0.1 Delone dynamical systems: ergodic features and applications

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0.1.1 Introduction

The effect of disorder (i.e. deviation from periodicity) in solid state models is of fundamental importance. It has stimulated an enormous effort that has led to quite a number of results since the late 1950's. From mathematical point of view, there is still a lot to be done until basic questions can be considered as rigorously settled. Quasicrystals provide an interesting and very challenging type of disorder.

In our research project we contribute to the rigorous study of the underlying mathematical models.

The characteristic properties of quasicrystals suggest a form of aperiodicity which is very close to periodicity. Thus, the relevant models exhibit a behaviour between order and disorder which is very close to the ordered case. To describe this phenomenon the term long range aperiodic order has been introduced. This leads to a number of conjectures concerning the spectral properties of the hamiltonians of quasicrystals.

But let us set the stage and review how order as well as disorder can be cast in a common mathematical framework. The main idea is to pass from single models to whole families whose parametrization encodes the internal symmetries.

Let us start by discussing a periodic solid. It can naturally be represented by a periodic hamiltonian H_{per} on $L^2(\mathbb{R}^d)$. Here, $L^2(\mathbb{R}^d)$ is the set of all square-integrable functions on the d-dimensional euclidean space $\mathbb{R}^d$. Typically, $H_{per} = \Delta + V_{per}$ with a periodic potential V_{per} that is invariant under shifts from a periodicity lattice Γ. Thus, periodicity of V_{per} is reflected in invariance properties of the function

$$\tilde{H} : \mathbb{R}^d \to S(L^2(\mathbb{R}^d)), \quad t \mapsto -\Delta + V_{per}(\cdot + t),$$

where $V_{per}(\cdot + t)$ is the function V_{per} translated. Here, $S(L^2(\mathbb{R}^d))$ denotes the self adjoint operators on $L^2(\mathbb{R}^d)$. By invariance, the mapping $\tilde{H}$ above reduces to a mapping $H : \mathbb{R}^d/\Gamma \to S(L^2(\mathbb{R}^d))$, if one factors out the periodicity lattice. Although this manipulation to go from H_{per} to a whole family may seem to be quite innocent, there are deep consequences on the level of spectral theory. In fact, this altered point of view is at the basis of the insight that the associated operator will exhibit purely absolutely continuous spectrum. This latter mathematical statement can be recast by saying that there are no localized but only extended states. Thus, we have seen that expressing order, periodicity namely, in terms of passing to a family of operators can be fruitful.

For the strongly disordered case this is in fact the starting point of the whole study. There one adopts the point of view that disorder is better not modeled by a single deterministic hamiltonian. Instead one consideres a collection (family) of possible hamiltonians along with the probabilities with which these realization are supposed to occur. Typical examples are the Anderson models, in which case the hamiltonian reads

$$H(\omega) = -\Delta + V_\omega \ \text{ on } \ \ell^2(\mathbb{Z}^d),$$

where $\Omega = I^{\mathbb{Z}^d}$, $I \subset \mathbb{R}$ some interval, $V_\omega(k) = \omega(k)$ for $k \in \mathbb{Z}^d$, $\omega = (\omega(k))_{k\in\mathbb{Z}^d} \in \Omega$ and the ω is picked with a product probability $\mathbb{P}$. Now, we face a situation in which the function H is much more complicated than in the first case. The different hamiltonians $H(\omega_1)$ and $H(\omega_2)$ need no longer be translates of each other nor are they similar, in general. Therefore, we really face a nontrivial operator function. Nevertheless, every $\omega \in \Omega$ can be thought of as one specific realisation of a disordered model, whose statistical properties are entirely encoded in the probability measure $\mathbb{P}$.

The first step in our program was to identify the right parameter spaces Ω. In order to decide what consequences order - disorder aspect is going to have, the properties of this space are to be studied. In the periodic case, we found a compact parameter space and a smooth operator valued function.

In the Anderson model, independence is the fundamental property and leads to rigorous proofs of localization in certain energy regions (see [1, 2, 3]).

Both cases have one important aspect in common: ergodicity with respect to the natural translations. Thus we are seeking, in fact, an ergodic dynamical system encoding the properties of a quasicrystal.

A natural first approach is to consider the set $\omega \subset \mathbb{R}^d$ of sites occupied by atoms/ions of a quasicrystal. This set ω should at least share the properties of a *Delone* set. Moreover, together with ω, also its translates $\omega + t =: T_t\omega$ have the same right to be considered. The relevant notion here is that of Delone sets and *Delone dynamical systems* (DDS). We discuss this point in Section 0.1.2 below. Most of the basic issues here had already been studied either in the Delone dynamical or in the more or less equivalent tiling dynamical framework, at least under the assumption of finite local complexity (FLC, see below), [4, 5]. However, it turned out that in the non-FLC case important questions concerning the topology had not been settled completely before. Our contribution in [6] was to define a suitable topology called the natural topology on the set of closed subsets of $\mathbb{R}^d$ that has the desired properties when restricted to Delone sets. It is worthwhile to point out that our topology works without assumptions of finite local complexity. The third section is devoted to the study of ergodic and combinatorical features of Delone dynamical systems. After what we said above it is not too astonishing that suitable parameter spaces are Delone dynamical systems (Ω, T). By this we simply mean that a set Ω of Delone sets is given such that Ω is invariant under translations $T = (T_t)_{t\in\mathbb{R}^d}$ and closed in the natural topology. By the results from Section 0.1.2 this will imply that Ω is a compact set.

