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Aperiodic Order and Quasicrystals: Spectral Properties

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Abstract. We present spectral theoretic results for Hamiltonians associated with Delone sets. For a family of discrete models we characterize the appearance of jumps in the integrated density of states. For a family of continuum models on the set of all Delone sets with suitable parameters we prove that generically purely singular continuous spectrum occurs.

Introduction

In this paper we continue our study of aperiodic order and quasicrystals with results concerning the nature of the spectrum of the associated Hamiltonians. It is a sequel to [21, 22, 23, 24].

We use the framework of Delone (Delaunay) [5] sets to describe the aperiodic order of positions of ions in a quasicrystal or a more general aperiodic solid. This approach is quite common, [1, 15, 16, 17, 28] with an equivalent alternative description available via tilings, [6, 7, 9, 10, 11, 18, 27]. We elaborate on this issue and introduce Delone dynamical systems in the next section. We also provide some necessary background concerning the natural topology on the set of all Delone sets. Moreover, we mention the von Neumann algebra of observables that can naturally be associated with a Delone dynamical system and an invariant measure on the latter.

With these preparations the stage is set for the study of spectral properties we are aiming at. In Section 2 we are concerned with discrete models. We investigate the possibility of jumps in the integrated density of states of the Hamiltonians in question. This latter quantity is a function $N(E)$ of the energy E that measures the number of eigenstates with eigenvalue lying below E. Since this quantity is self averaging and typically rather smooth it is at first sight very strange that it can exhibit jumps. For the Penrose tiling this effect had already been discovered and studied earlier [13, 14]. It turns out that it is based on the fact that the tilings in question allow for compactly supported eigenfunctions of the associated laplacian. Our results from [12] show two facts: firstly, the Penrose tiling is not exceptional in the sense that with a "local modification" any Delone set can be turned into one that shows compactly supported eigenfunctions. Secondly, discontinuities of the integrated density of states can only appear in that way, provided the Delone sets one starts with satisfies certain quite natural complexity conditions. As the main input, we use a particularly strong ergodic theorem from [24].

In the last section we announce a new result on spectral properties, this time for continuum models. In fact we are able to prove that a certain family of models exhibits the spectral behaviour that is conjectured to be typical for quasicrystal Hamiltonians: purely singular continuous spectrum. To this end we consider a complete metric space consisting of all Delone sets with suitable parameters and associate a Hamiltonian with each of the sets. Our result then tells us that a certain energy region consists of purely singular continuous spectrum for a dense subset of the metric space in question. To our knowledge this is the first result establishing a particular spectral type for multidimensional Hamiltonians associated to Delone sets. The proof we sketch is based on Barry Simon's "Alice in Wonderland" technique from [26].

1 Delone sets and Delone dynamical systems: topology and algebra

We now sketch how to define a suitable topology on the set of all Delone sets following [22] to which the reader is referred for details. Let us start with $\mathcal{F}(\mathbb{R}^d)$, the set of closed subsets of $\mathbb{R}^d$ and recall that there is a natural action T of $\mathbb{R}^d$ on $\mathcal{F}(\mathbb{R}^d)$ given by $T_tG = G + t$. We aim at a topology on $\mathcal{F}(\mathbb{R}^d)$ that fulfills two requirements: the action T should be continuous and two sets that are close to each other with respect to the topology are supposed to be such that their finite parts have small *Hausdorff distance*. The latter can be defined by

$$d_H(K_1, K_2) := \inf(\{\epsilon > 0 : K_1 \subset U_\epsilon(K_2) \wedge K_2 \subset U_\epsilon(K_1)\} \cup \{1\}),$$

where K_1, K_2 are compact subsets of a metric space (X, d) and $U_\epsilon(K)$ denotes the open ϵ-neighborhood around K. The extra 1 is to deal with the empty set that is included in $\mathcal{K}(X) := \{K \subset X : K \text{ compact}\}$. It is well known that $(\mathcal{K}(X), d_H)$ is complete if (X, d) is complete and compact if (X, d) is compact.

We use the stereographic projection to identify points $x \in \mathbb{R}^d \cup \{\infty\}$ in the one-point-compactification of $\mathbb{R}^d$ with the corresponding points $\tilde{x} \in \mathbb{S}^d$. Clearly, the latter denotes the d-dimensional unit sphere $\mathbb{S}^d = \{\xi \in \mathbb{R}^{d+1} : \|\xi\| = 1\}$. Now $\mathbb{S}^d$ carries the euclidian metric ρ. Since the unit sphere is compact and complete, we can associate a complete metric ρ_H on $\mathcal{K}(\mathbb{S}^d)$ by what we said above.

