Between order and disorder: Hamiltonians for quasicrystals

Peter Stollmann

Chemnitz University of Technology

Minisymposium Spectral Theory and Ergodic Operators, Bonn, 18.9.2006

Outline

- Quasicrystals?
- Mathematical models of aperiodic order
- Hamiltonians
  - Continuum models
  - Discrete models
- Dynamical systems
- Spectral properties
  - Continuum models
  - Discrete models
- Algebras of Hamiltonians
- Conclusion

Based on collaboration with D. Lenz and S. Klassert.

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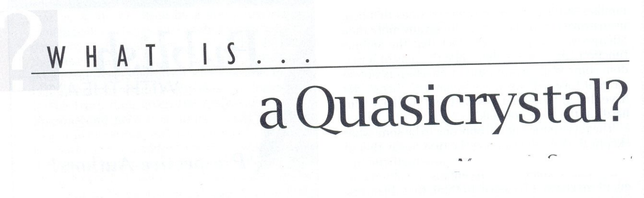
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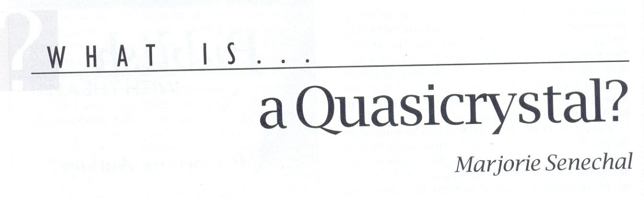

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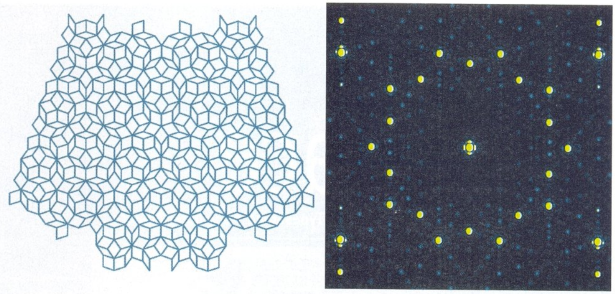

Figure 1. (a). A patch of a Penrose tiling. (b). The diffraction diagram of the vertex set V of (a) is essentially discrete; thus F is an aperiodic crystal, according to the new definition.

As a rule of thumb quasicrystals exhibit:

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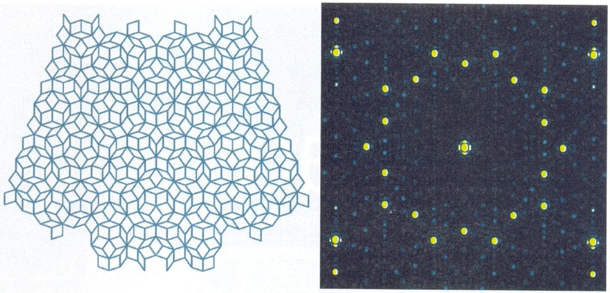

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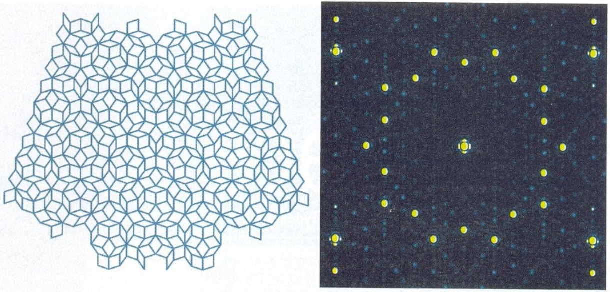

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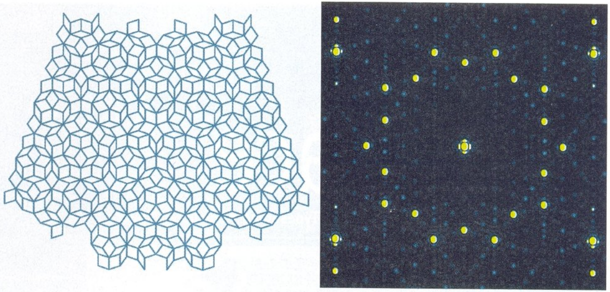