Now there are two different levels of combinatorical properties that are intimately linked. On the one hand, every Delone set $\omega \in \Omega$ has its intrinsic complexity. In many interesting cases, only finitely many different (up to translation) patterns occur in balls of finite radii. This situation is described by the notion of finite local complextiy (FLC). It is now natural to ask for frequencies of patterns, whenever such frequencies exists, and so on. On the other hand there are the ergodic properties of the DDS. It turns out that the latter are often determined by combinatorical properties of the individual Delone sets ω that build the DDS (Ω, T). Moreover, these ergodic properties can be phrased in terms of the validity of certain forms of the ergodic theorem. Another aspect concerns the consequences for the naturally associated operator algebras as well as for the individual operators (rather operator families) that constitute these algebras.

This leads us to Section 0.1.4 in which the relevant operators are introduced. Looking back to what we said above, it still remains to specify the operator function H on Ω. Here we meet a fundamental difference when compared to the cases above. The natural tight binding approach leads to a family $(\ell^2(\omega))_{\omega\in\Omega}$ of different Hilbert spaces. The natural candidate from the point of view of parametrising the order - disorder aspect present in a DDS Ω is now a family $(H(\omega))_{\omega\in\Omega}$ in which $H(\omega)$ acts in $\ell^2(\omega)$ for each $\omega \in \Omega$. The natural requirement that this family should respect translations leads to the notion of covariant operator families. We define an associated algebra $\mathcal{N}(\Omega, T, \mu)$ given any invariant measure μ on (Ω, T). Using noncommutative integration theory, one can prove that these algebras are von Neumann algebras. We discuss almost sure constancy of spectral features of selfadjoint families of random operators. Here, almost sure means that these features hold for all $\omega \in \Omega$ not belonging to a certain set of μ-measure zero. A $C^\star$- subalgebra is the algebra generated by finite range operators. Here we rely on topological properties to define a suitabe bundle over Ω. Some important properties concern almost sure constancy of the spectrum. The existence of the integrated density of states (IDOS) for operators of finite range is discussed in Section 0.1.5. It is the strong ergodic theorem that allows one to realize that the IDOS is given by a uniform limit. This has a striking application: it has been known since quite some time that the nearest neighbor laplacian of the Penrose tiling allows for eigenfunctions of finite support. Of course this leads to a jump in the integrated density of states. Using the uniform convergence, we can see that finitely supported eigenfunctions are the only possible means to get a discontinuity of the IDOS. Moreover, we proved a Shubin's trace formula that relates the integrated density of states with a trace on the corresponding von Neumann algebra.

0.1.2 Delone sets and Delone dynamical systems

We start with defining a suitable mathematical model to describe quasicristals. We use the language of Delone sets to describe these kind of models. Roughly speaking, a Delone set Ω is a discrete point set in $\mathbb{R}^d$ whose points are not too close and not too far apart.

More precisely, led $d \geq 1$ be fixed. All Delone sets, patterns etc. will be subsets of $\mathbb{R}^d$. The Euclidean norm on $\mathbb{R}^d$ will be denoted by $\|\cdot\|$. For $r \in \mathbb{R}^+$ and $p \in \mathbb{R}^d$, we let $B(p, r)$ be the closed ball in $\mathbb{R}^d$ centered at p with radius r.

A subset ω of $\mathbb{R}^d$ is called Delone set if there exist $r(\omega)$ and $R(\omega) > 0$ such that $2r(\omega) \leq \|x - y\|$ whenever $x, y \in \omega$ with $x \neq y$, and $B(x, R(\omega)) \cap \omega \neq \emptyset$ for all $x \in \mathbb{R}^d$.

Note that this definition includes sets with global translation symmetries. In this point of view a perfect crystal is a special kind of a quasicrystal. In the general case we have only local symmetries.

Therefore we have to deal with local structures of Delone sets and the restrictions of ω to bounded subsets of $\mathbb{R}^d$ are of particular interest. In order to treat these restrictions, we introduce the following definition.