For $F \in \mathcal{F}(\mathbb{R}^d)$ write $\tilde{F}$ for the corresponding subset of $\mathbb{S}^d$ and define

$$\rho(F, G) := \rho_H(\widetilde{F \cup \{\infty\}}, \widetilde{G \cup \{\infty\}}) \text{ for } F, G \in \mathcal{F}(\mathbb{R}^d).$$

Although this constitutes a slight abuse of notation it makes sense since $\widetilde{F \cup \{\infty\}}, \widetilde{G \cup \{\infty\}}$ are compact in $\mathbb{S}^d$ provided F, G are closed in $\mathbb{R}^d$.

We have the following result:

Proposition 1.1 *The metric ρ above induces the natural topology on $\mathcal{F}(\mathbb{R}^d)$.*

Denote by $B_r(x)$ $(U_r(x))$ the closed (open) ball in $\mathbb{R}^d$ around x with radius r.

A subset ω of $\mathbb{R}^d$ is called a *Delone set* if there exist $r(\omega) > 0$ and $R(\omega) > 0$ such that $2r(\omega) \leq \|x - y\|$ whenever $x, y \in \omega$ with $x \neq y$, and $B_{R(\omega)}(x) \cap \omega \neq \emptyset$ for all $x \in \mathbb{R}^d$. If $0 < r \leq r(\omega) \leq R(\omega) \leq R$ we speak of an (r, R)-*set* and denote the set of all (r, R)-sets by $\mathcal{D}_{r,R}$. From the basic properties of the metric ρ above it follows that $\mathcal{D}_{r,R}$ is a compact, complete metric space, a fact that will be useful in the sequel. The set of all Delone sets is denoted by $\mathcal{D}$.

The convergence of a sequence of Delone sets with respect to the natural topology can easily be visualized:

Lemma 1.2 *A sequence (ω_n) of Delone sets converges to $\omega \in \mathcal{D}$ in the natural topology if and only if there exists for any $l > 0$ an $L > l$ such that the $\omega_n \cap U_L(0)$ converge to $\omega \cap U_L(0)$ with respect to the Hausdorff distance as $n \to \infty$.*

We call a closed, translation invariant subset $\Omega \subset \mathcal{D}$ a *Delone dynamical system*, DDS. Note that compactness and hence completeness of Ω follows, since $\mathcal{F}(\mathbb{R}^d)$ is compact. A DDS is said to be an (r, R)-*system* if, furthermore, $\Omega \subset \mathcal{D}_{r,R}$. A further notion is to be introduced: we say that $\omega \in \mathcal{D}$ is of *finite local complexity*, if only finitely many different (up to translation) pattern of bounded diameter occur in ω, i.e., if the set $\{U_L(0) \cap (\omega - x) : x \in \omega\}$ is finite for every $L > 0$.

We speak of a *Delone dynamical system of finite type*, DDSF, if this latter finiteness condition extends to all of Ω, i.e. if the set $\{U_L(0) \cap (\omega - x) : x \in \omega, \omega \in \Omega\}$ is finite for every $L > 0$.

We often keep the translations in our notation and write (Ω, T) for a DDS. The next topic will concern a natural von Neumann algebra that contains the Hamiltonians we are interested in. For details and proofs see [23]. These Hamiltonians are in fact families $A = (A_\omega)$, indexed by the elements ω of a DDS (Ω, T). Each A_ω acts in the Hilbert space $\ell^2(\omega, \alpha^\omega)$, where α^ω denotes the counting measure on the discrete subset $\omega \subset \mathbb{R}^d$. These spaces are "glued" together by the following bundle:

$$\mathcal{X} = \{(\omega, x) \in \mathcal{G} : x \in \omega\} \subset \Omega \times \mathbb{R}^d.$$

Here is the definition:

Definition 1.3 *Let (Ω, T) be an (r, R)-system and let μ be an invariant measure on Ω. Denote by $\mathcal{V}_1$ the set of all $f : \mathcal{X} \longrightarrow \mathbb{C}$ which are measurable and satisfy $f(\omega, \cdot) \in \ell^2(\mathcal{X}^\omega, \alpha^\omega)$ for every $\omega \in \Omega$.*

A family $(A_\omega)_{\omega \in \Omega}$ of bounded operators $A_\omega : \ell^2(\omega, \alpha^\omega) \longrightarrow \ell^2(\omega, \alpha^\omega)$ is called measurable if $\omega \mapsto \langle f(\omega), (A_\omega g)(\omega)\rangle_\omega$ is measurable *for all $f, g \in \mathcal{V}_1$. It is called* bounded *if the norms of the A_ω are uniformly bounded. It is called* covariant *if it satisfies the covariance condition*

$$H_{\omega+t} = U_t H_\omega U_t^*, \ \omega \in \Omega, t \in \mathbb{R}^d,$$

where $U_t : \ell^2(\omega) \longrightarrow \ell^2(\omega + t)$ is the unitary operator induced by translation. Now, we can define

$$\mathcal{N}(\Omega, T, \mu) := \{A = (A_\omega)_{\omega \in \Omega} | A \text{ covariant, measurable and bounded}\} / \sim,$$

where $\sim$ means that we identify families which agree μ almost everywhere.