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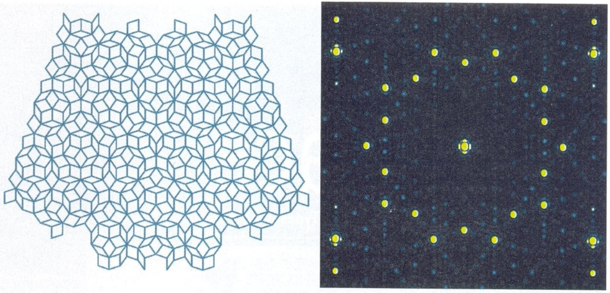

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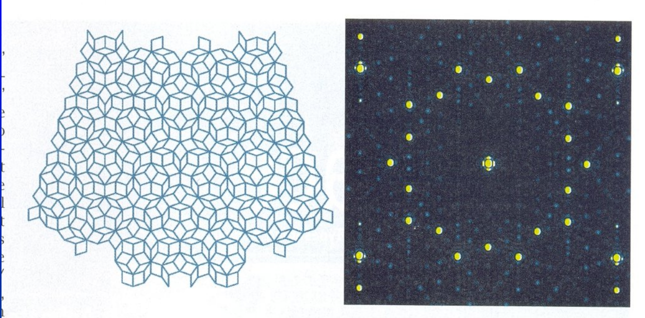

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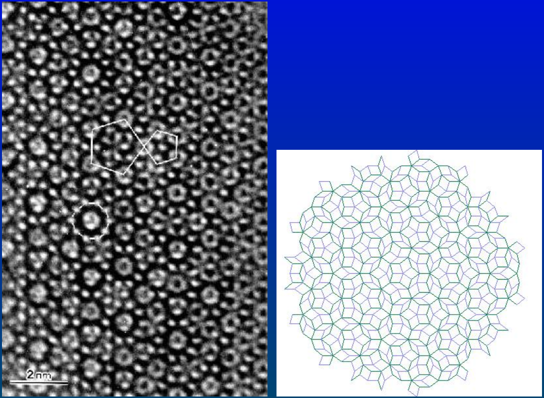
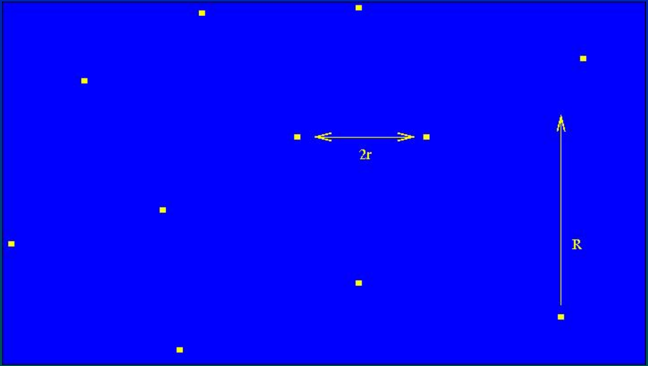


Figure: Original und Fälschung

Delone (Delaunay) sets

A tiling with only finitely many tiles will lead to a model with finite local complexity - there are only finitely many different pattern of a fixed diameter. This can easily be described by Delone sets. A set $\omega \subset \mathbb{R}^d$ is called a Delone set, if there exist $r, R \in \mathbb{R}$ such that



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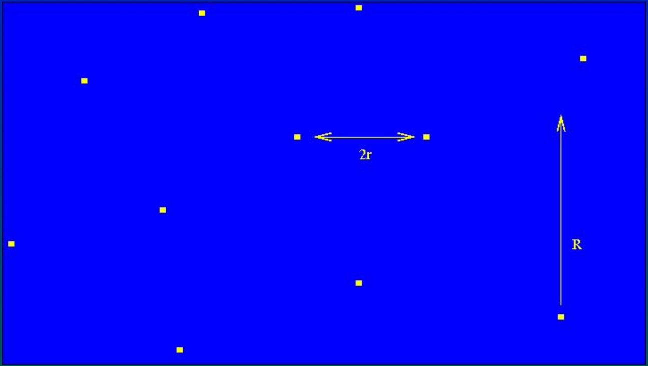

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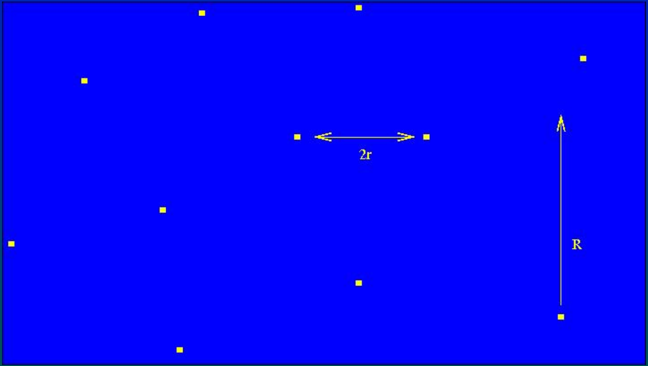

