Quasicrystals in Wonderland

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Chemnitz University of Technology

AIMS conference May 2008

Outline

- Quasicrystals?
  - Mathematical models of aperiodic order
  - Hamiltonians
- Dynamical systems
- Spectral properties: The Wonderland theorem.

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Based on collaboration with D. Lenz.

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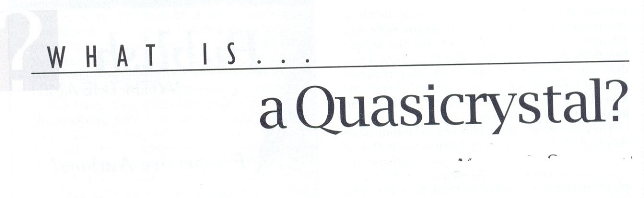
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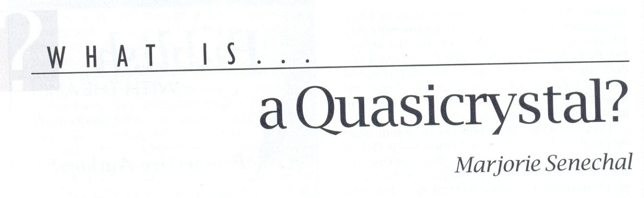
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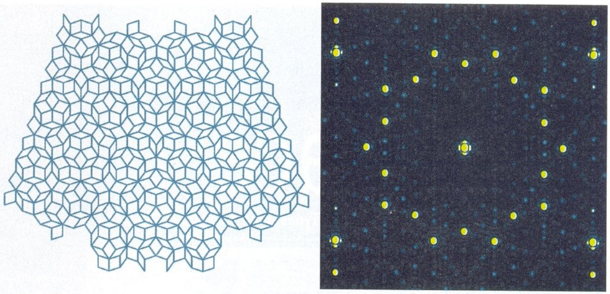

Figure 1. (a). A patch of a Penrose tiling. (b). The diffraction diagram of the vertex set V of (a) is essentially discrete; thus F is an aperiodic crystal, according to the new definition.

As a rule of thumb quasicrystals exhibit:

- Sharp diffraction peaks - usually coming with long range order.
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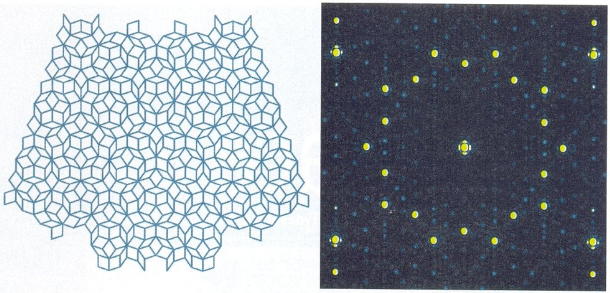

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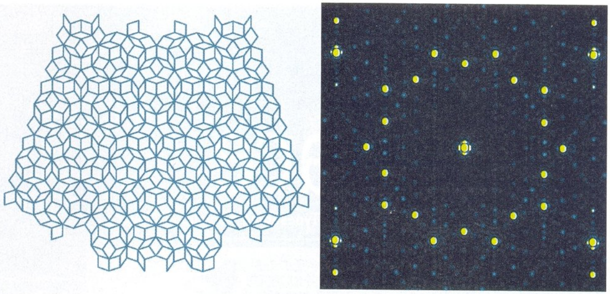

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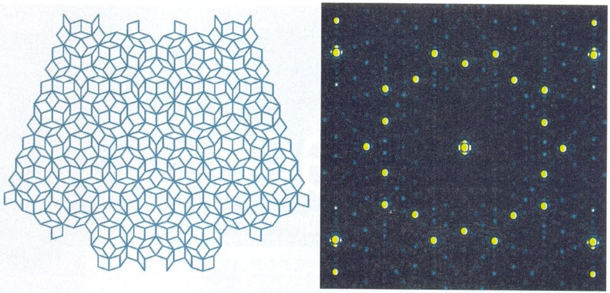

