Quasicrystals, aperiodic order, and groupoid von Neumann algebras

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Abstract

We introduce tight binding operators for quasicrystals that are parametrized by Delone sets. These operators can be regarded in a natural operator algebra framework that encodes the long range aperiodic order. This algebraic point of view allows us to study spectral theoretic properties. In particular, the integrated density of states of the tight binding operators is related to a canonical trace on the associated von Neumann algebra.

1 Introduction: Quasicrystals and Delone dynamical systems

Quasicrystals have been discovered as solids that exhibit sharp Bragg peaks in diffraction experiments with symmetries disallowed for periodic order, see [26]. Due to that phenomenon, quasicrystals are supposed to have long range aperiodic order as explained in [12], which also contains useful information on the literature.

It is nowadays quite common to model this long range order by tilings or, equivalently, Delone sets. We adopt the second point of view and refer to [18, 25, 28, 29] for standard notions and bibliographic information. In this section, we briefly introduce the necessary notions. Details will be given in [21].

Definition 1.1. *A subset* $\omega \subset \mathbb{R}^d$ *is called a* Delone set *if there exist* $0 < r_0 < r_1$ *such that for any* $p \in \mathbb{R}^d$ *the ball* $B_{r_0}(p)$ *contains at most one and* $B_{r_1}(p)$ *contains at least one element of* ω.

Here $B_r(p)$ denotes the closed ball centered at p with radius r. The points of a Delone set ω are interpreted as the positions of the atoms of a quasicrystal. Thus a natural attempt to describe a quasicrystal quantum mechanically is to associate with ω a tight binding operator H_ω defined on $\ell^2(\omega)$ whose matrix elements represent the effective interaction and potentials. Clearly, such a hamiltonian should be shift invariant in the sense that $H_{\omega+t}$ is obtained from H_ω by translation. This leads to considering along with ω all the translations $\omega + t$. (The shift $T = (T_t)_{t\in\mathbb{R}^d}, T_t\omega := \omega + t$ obviously maps Delone sets to Delone sets.)

According to [21] there is a topology on the set of closed subsets of $\mathbb{R}^d$ that is compact and has the property that translations are continuous. It is called the *natural topology*. See also [18], which we follow in the first part of the following Definition:

Definition 1.2. (1) *If Ω is a closed set of Delone sets and invariant under the shift we call (Ω, T) a* Delone dynamical system, DDS *for short.*
(2) *A DDS is said to be of* finite type, DDSF *for short, if, furthermore,*

$$\{\omega - p | p \in \omega, \omega \in \Omega\} \cap B_r(0)$$

is finite for every $r > 0$.

The important finiteness condition in (2) above can be rephrased by saying that there are only finitely many non-equivalent (with respect to translation) patches $\omega \cap B_r(p)$ of radius r around $p \in \omega$. By what we said above Ω is compact for every DDS. See also [5, 18] for compactness results under more restrictive conditions, as well as [24]. Now a Delone dynamical system Ω can be used as a natural parameter space of a family of hamiltonians describing quasicrystals. It should be regarded as the analog of the hull of a quasiperiodic potential or the probability space of a random potential. Moreover it captures the symmetry inherent in the Delone sets.

We shall say that a DDSF is *aperiodic* if $\omega + t = \omega$ (for some ω) implies $t = 0$. In this respect we follow the terminology of [28] and differ from [18].

It is our aim to prove that one has the same sort of results for families of Hamiltonians associated to Delone sets as in the almost periodic or random case. This includes results on

- (almost sure) constancy of spectral properties as well as absence of discrete spectrum under suitable conditions,
- a trace on a canonically associated von Neumann algebra giving rise to a spectral measure which is just the integrated density of states,
- a local procedure to calculate the density of states, yielding a strong type of Pastur-Shubin trace formula.