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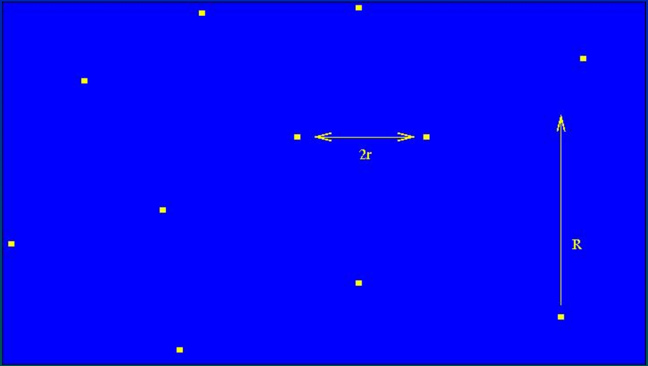

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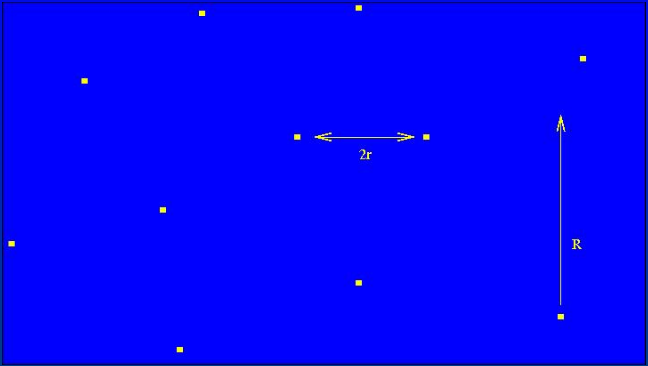

$\omega \subset \mathbb{R}^d$ is called a Delone set, if there exist $r, R \in \mathbb{R}$ such that

- $\forall x, y \in \omega, x \neq y : U_r(x) \cap U_r(y) = \emptyset$,
- $\bigcup_{x \in \omega} B_R(x) = \mathbb{R}^d$.

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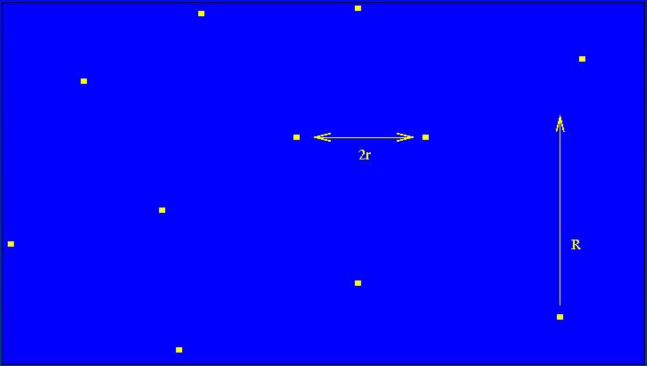

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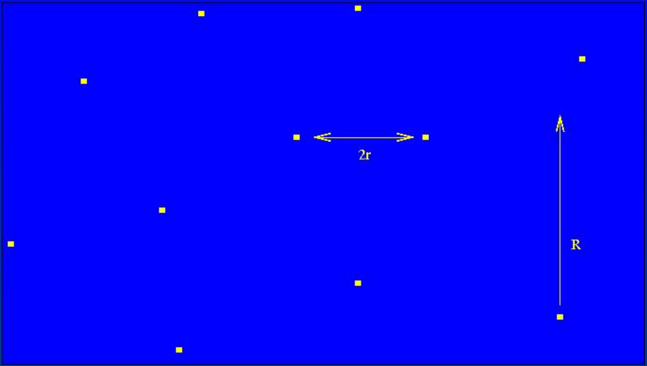