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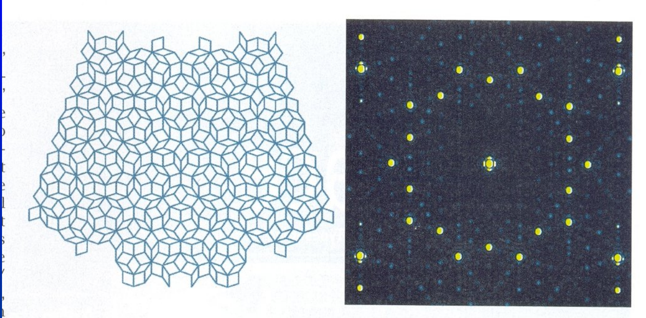

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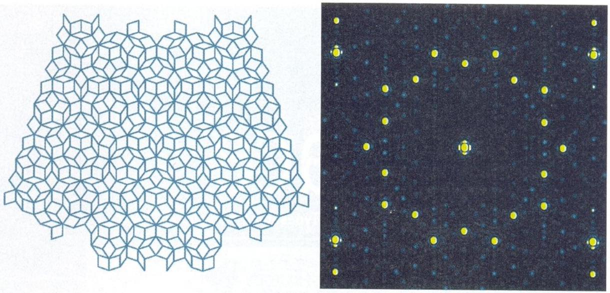

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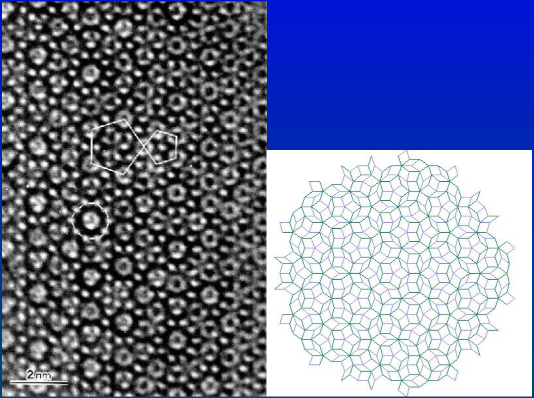

Figure: A real quasicrystal and the Penrose tiling

Delone (Delaunay) sets

An alternative to tilings are Delone sets.

$\omega \subset \mathbb{R}^d$ is called a Delone set, if there exist $r, R \in \mathbb{R}$ such that

- $\forall x, y \in \omega, x \neq y : U_r(x) \cap U_r(y) = \emptyset$,
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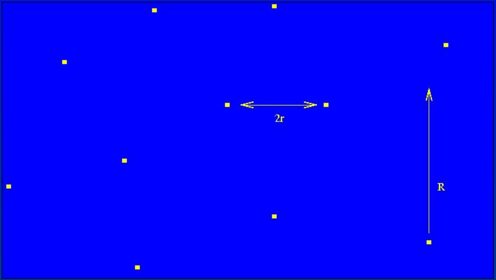

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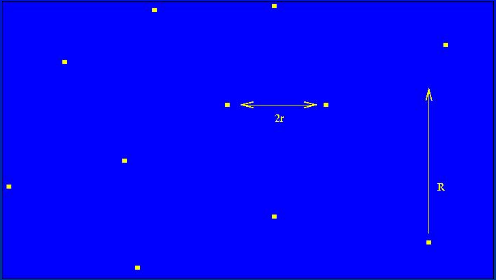

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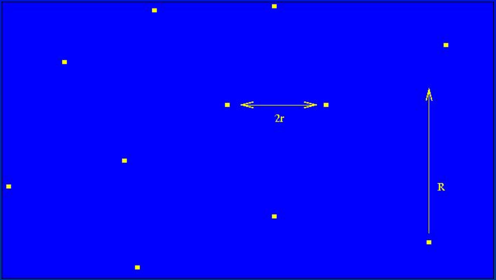

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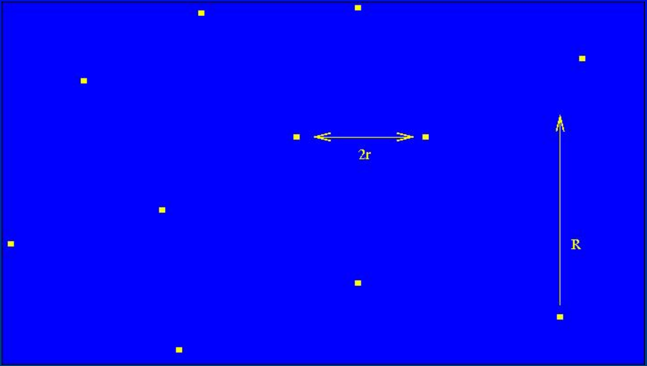

By $\mathbb{D}_{r,R}(\mathbb{R}^d) = \mathbb{D}_{r,R}$ we denote the set of all (r, R)-sets; it is a compact metric space in the natural topology.