The study of random operators by means of operator algebras is not new. It goes back at least to the seminal work of Shubin [27] and Coburn/Moyer/Singer

[7]. Later C^*-algebras associated to almost-periodic operators became a key tool in a program initiated by Bellissard centered around the so called gap-labelling (see e.g. [2, 3, 4]). These works focus on K-theory for almost-periodic operators. However, they also establish versions of Pastur-Shubin formulas (which are needed to calculate a certain functional on the K_0-groups) as well as certain spectral features. However, all these results are phrased and proven within the framework of crossed products. This means, the underlying Hamiltonians are all assumed to act on the same Hilbert space which is just the ℓ^2-space of the underlying (mostly discrete) group. While this is a quite general framework it is not sufficiently general to treat discrete random operators associated to tilings or Delone sets (unless of course the Delone set is a lattice). Namely, in this case each Hamiltonian H_ω has its own Hilbert space $\ell^2(\omega)$ attached and this Hilbert space depends on ω and is not the ℓ^2 space of a group.

This difficulty is overcame in our present work by the use of Connes' Noncommutative integration theory combined with certain direct integrals based on naturally arising fibred spaces.

This new setting allows us to directly tackle the first two points of our program. Our treatment of Pastur-Shubin-type formulas then consists of two results. The first result, giving weak convergence of certain measures, is analogous to corresponding results for random or almost periodic operators as e.g. [27, 2, 3], see work of Kellendonk [13] for a treatment of special tilings as well. It uses ideas of the cited works of Bellissard (see [13] as well) and of Hof [11]. The second result gives a very strong type of convergence for a large class of models. It is the very first result of its kind. Its proof relies on a new technique based on a recently established Banach-space-valued ergodic theorem.

Finally, let us mention that starting with the work of Kellendonk [13, 14], much has been established about the K-theory of certain tiling C^*-algebras. We refer the reader to the survey articles by Kellendonk and Putnam [15] and the article by Bellissard/Herrmann/Zarrouati [5].

2 The associated von Neumann algebra

We shall use Delone dynamical systems as parameter spaces for operators associated with quasicrystals. A DDS Ω is viewed as standing for a type of quasicrystals and the elements $\omega \in \Omega$ are considered as specific realizations, the points of ω representing the positions of the atoms of a quasicrystal. Notation is chosen to underline the analogy with random models [6, 23, 30], see also the almost random framework introduced in [2, 3]. However, there is a fundamental difference: in the situation at hand the hamiltonian H_ω is naturally defined on $\ell^2(\omega)$ and the latter space varies with $\omega \in \Omega$. Clearly, a reasonable family $(H_\omega)_{\omega\in\Omega}$ should satisfy the *covariance condition*

$$H_{\omega+t} = U_t H_\omega U_t^*,$$

where $U_t : \ell^2(\omega) \to \ell^2(\omega + t)$ is the unitary operator induced by translation. For a DDSF (Ω, T) consider the bundle

$$\Xi := \{(\omega, x) | \omega \in \Omega, x \in \omega\} \subset \Omega \times \mathbb{R}^d,$$

that carries a natural measurable structure induced by $C(\Omega) \otimes C_c(\mathbb{R}^d)$. Since Ω is compact, there exist T–invariant measures on Ω. Given such an invariant measure μ we can introduce the measure

$$m = \int_\Omega \left(\sum_{x \in \omega} \epsilon_x \right) d\mu(\omega),$$

ϵ_x the unit mass, and get

$$L^2(\Xi, m) = \int_\Omega^\oplus \ell^2(\omega) d\mu(\omega).$$

For a measurable, essentially bounded $H = (H_\omega)_{\omega \in \Omega}$ let

$$\pi(H) = \int_\Omega^\oplus H_\omega d\mu(\omega) \in \mathcal{B}(L^2(\Xi, m)).$$

Define

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

where $\sim$ means that we identify families that agree μ almost everywhere. In the notation of Connes' [8] we would have $\mathcal{H} = (\ell^2(\omega))_{\omega \in \Omega}$, Λ the transversal measure corresponding to the invariant measure μ on Ω and $\mathcal{N}(\Omega, \mu) = \mathrm{End}_\Lambda(\mathcal{H})$, where Ω is considered as a groupoid with respect to translations. We get the following result, details of which will be given in [21].