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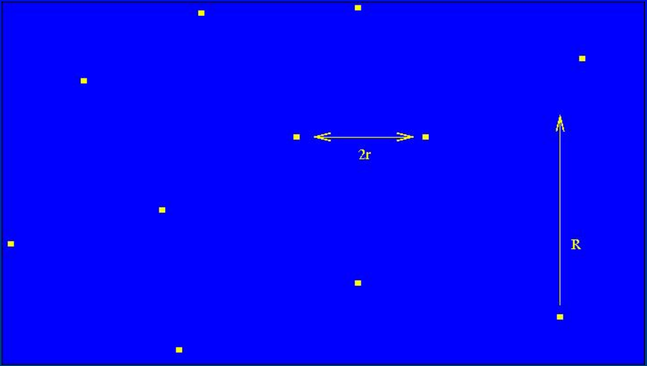

By $\mathbb{D}_{r,R}(\mathbb{R}^d) = \mathbb{D}_{r,R}$ we denote the set of all (r, R)-sets; it is a compact metric space in the natural topology.

$\mathbb{D}(\mathbb{R}^d) = \bigcup_{0<r\leq R} \mathbb{D}_{r,R}(\mathbb{R}^d)$ is the set of all Delone sets.

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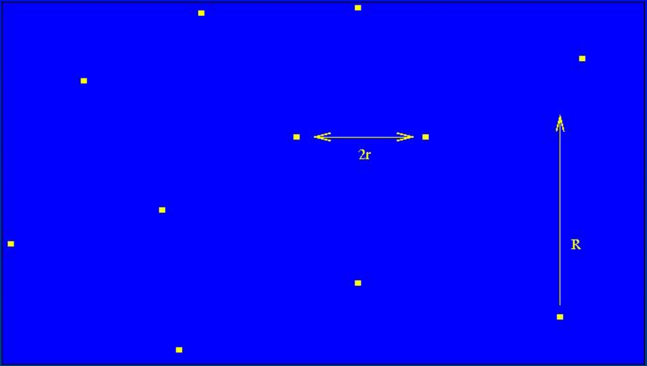

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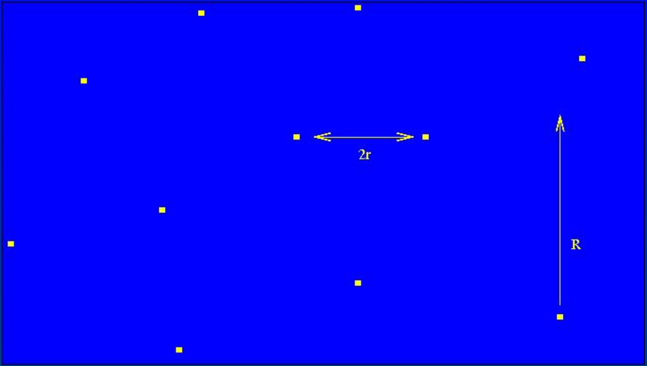

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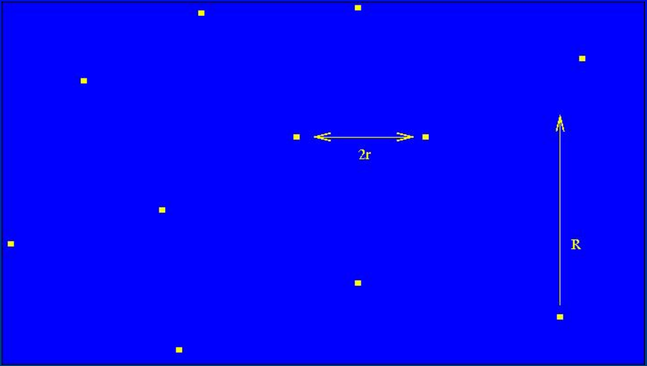

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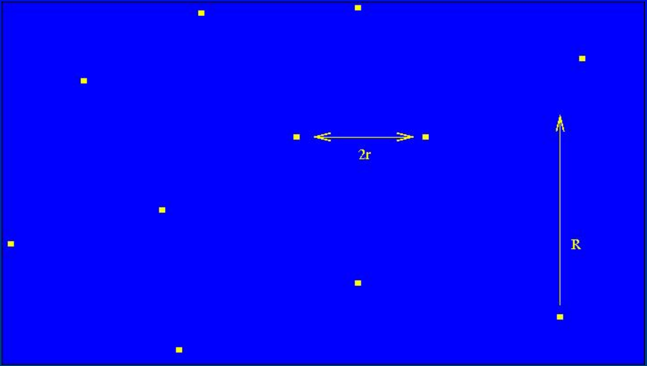

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Finite local complexity is phrase in terms of *pattern*. A pattern is a pair (U, λ), consisting of an open bounded subset of $U \subset \mathbb{R}^d$ and a finite subset $\lambda \subset U$. For a Delone set ω and U as above, $(U, U \cap \omega)$ is a pattern. We say that ω has finite local complexity if for any $L > 0$ the number

$$n_L := \#\{(\omega - x) \cap U_L(0) | x \in \omega\} < \infty.$$

An obvious extension is defined for subsets $\Omega \subset \mathbb{D}$. The growth of n_L in L is an important combinatorial manifestation of (dis-)order. Periodic vs Bernoulli.