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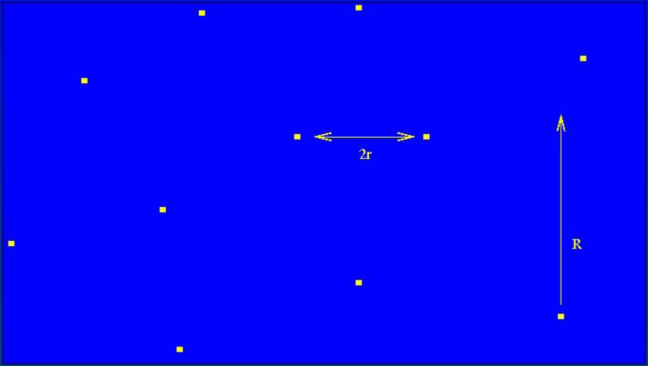

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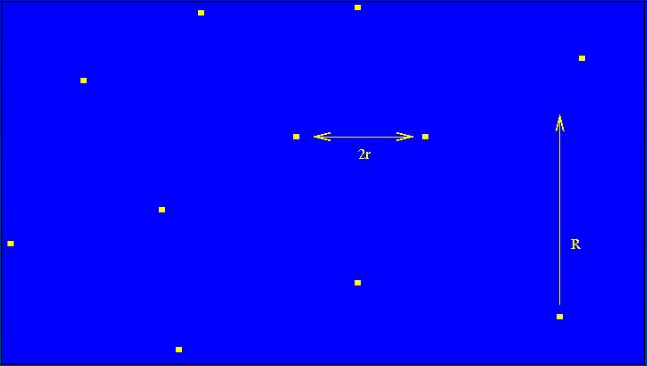

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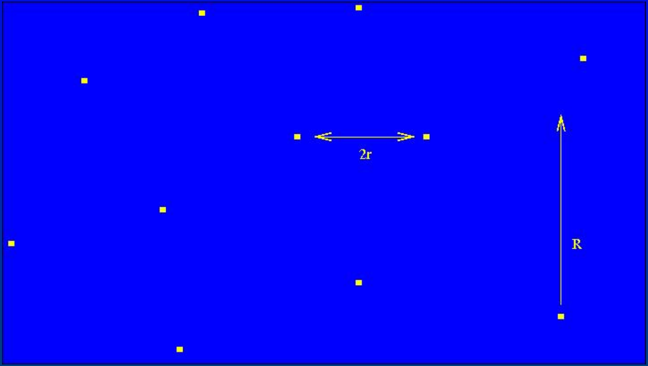

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Hamiltonians: continuum models

The basic idea is very simple: at each point of a Delone set ω an ion is sitting, whose potential is given by v. This leads to the Hamiltonian

$$H(\omega) := -\Delta + \sum_{x\in\omega} v(\cdot - x)$$

The potential

$$V_\omega = \sum_{x\in\omega} v(\cdot - x)$$

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If the Delone set ω is periodic, then $H(\omega)$ describes a crystal. If we choose the point set ω as the points of a Poisson process (typically no Delone set) then $H(\omega)$ describes a disordered solid. If ω is aperiodically ordered, then $H(\omega)$ can be used to describe electronic properties of a quasicrystal.

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Hamiltonians

We are interested in the Schrödinger equation

$$\psi'(t) = -iH(\omega)\psi(t) \qquad (SE)$$

it describes the time evolution of a wave function $\psi(t)$.
Spectral properties of $H(\omega)$ can be translated into qualitative properties of solutions of (SE).
The specific form of (dis-)order is encoded in $H(\omega)$.
It will be very useful to consider a whole collection $(H(\omega), \omega \in \Omega)$ at the same time, for physical reasons and for analytical reasons.