Obviously, $\mathcal{N}(\Omega,T,\mu)$ depends on the measure class of μ only. Hence, for uniquely ergodic (Ω,T), $\mathcal{N}(\Omega,T,\mu) =: \mathcal{N}(\Omega,T)$ gives a canonical algebra. This special case has been considered in [21, 22]. Apparently, $\mathcal{N}(\Omega,T,\mu)$ is an involutive algebra under the obvious operations. The following result is taken from [23], where we prove it using Connes' noncommutative integration theory, [3].

Theorem 1.4 *Let (Ω,T) be an (r,R)-system and let μ be an invariant measure on Ω. Then $\mathcal{N}(\Omega,T,\mu)$ is a weak-*-algebra.*

This algebra carries a particular trace that is related to the integrated density of states we will meet later. Now, choose a nonnegative measurable u on $\mathbb{R}^d$ with compact support and $\int_{\mathbb{R}^d} u(x)dx = 1$. Letting $f(\omega,p) := u(p)$, it can be shown that the map

$$\tau : \mathcal{N}(\Omega,T,\mu) \longrightarrow \mathbb{C}, \quad \tau(A) = \int_\Omega \mathrm{tr}(A_\omega M_u)\, d\mu(\omega)$$

does not depend on the choice of f viz u as long as the integral is one. Moreover, τ is a trace on $\mathcal{N}(\Omega,T,\mu)$; see [23] for details.

Let us now introduce the C*-subalgebra of $\mathcal{N}(\Omega,T,\mu)$ that contains those operators that might be used as Hamiltonians for quasicrystals. We define

$$\mathcal{X} \times_\Omega \mathcal{X} := \{(p,\omega,q) \in \mathbb{R}^d \times \Omega \times \mathbb{R}^d : p,q \in \omega\},$$

which is a closed subspace of $\mathbb{R}^d \times \Omega \times \mathbb{R}^d$ for any DDS Ω.

Definition 1.5 *A* kernel of finite range *is a function $k \in C(\mathcal{X} \times_\Omega \mathcal{X})$ that satisfies the following properties:*

(i) *k is bounded.*

(ii) *k has finite range, i.e., there exists $R_k > 0$ such that $k(p,\omega,q) = 0$, whenever $|p-q| \geq R_k$.*

(iii) *k is invariant, i.e.,*

$$k(p+t,\omega+t,q+t) = k(p,\omega,q),$$

for $(p,\omega,q) \in \mathcal{X} \times_\Omega \mathcal{X}$ and $t \in \mathbb{R}^d$.

The set of these kernels is denoted by $\mathcal{K}^{fin}(\Omega,T)$.

We record a few quite elementary observations. For any kernel $k \in \mathcal{K}^{fin}(\Omega,T)$ denote by $\pi_\omega k := K_\omega$ the operator $K_\omega \in \mathcal{B}(\ell^2(\omega))$, induced by

$$(K_\omega \delta_q | \delta_p) := k(p,\omega,q) \text{ for } p,q \in \omega.$$

Clearly, the family $K := \pi k$, $K = (K_\omega)_{\omega\in\Omega}$, is bounded in the product (equipped with the supremum norm) $\Pi_{\omega\in\Omega}\mathcal{B}(\ell^2(\omega))$. Thus, it belongs to $\mathcal{N}(\Omega,T,\mu)$. Now, pointwise sum, the convolution (matrix) product

$$(k_1 \cdot k_2)(p,\omega,q) := \sum_{x\in\omega} k_1(p,\omega,x)k_2(x,\omega,q)$$