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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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Hamiltonians: discrete models

In the tight binding approximation which has proved to be quite useful in solid state physics, the Hilbert space is $\ell^2(\omega)$. The operator is a difference operator, defined by its matrix elements

$$(H(\omega)\delta_x|\delta_y).$$

We assume that $(H(\omega)\delta_x|\delta_y)$ is 0 if the distance of x and y is large enough; and that this matrix element only depends on the pattern around x and y and call these operators of finite range.

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We assume that $(H(\omega)\delta_x|\delta_y)$ is 0 if the distance of x and y is large enough; and that this matrix element only depends on the pattern around x and y and call these operators of finite range.

Hamiltonians

Independent of the use of discrete or continuum models, 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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$$\sigma(H(\omega)) = \sigma(H(\omega')) \text{ for all } \omega, \omega' \in \Omega.$$

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Spectral properties: continuum models

A very modest step has been taken in showing that generically (in the topological sense) singular continuous spectrum occurs.

Theorem

Let $r, R > 0$ with $2r < R$ and $v \neq 0$. 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.

This follows from Barry Simon's Wonderland Theorem and uses heavily the spectral properties of periodic operators.

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Recall that here we are talking about operators on $\ell^2(\omega)$ whose matrix elements reflect the pattern of ω. E.g. nearest neighbor Laplacians on certain graphs. This may lead to compactly supported eigenfunctions sometimes called *scars* and this of course contradicts purely singular continuous spectrum. Scars can be excluded by a curvature condition.

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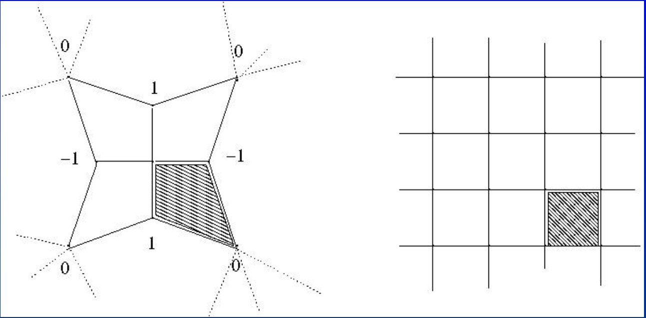

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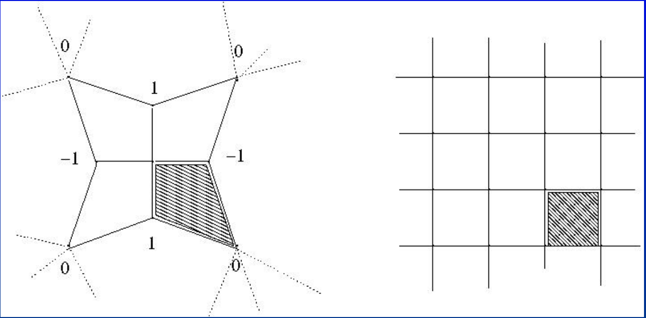

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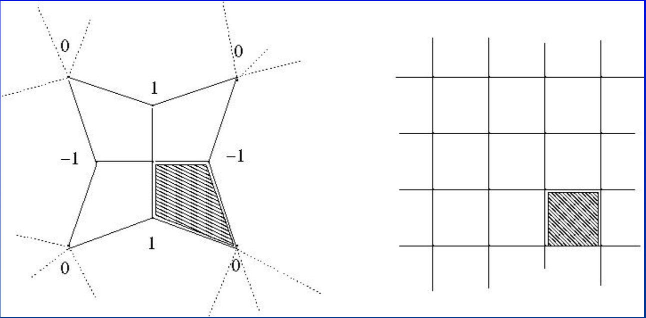