Theorem 2.1. *Consider an aperiodic and uniquely ergodic DDSF (Ω, T). Let μ be the unique invariant probability measure. Then $\mathcal{N}(\Omega, \mu)$ is a factor of type II_D, where*

$$D = lim_{R \to \infty} \frac{\#(\omega \cap B_R(0))}{|B_R(0)|}$$

is the density *of ω.*

Of course, the existence of the limit that gives D had already be known and can be found, e.g., in [5]. This theorem is a consequence of the results in [8] and a direct calculation of the canonical trace

$$\tau(H) = \int_\Omega \mathrm{tr}(H_\omega M_f) d\mu(\omega)$$

that does not depend upon the choice of $f \in C_c(\mathbb{R}^d)$ as long as $f \geq 0$ and $\int f(x)dx = 1$. Note that the multiplication operator M_f acts on $\ell^2(\omega)$ by restriction and that the resulting operator $H_\omega M_f$ has finite rank, since only finitely many points of ω lie in the support of f. This canonical trace is connected with the integrated density of states as will be seen in the next section. It can be defined on $\mathcal{N}(\Omega,\mu)$ whenever μ is an invariant measure. The relation to spectral theoretic properties of H is provided by the following measure ρ_H on $\mathbb{R}$, defined by

$$\langle \rho_H, \varphi\rangle := \tau(\varphi(H)) \text{ for } \varphi \in C_b(\mathbb{R}),$$

for any $H \in \mathcal{N}(\Omega,\mu)$. Its fundamental importance is illustrated by:

Proposition 2.1. *Let (Ω, T) be an aperiodic DDSF, μ an invariant measure and $H \in \mathcal{N}(\Omega,\mu)$ selfadjoint. Then ρ_H is a spectral measure of H and $\pi(H)$. If, moreover, μ is ergodic, then for μ–a.e. $\omega \in \Omega$ we have that $supp\rho_H = \sigma(H_\omega)$ and that the discrete spectrum of H_ω is void.*

Details will be given in [21]. Note that this is the analog of one of the basic results for random operators, [6, 23, 30]. In different context it can be found in [19, 20].

3 Tight binding operators

In order to describe the properties of disordered models quantum mechanically it is common to use a tight binding approach. E.g., a random model is often described by an operator on $\ell^2(\mathbb{Z}^d)$ consisting of the Laplacian that stands for nearest neighbor interactions plus a random potential perturbation. We search for an analogous description of quasicrystals, introducing the following notion that still leaves a lot of flexibility. In comparison with the random or almost random case it is again the fact that the space varies that makes the fundamental difference. Details will appear in [22].

Definition 3.1. *Let Ω ba a DDSF. A family $A = (A_\omega)$, $A_\omega \in \mathcal{B}(\ell^2(\omega))$ is said to be an* operator (family) of finite range *if there exists $R > 0$ such that*

- $(A_\omega\delta_x|\delta_y) = 0$ *if $x, y \in \omega$ and $|x - y| \geq R$.*
- $(A_{\omega+t}\delta_{x+t}|\delta_{y+t}) = (A_{\tilde\omega}\delta_x|\delta_y)$ *if $\omega\cap B_R(x+t) = \tilde\omega\cap B_R(x)+t$ and $x, y \in \tilde\omega$.*

This merely says that the matrix elements $A_\omega(x, y) = (A_\omega\delta_x|\delta_y)$ of A_ω only depend on a sufficiently large patch around x and vanish if the distance between x and y is too large. Since there are only finitely many nonequivalent patches, an operator of finite range is bounded in the sense that $\|A\| = \sup_{\omega\in\Omega} \|A_\omega\| < \infty$. Moreover it is clear that every such A is covariant and consequently $A \in \mathcal{N}(\Omega,\mu)$ for every invariant measure μ. The completion of the space of all finite range operators with respect to the above norm is a C^*–algebra that we denote by $\mathcal{A}(\Omega)$. The representations $\pi_\omega : A \mapsto A_\omega$ can be uniquely extended to representations of $\mathcal{A}(\Omega)$ and are again denoted by $\pi_\omega : \mathcal{A}(\Omega) \to \mathcal{B}(\ell^2(\omega))$. We have the following result:

Theorem 3.2. *The following conditions on Ω are equivalent:*

(i) (Ω, T) *is minimal.*

(ii) *For any selfadjoint* $A \in \mathcal{A}(\Omega)$ *the spectrum* $\sigma(A_\omega)$ *is independent of* $\omega \in \Omega$.

(iii) π_ω *is faithful for every* $\omega \in \Omega$.

Next we relate the "abstract integrated density of states" ρ_H to the integrated density of states as considered in random or almost random models and defined by a volume limit over finite parts of the operator.

Note that for selfadjoint $A \in \mathcal{A}(\Omega)$ and bounded $Q \subset \mathbb{R}^d$ the restriction $A_\omega|_Q$ defined on $\ell^2(Q \cap \omega)$ has finite rank. Therefore, the spectral counting function

$$n(A_\omega, Q)(E) := \#\{\text{ eigenvalues of } A_\omega|_Q \text{ below } E\}$$

is finite and that $\frac{1}{|Q|} n(A_\omega, Q)$ is the distribution function of the measure $\rho(A_\omega, Q)$, defined by

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

One of the fundamentals of random operator theory is the existence of the infinite volume limit

$$N(E) = \lim_{Q \nearrow \mathbb{R}^d} \frac{1}{|Q|} n(A_\omega, Q)(E)$$

independently of ω a.s. This amounts to the convergence in distribution of the measures $\rho(A_\omega, Q)$ just defined. As a first result on weak convergence we get:

Theorem 3.3. *Let* (Ω, T) *be a uniquely ergodic DDSF and* $A \in \mathcal{A}(\Omega)$ *selfadjoint. Then, for any van Hove sequence* Q_n,

$$\rho(A_\omega, Q_n) \to \rho_A \text{ weakly as } n \to \infty.$$

Recall that a van Hove sequence consists of bounded sets Q_n that satisfy $\frac{|\partial_R Q_n|}{|Q_n|} \to 0$ as $n \to \infty$ for $R > 0$. This latter condition signifies that for every $R > 0$ the fattened surface $\partial_R Q_n = \{p \in \mathbb{R}^d : \mathrm{dist}(y, \partial Q_n) \leq R\}$ of Q_n is negligible compared to the volume. This generalizes results implicit in Geerse and Hof [9] and Kellendonk [13], see also [10] and is an analog of results of Bellissard [2, 3] in the almost random setting. General arguments now yield the convergence in distribution for E a continuity point of the limit distribution. However, as we will show by examples in [22], discontinuities cannot be excluded. This may seem rather astonishing in view of what is known for random models as well as onedimensional quasicrystals. The reason is the more complicated geometry in dimensions $d \geq 2$. In virtue of this remark the next result is of particular interest. It is based upon an ergodic theorem for Delone sets, details will be given in [22].

Theorem 3.4. *Let* (Ω, T) *be a minimal, uniquely ergodic, aperiodic DDSF. Then, for any van Hoove sequence* Q_n,

$$\rho(A_\omega, Q_n) \to \rho_A \text{ in distribution as } n \to \infty,$$

uniformly in $\omega \in \Omega$ *for every selfadjoint* A *of finite range.*

Note that both these last results can be regarded as abstract versions of the celebrated Shubin's trace formula [27]. See also the discussion in [19] as well as [1, 6, 23, 2, 3] for the almost periodic, random and almost random case. The result holds as well for primitive substitutions. For the special case of the Penrose tiling related but weaker results can be found [9, 10], see [11] as well.

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