and the involution $k^*(p,\omega,q) := \overline{k}(q,\omega,p)$ make $\mathcal{K}^{fin}(\Omega,T)$ into a $*$-algebra. Then, the mapping $\pi : \mathcal{K}^{fin}(\Omega,T) \to \Pi_{\omega\in\Omega}\mathcal{B}(\ell^2(\omega))$ is a faithful $*$-representation. We denote $\mathcal{A}^{fin}(\Omega,T) := \pi(\mathcal{K}^{fin}(\Omega,T))$ and call it the *operators of finite range.* This gives a subalgebra of $\mathcal{N}(\Omega,T,\mu)$, as can easily be seen. The completion of $\mathcal{A}^{fin}(\Omega,T)$ with respect to the norm $\|A\| := \sup_{\omega\in\Omega}\|A_\omega\|$ is denoted by $\mathcal{A}(\Omega,T)$. This again is a subalgebra of $\mathcal{N}(\Omega,T,\mu)$. Moreover, it is not hard to see that the mapping $\pi_\omega : \mathcal{A}^{fin}(\Omega,T) \to \mathcal{B}(\ell^2(\omega)), K \mapsto K_\omega$ is a representation that extends by continuity to a representation of $\mathcal{A}(\Omega,T)$ that we denote by the same symbol.

2 Integrated density of states and its discontinuities

In this section, we first relate the abstract trace τ defined above to the mean trace per unit volume. The latter object is quite often considered by physicists and bears the name *integrated density of states.* We then study discontinuities of the integrated density of states and characterize their occurence by existence of locally supported eigenfunctions.

The proper definition of the integrated density of states rests on ergodicity; we need the notion of a van Hove sequence of sets.For $s > 0$ and $Q \subset \mathbb{R}^d$, we denote by $\partial_s Q$ the set of points in $\mathbb{R}^d$ whose distance to the boundary of Q is less than s. A sequence (Q_n) of bounded subsets of $\mathbb{R}^d$ is called a *van Hove sequence* if $|Q_n|^{-1}|\partial_s Q_n| \longrightarrow 0, n \longrightarrow 0$ for every $s > 0$. The following result from [23] establishes an identity that one might call an abstract Shubin's trace formula. It says that the abstractly defined trace τ is determined by the integrated density of states. The latter is the limit of the following eigenvalue counting measures. Let, for selfadjoint $A \in \mathcal{A}(\Omega,T)$ and $Q \subset \mathbb{R}^d$:

$$\langle\rho[A_\omega,Q],\varphi\rangle := \frac{1}{|Q|}\mathrm{tr}(\varphi(A_\omega|_Q)), \varphi \in C(\mathbb{R}).$$

Its distribution function is denoted by $n[A_\omega,Q]$, i.e. $n[A_\omega,Q](E)$ gives the number of eigenvalues below E per volume (counting multiplicities).

Theorem 2.1 *Let (Ω,T) be a uniquely ergodic (r,R)-system and μ its ergodic probability measure. Then, for selfadjoint $A \in \mathcal{A}(\Omega,T)$ and any van Hove sequence (Q_n),*

$$\langle\rho[A_\omega,Q_n],\varphi\rangle \to \tau(\varphi(A)) \text{ as } n \to \infty$$

for every $\varphi \in C(\mathbb{R})$ and every $\omega \in \Omega$. Consequently, the measures $\rho_\omega^{Q_n}$ converge weakly to the measure ρ_A defined above by $\langle\rho_A,\varphi\rangle := \tau(\varphi(A))$, for every $\omega \in \Omega$.

Remark 2.2 This generalizes results in Kellendonk [9] (see [7, 8] for related material as well) and is an analog of results of Bellissard [2] in the almost periodic setting. The proof is based on ideas from these works.

For a special class of operators we can actually say more. This class is defined next. It includes all Hamiltonians based on a next neighbor Laplacian and a locally determined potential.

Definition 2.3 *Let (Ω, T) be a DDSF. A finite range operator $A = (A_\omega)$ is called locally constant if there exists a constant r_A such that $A_\omega(x, y) = A_{\omega'}(x', y')$ whenever $(B_{r_A}(x) \cup B_{r_A}(y)) \wedge \omega = t + (B_{r_A}(x') \cup B_{r_A}(y')) \wedge \omega'$ for some $t \in \mathbb{R}^d$.*

For such operators we can characterize the appearance of a discontinuity in the integrated density of states ρ^A (see [12] for details and proofs).

Theorem 2.4 *Let (Ω, T) be a strictly ergodic DDSF. Let A be a locally constant finite range operator. Then E is a point of discontinuity of ρ^A if and only if there exists a locally supported eigenfunction of A_ω to E for one (all) $\omega \in \Omega$.*

Remark 2.5 Let us emphasize that locally supported eigenfunctions do exist for DDSF (see [12] and the references given in the introduction). Thus, the theorem gives that the integrated density of states is not continuous for DDSF. This contrasts with what is known for one dimensional operators as well as for random operators. On the other hand the theorem also tells us that these discontinuities can only arise in a certain way which is linked to the geometry of the Delone sets in question.