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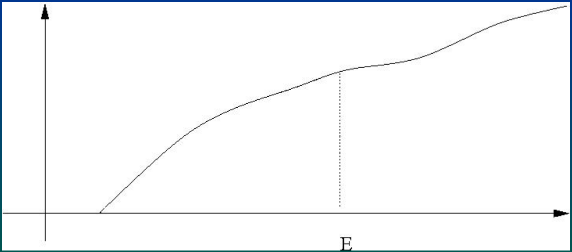
Spectral properties: the integrated density of states

Assume that (Ω, T) is minimal and uniquely ergodic with invariant measure μ. In this case

$$\lim_{|C|\to\infty} \frac{tr[\chi_{(-\infty,E]}(H_\omega|_C)]}{|C|} =: N(E)$$

exists, is independent of ω and is the distribution function of a measure on the real line. $N(E)$ is interpreted as the number of enery levels below E per unit volume.



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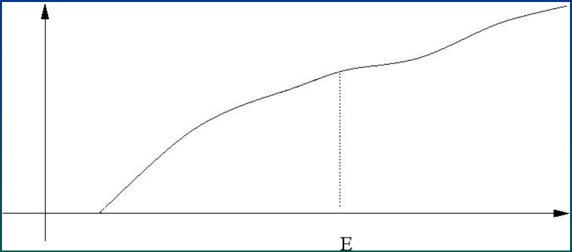

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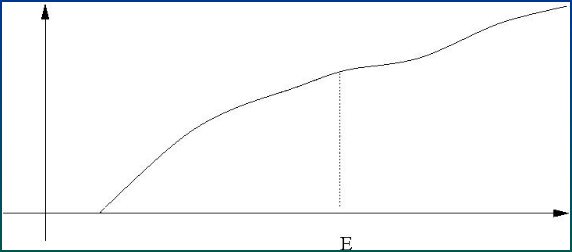

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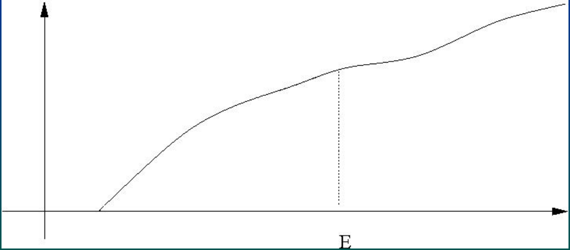

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Algebras of Hamiltonians

Assume that (Ω, T) is minimal and uniquely ergodic with invariant measure μ. Then we can define a type II_1 factor $\mathcal{N}(\Omega, T)$ with a trace τ such that

$$H = (H(\omega), \omega \in \Omega) \in \mathcal{N}(\Omega, T)$$

and

$$N(E) = \tau(\chi_{(-\infty, E]}(H))$$

For any $f \in C_c(\mathbb{R}^d)$ with $\int f(x)dx = 1$ we have

$$N(E) = \int_\Omega tr[M_f \chi_{(-\infty,E]}(H_\omega)] d\mu(\omega)$$

This is intimately related to Connes noncommutative integration theory.
(Precursors: Bellissard et. al., Hof, Kellendonk. More general framework: Lenz, Peyerimhoff Veselic)

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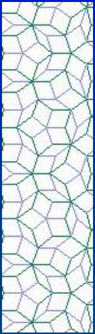

The geometry of quasicrystals can be studied by tilings or equivalently Delone sets. That leads to the study of Hamiltonians $H(\omega)$ indexed by the elements of a dynamical system (Ω, T). these operators are expected to exhibit exotic spectral properties but only few rigorous results are available. The methods used combine combinatorics, ergodic theory and algebra with more traditional spectral theory.

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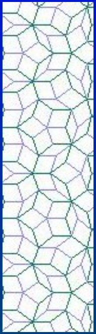

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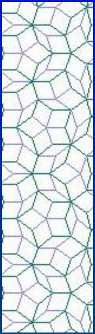

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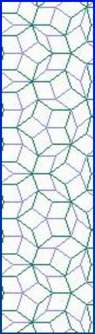

The geometry of quasicrystals can be studied by tilings or equivalently Delone sets. That leads to the study of Hamiltonians $H(\omega)$ indexed by the elements of a dynamical system (Ω, T). these operators are expected to exhibit exotic spectral properties but only few rigorous results are available. The methods used combine combinatorics, ergodic theory and algebra with more traditional spectral theory.

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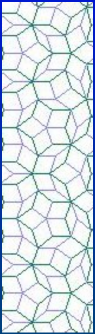

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