Quasicrystals in Wonderland

Peter Stollmann

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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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WHAT IS...

a Quasicrystal?

Marjorie Senechal
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▶ Sharp diffraction peaks - usually coming with long range order.
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Mathematical models for aperiodic order

Aperiodic order can mathematically be described by tilings:
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Mathematical models for aperiodic order

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Figure: A real quasicrystal and the Penrose tiling
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

- \( \forall x, y \in \omega, x \neq y : U_r(x) \cap U_r(y) = \emptyset \),
- \( \bigcup_{x \in \omega} B_R(x) = \mathbb{R}^d \).
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ω ⊂ R^d is called a Delone set, if there exist r, R ∈ R such that

1. ∀x, y ∈ ω, x ≠ y : U_r(x) ∩ U_r(y) = ∅,
2. ∪_{x ∈ ω} B_R(x) = R^d.
By \( \mathcal{D}_{r,R}(\mathbb{R}^d) = \mathcal{D}_{r,R} \) we denote the set of all \((r, R)\)-sets; it is a compact metric space in the natural topology. \( \mathcal{D}(\mathbb{R}^d) = \bigcup_{0 < r \leq R} \mathcal{D}_{r,R}(\mathbb{R}^d) \) is the set of all Delone sets.
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Hamiltonians: continuum models

The basic idea is very simple: at each point of a Delone set $\omega$ 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 $\omega$ is periodic, then $H(\omega)$ describes a crystal. If we choose the point set $\omega$ as the points of a Poisson process (typically no Delone set) then $H(\omega)$ describes a disordered solid. If $\omega$ is aperiodically ordered, then $H(\omega)$ can be used to describe electronic properties of a quasicrystal.
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We are interested in the Schrödinger equation

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

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 $\Omega \subset D(\mathbb{R}^d)$, 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 $(\Omega, T)$. We interpret such a DDS $(\Omega, T)$ as a model for a certain type of (dis-)order. Ergodic properties of $(\Omega, T)$ 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.

$$(\Omega, T) \text{ minimal} \quad \Downarrow$$

$$\sigma(H(\omega)) = \sigma(H(\omega')) \text{ for all } \omega, \omega' \in \Omega.$$ 

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Minimality and unique ergodicity are equivalent to certain combinatorial properties of the \( \omega \)'s.
For a DDS \((\Omega, T)\) that describes aperiodic order one is tempted to expect purely singular continuous spectrum and this has been verified in some classes of discrete examples in one dimension (quasiperiodic Hamiltonians, substitution potentials) as well as continuum models in one dimension, see the talk of D. Lenz. However in higher dimensions there are only very few rigorous results :-( .
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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.

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 \( G_\delta \)-set \( \Omega_{sc} \subset D_{r,R} \) 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 a variant of Barry Simon’s Wonderland Theorem and uses heavily the spectral properties of periodic operators.
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Fix a separable Hilbert space $\mathcal{H}$, consider the space $\mathcal{G} = \mathcal{G}(\mathcal{H})$ of self-adjoint operators in $\mathcal{H}$ with the strong resolvent topology $\tau_{srs}$.

Let $(X, \rho)$ be a complete metric space and $H : (X, \rho) \to (\mathcal{G}, \tau_{srs})$ a continuous mapping. Assume that, for an open set $U \subset \mathbb{R}$,
(1) the set $X_1 = \{x \in X \mid \sigma_{pp}(H(x)) \cap U = \emptyset\}$ is dense in $X$,
(2) the set $X_2 = \{x \in X \mid \sigma_{ac}(H(x)) \cap U = \emptyset\}$ is dense in $X$,
(3) the set $X_3 = \{x \in X \mid U \subset \sigma(H(x))\}$ is dense in $X$.
Then, their intersection
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\{x \in X \mid U \subset \sigma(H(x)), \sigma_{ac}(H(x)) \cap U = \emptyset, \sigma_{pp}(H(x)) \cap U = \emptyset\}
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1. the set $X_1 = \{x \in X| \sigma_{pp}(H(x)) \cap U = \emptyset\}$ is dense in $X$,
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$$ X \rightarrow M_+(U) := \{\text{measures on } U\}, x \mapsto \rho_{\xi}^{H(x)}|_U $$

is continuous. For every dense $\{\xi_n| n \in \mathbb{N}\} \subset \mathcal{H}$:

$$ X_1 = \bigcap_{n \in \mathbb{N}} \{x| \rho_{\xi_n}^{H(x)}|_U \in M_c(U)\}. $$

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Analysis in spaces of measures

Fix \( S \), a locally compact, \( \sigma \)-compact, separable metric space. Consider \( \mathcal{M}_+(S) \), the set of positive, regular Borel measures. \( \mu \in \mathcal{M}_+(S) \) diffusive or continuous if and only if \( \mu(\{x\}) = 0 \) for every \( x \in S \).

\( \mu \perp \nu \), mutually singular if and only if \( \exists \ C \subset S \) such that \( \mu(C) = 0 = \nu(S \setminus C) \).


Let \( S \) be as above. Then

1. The set \( \mathcal{M}_c(S) := \{ \mu \in \mathcal{M}_+(S) | \mu \) is diffusive\} is a \( G_\delta \)-set in \( \mathcal{M}_+(S) \).
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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.,
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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
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Proof of generic appearance of singular continuous spectrum using the Wonderland theorem. If $\rho \in \mathcal{D}_{r,R}$ is crystallographic, i.e.,

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

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 $U := \sigma(H(\gamma))^\circ \setminus \sigma(H(\tilde{\gamma})) \neq \emptyset$.

Figure: crystallographic $\gamma$ (green) and $\tilde{\gamma}$ (green+blue)
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This will be the $U$ whose existence is stated in the theorem. For $\omega \in \mathbb{D}_{r,R}$ we have to find

1. one sequence $(\omega_n^1)_n$ s.t. $H(\omega_n^1)$ is purely singular in $U$ and $\omega_n^1 \to \omega$.
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Quasicrystals in Wonderland
Peter Stollmann

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Since $H(\omega^1_n)$ and $H(\tilde{\gamma})$ only differ by a compactly supported potential, $\sigma_{ac}(H(\omega^1_n)) \cap U = \sigma_{ac}(H(\tilde{\gamma})) \cap U = \emptyset$. To get $\omega^2_n$ we extend $\omega \cap [-n, n]^d$ periodically. The corresponding operator has purely absolutely continuous spectrum, in particular purely continuous spectrum. Finally, we let $\omega^3_n \in \mathbb{D}_{r,R}$ s.t. $\omega^3_n \cap [-n, n]^d = \omega \cap [-n, n]^d$ and $\omega^3_n \cap ([-n-R, n+R]^d)^c = \gamma \cap ([-n-R, n+R]^d)^c$. Since $H(\omega^3_n)$ and $H(\gamma)$ only differ by a compactly supported potential, $\sigma_{ac}(H(\omega^3_n)) \cap U = \sigma_{ac}(H(\tilde{\gamma})) \cap U = U$, by choice of $U$ and the fact that $H(\gamma)$ has purely absolutely continuous spectrum. QED
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Conclusion

- $M_c(S)$ and $M_s(S)$ are $G_δ$-sets, for polish $S$.
- 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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