3 Generic purely singular continuous spectrum

In the sequel we consider Hamiltonians in $L^2(\mathbb{R}^d)$ that can be considered for the description of aperiodic solids. We fix a compactly supported, bounded $f \leq 0$ that gives the attractive potential of an ion. If these ions are distributed according to the sites of a Delone set ω we arrive at

$$H(\omega) = -\Delta + \sum_{t \in \omega} f(\cdot - t).$$

Since we consider a fixed $f \neq 0$ as above we omit it from the notation. We now fix $0 < r < R$ in such a way that there exists a lattices $\gamma, \tilde{\gamma} \in \mathcal{D}_{r,R}$ with the property that the corresponding Hamiltonians $H(\gamma)$ and $H(\tilde{\gamma})$ satisfy:

$$a := \inf \sigma \left(-\Delta + \sum_{t \in \gamma} f(\cdot - t) \right) < \tilde{b} := \inf \sigma \left(-\Delta + \sum_{t \in \tilde{\gamma}} f(\cdot - t) \right).$$

Our aim is the following result; details will appear elsewhere [25].

Theorem 3.1 *There is an nonempty open interval I and a dense G_δ-set Ω_{sc} such that for all $\omega \in \Omega_{sc}$ the spectrum of $H(\omega)$ contains I and is purely singular continuous there.*

Let us stress that singular continuous spectrum is in fact what one expects for quasicrystals. One reason is that the latter are in between highly disordered media (for which pure point spectrum is typical) and ordered media (for which absolutely continuous spectrum is characteristic). Moreover, there are by now a number of rigorous results in this direction for one-dimensional operators, starting from [29]; references to more recent papers can be found in the survey papers [4, 30]. We are not aware of any result concerning higher dimensions, however.

Of course, a more realistic Hamiltonian would allow for a finite number of different ions. The framework of *colored Delone sets* as considered in [23] provides the appropriate notions.

The main tool to prove the above result is the following Theorem 2.1 from [26] that we include for the readers convenience.

Theorem 3.2 *Let X be a regular metric space of self-adjoint operators. Suppose that for some interval (a,b), we have that*

(i) $\{A \in X |$ *has purely continuous spectrum on* $(a,b)\}$ *is dense in* X.

(ii) $\{A \in X |$ *has purely singular spectrum on* $(a,b)\}$ *is dense in* X.

(iii) $\{A \in X |$ *has* (a,b) *in its spectrum*$\}$ *is dense in* X.

Then $\{A | (a,b) \subset \sigma(A), (a,b) \cap \sigma_{pp}(A) = \emptyset, (a,b) \cap \sigma_{ac}(A) = \emptyset\}$ *is a dense* G_δ.

Clearly, the conclusion of this latter theorem is exactly the assertion of our Theorem 3.1. Thus, we have to associate the right space of operators with $\mathcal{D}_{r,R}$ and verify properties (i)-(iii) from the preceding Theorem.

Of course, the appropriate space is

$$X_{r,R} = \{H(\omega) | \omega \in \mathcal{D}_{r,R}\}$$

equipped with the metric from $\mathcal{D}_{r,R}$. Metrizability and completeness have already been discussed in Section 1; they follow from the results in [22]. Moreover, one can see that convergence with respect to the natural topology implies strong resolvent convergence of the respective operators so that $X_{r,R}$ is a regular metric space of self-adjoint operators in the sense of [26].

Let us finally sketch how to prove property (iii). Recall the lattices $\gamma, \tilde{\gamma}$ from above. This gives the energy interval (a,b) in the following way: We take $a, \tilde{b}$ as above and define $b := \min\{\tilde{b}, b^*\}$ where b^* is the upper edge of the spectral band of $-\Delta + \sum_{t\in\gamma} f(\cdot - t)$ that starts at a, i.e.,

$$b^* := \sup\{\lambda | [a,\lambda] \subset \sigma\left(-\Delta + \sum_{t\in\gamma} f(\cdot - t)\right)\}.$$

We can now use suitable perturbations of γ to see that (iii) is fulfilled. In fact, given $\omega \in \mathcal{D}_{r,R}$ find ω_n that coincides with ω in the box centered at 0 with sidelength n and coincides with γ outside the box centered at 0 with sidelength $2n$. By Lemma 1.2 above we get convergence $\omega_n \to \omega$ in the natural topology. Moreover, the essential spectrum of $H(\omega_n)$ coincides with the essential spectrum of $H(\omega)$, hence $[a,b] \subset \sigma(H(\omega_n))$ for all $n \in \mathbb{N}$.

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