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Delone dynamical systems

... simply consist of a translation invariant, compact set $\Omega \subset \mathbb{D}(\mathbb{R}^d)$, on which the group $T_t : \mathbb{R}^d \to \mathbb{R}^d (t \in \mathbb{R}^d)$ of translations acts; we denote such a system by (Ω, T). We interpret such a DDS (Ω, T) as a model for a certain type of (dis-)order. Ergodic properties of (Ω, T) reflect combinatorial properties of the elements $\omega \in \Omega$ and vice versa. Moreover, spectral properties of the $H(\omega)$ are sometimes related to ergodic properties of the DDS. E.g.

$$(\Omega, T) \text{ minimal}$$
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$$\sigma(H(\omega)) = \sigma(H(\omega')) \text{ for all } \omega, \omega' \in \Omega.$$

Minimality and unique ergodicity are equivalent to certain combinatorial properties of the ω's.

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Let $r, R > 0$ with $2r < R$ and $v \geq 0$, $v \neq 0$. Then there exists an open $\emptyset \neq U \subset \mathbb{R}$ and a dense G_δ-set $\Omega_{sc} \subset \mathbb{D}_{r,R}$ such that for every $\omega \in \Omega_{sc}$ the spectrum of $H(\omega)$ contains U and is purely singular continuous in U.

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Fix S, a locally compact, σ-compact, separable metric space.
Consider $\mathcal{M}_+(S)$, the set of positive, regular Borel measures.
$\mu \in \mathcal{M}_+(S)$ *diffusive* or *continuous*:$\iff \mu(\{x\}) = 0$ for every $x \in S$.
$\mu \perp \nu$, *mutually singular*:$\iff \exists\ C \subset S$ such that $\mu(C) = 0 = \nu(S \setminus C)$.

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Proof of generic appearance of singular continuous spectrum using the Wonderland theorem. If $\rho \in \mathbb{D}_{r,R}$ is *crystallographic*, i.e.,

$$Per(\rho) := \{t \in \mathbb{R}^d : \rho = t + \rho\}$$

is a lattice, then $H(\rho)$ is periodic. Consequently, $H(\rho)$ has purely absolutely continuous spectrum.

Since $2r < R$, there exist crystallographic $\gamma, \tilde{\gamma}$ such that $U := \sigma(H(\gamma))^\circ \setminus \sigma(H(\tilde{\gamma})) \neq \emptyset$.

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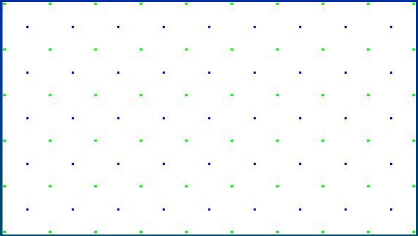

Figure: crystallographic γ (green) and $\tilde{\gamma}$ (green+blue)

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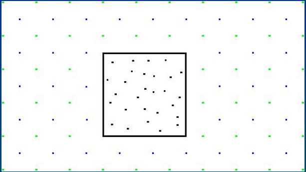

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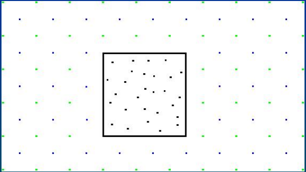

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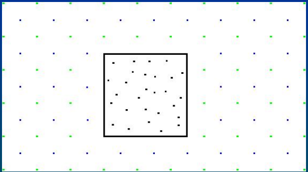

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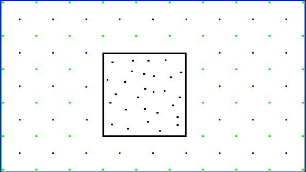

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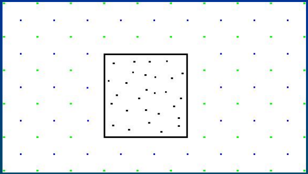

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- This implies the Wonderland theorem and the fact that generic measures are singular continuous in "nice spaces".
- A particular example is given by "geometric disorder" (= Delone Hamiltonians) for which we can prove that purely singular continuous components turn up, generically.

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