambda$ 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 $y \in \mathbb{R}^d$
  
  $$B_R(y) \cap \Lambda \text{ contains at least one element.}$$
Mathematical diffraction theory

Dirac Comb

\[ \delta \Lambda := \sum_{x \in \Lambda} \delta_x \]

for \( \Lambda \subset \mathbb{R}^d \).

Autocorrelation restricted to \([-L, L]^d\):

\[ \sum_{x, y \in \Lambda \cap [-L, L]^d} \delta_{x - y} \]

Autocorrelation measure \( \gamma \):

\[ \gamma = \lim_{L \to \infty} \frac{1}{\text{vol}[-L, L]^d} \sum_{x, y \in \Lambda \cap [-L, L]^d} \delta_{x - y} \]

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 \( \Lambda \) with \( \hat{\gamma}_d \neq 0 \).

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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 $\Lambda$ with $\hat{\gamma}_d \neq 0$. 

What is a Quasicrystal?
Example: a lattice

- $L \subset \mathbb{R}^d$ a lattice, i.e., $L = A(\mathbb{Z}^d)$,
  - $A$ is $d \times d$ invertible matrix.
  - $L^* = \{y : e^{ix \cdot y} = 1, \ \forall x \in L\}$

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- $L - L = L$ implies
  $$\gamma = \delta_L = \sum_{x \in L} \delta_x$$
- Poisson summation formula says that
  $$\hat{\gamma} = \frac{1}{|\det A|} \sum_{x \in L^*} \delta_x$$

What is a Quasicrystal?
Meyer sets

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$$\exists \text{ a finite set } F : \Lambda - \Lambda \subset \Lambda + F.$$
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   \[ \exists \text{ a finite set } F : \Lambda - \Lambda \subset \Lambda + F. \]
3. $\Lambda$ is harmonious:
   \[ \forall \epsilon > 0, \Lambda^*_\epsilon = \{ y \in \mathbb{R}^d : |e^{ix\cdot y} - 1| \leq \epsilon \} \text{ is relatively dense.} \]
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**Theorem** If $\Lambda$ is a Delone set, then the above three conditions are equivalent.

What is a Quasicrystal?
Cut and Project method

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What is a Quasicrystal?
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.
Some results

A model set is a Meyer set. Schlottman, 1998

A model set $\Lambda$ has a purely discrete diffraction spectrum. ($\hat{\gamma} = \hat{\gamma}_d$).

A Meyer is a subset of some model sets. Strungaru, 2005

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  A Meyer set has a discrete diffraction spectrum. ($\hat{\gamma}_d \neq 0$).
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.
Pisot and Salem numbers

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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.

What is a Quasicrystal?
Quasicrystals corresponding to Pisot or Salem numbers

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

Theorem

- Given a Pisot or Salem number \( \theta \), there exists a model set \( \Lambda \) such that \( \theta\Lambda \subset \Lambda \).
- Given a model set \( \Lambda \), if \( \theta \) is a positive real number with \( \theta\Lambda \subset \Lambda \), then \( \theta \) is a Pisot or Salem number.
Riemann Hypothesis

- Riemann zeta function:

\[ \zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}. \]

- Riemann hypothesis: the non-trivial zeros should lie on the critical line \( \frac{1}{2} + it \).

- \( \mathbb{Z} \): the set of imaginary parts of the complex zeros. \( \mathbb{Z} \) is not uniformly discrete.

- Truth of hypothesis implies that the Fourier transform of \( \mathbb{Z} \) is

\[ \sum_{n=1}^{\infty} \frac{1}{n^s}. \]

- Where \( p \) is a prime and \( m \) is a positive integer.

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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.

What is a Quasicrystal?
An aperiodic set $\Lambda$ is a generalized quasicrystal if

- it is locally finite, and has a points in every sphere of some radius $R$.
- it has a discrete Fourier transform.
A generalized quasicrystal

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- it has a discrete Fourier transform.

**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.
Y. Meyer (1995)
Quasicrystals, Diophantine approximations, and algebraic numbers

M. Senechal (1995)
Quasicrystals and Geometry

R. Moody (1997)
Meyer sets and their duals.

F. Dyson (MSRI Lecture Notes 2002)
Random Matrices, Neutron Capture Levels, Quasicrystals and Zeta-function zeros