Definition 0.1.1 (a) *A pair (Λ, Q) consisting of a bounded subset Q of $\mathbb{R}^d$ and $\Lambda \subset Q$ finite is called* pattern. *The set Q is called the* support of the pattern.
(b) *A pattern (Λ, Q) is called a* ball pattern *if $Q = B(x, r)$ with $x \in \Lambda$ for suitable $x \in \mathbb{R}^d$ and $r \in (0, \infty)$.*

The pattern (Λ_1, Q_1) is contained in the pattern (Λ_2, Q_2) written as $(\Lambda_1, Q_1) \subset (\Lambda_2, Q_2)$ if $Q_1 \subset Q_2$ and $\Lambda_1 = Q_1 \cap \Lambda_2$. Diameter, volume etc. of a pattern are defined to be the diameter, volume etc of its support. For patterns $X_1 = (\Lambda_1, Q_1)$ and $X_2 = (\Lambda_2, Q_2)$, we define $\sharp_{X_1} X_2$, *the number of occurences of X_1 in X_2*, to be the number of elements in $\{t \in \mathbb{R}^d : \Lambda_1 + t \subset \Lambda_2, Q_1 + t \subset Q_2\}$. Note the relation of ball patterns with s-patches as considered in [7]. We will identify patterns wich are equal up to translations. The notions of diameter, volume etc. can easily be carried over to pattern classes. The class of a pattern P will be denoted by $[P]$.

Every Delone set ω gives rise to a set of pattern classes, $\mathcal{P}(\omega) = \{[Q \wedge \omega] : Q \subset \mathbb{R}^d \text{ bounded and measurable}\}$, and to a set of ball pattern classes $\mathcal{P}_B(\omega) = \{[B(p, r) \wedge \omega] : p \in \omega, r \in \mathbb{R}^+\}$. Here we set $Q \wedge \omega = (\omega \cap Q, Q)$. We define the radius $s = s(P)$ of an arbitrary ball pattern P to be the radius of the underlying ball. For $s \in (0, \infty)$, we denote by $\mathcal{P}_B^s(\omega)$ the set of ball patterns with radius s. A Delone set is said to be of *finite type* or of *finite local complexity* if for every radius $s > 0$ the set $\mathcal{P}_B^s(\omega)$ is finite.

Examples

- The simplest example of a Delone set is the lattice $\mathbb{Z}^d$ in $\mathbb{R}^d$.
- The set of vertices of the Penrose tiling is a Delone set.

Next we introduce a suitable topology on the set $\mathcal{F}(\mathbb{R}^d)$ of closed subsets of $\mathbb{R}^d$. The method we are going to outline now has most definitely been pointed out to us by someone else. Unfortunately, we were not able to find out by whom.

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 euclidean metric ρ. Since the unit sphere is compact and complete, the Hausdorff metric ρ_H makes the set $\mathcal{K}(\mathbb{S}^d)$ of compact subsets of it into a complete and compact metric space.

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:

Theorem 1 *$\mathcal{F}(\mathbb{R}^d)$ endowed with the natural topology τ_{nat} is compact.*

Note that, interestingly, no additional properties are needed for compactness. Of course, this result immediately gives compactness of certain subsets of the set of all Delone sets, e.g. compactness of the union over R of the (r, R)-sets for any fixed value of r.

Let us note in passing that the metric ρ proposed in [5] as well as the metric in [8] do not satisfy the triangle inequality. See, however, [9], in which a metric on the set of Delone sets is constructed. A discussion in a more general framework can be found in [4], where the author constructs a topology on the set of closed discrete subsets of a locally compact σ-compact space. In the case of $\mathbb{R}^d$ this topology coincides with the restriction of the above given natural topology.

For a quite different approach to the topology on the set of Delone sets we refer to [10], where Delone sets are identified with the sum of delta measures sitting at the points of the Delone set. Then one has the w*-topology on the set of measures at ones disposal, providing good compactness properties. The approach presented here has the advantage that a topology is induced on the set of closed sets.

Next, we define Delone dynamical systems, following the study of repetitive Delone sets in [11] and single out some important properties:

Definition 0.1.2 (a) *Let Ω be a set of Delone sets. The pair (Ω, T) is called a* Delone dynamical system *(DDS) if Ω is invariant under the shift T and closed in the natural topology.*
(b) *A DDS (Ω, T) is said to be of* finite type *(DDSF) if $\cup_{\omega\in\Omega} P_B^s(\omega)$ is finite for every $s > 0$.*
(c) *Let $0 < r, R < \infty$ be given. A DDS (Ω, T) is said to be an* (r, R)-system *if every $\omega \in \Omega$ is an (r, R)-set.*
(d) *The set $\mathcal{P}(\Omega)$ of* pattern classes associated to a DDS Ω *is defined by $\mathcal{P}(\Omega) = \cup_{\omega\in\Omega}\mathcal{P}(\omega)$.*

Remark 0.1.3 (a) Whenever (Ω, T) is a Delone dynamical system, there exists an $R > 0$ with $B_R(x) \cap \omega \neq \emptyset$ for every $\omega \in \Omega$ and every $x \in \mathbb{R}^d$. This follows easily as Ω is closed and invariant under the action of T.
(b) Every DDSF is an (r, R)-system for suitable $0 < r, R < \infty$.
(c) For a thorough study of Delone sets of finite local complexity we refer the reader to [7] (d) Let ω be an (r, R)-set and let Ω_ω be the closure of $\{T_t\omega : t \in \mathbb{R}^d\}$ in $\mathcal{F}(\mathbb{R}^d)$ with respect to the natural topology. Then (Ω_ω, T) is an (r, R)-system.

For a DDSF, there is a simple way to describe convergence in the natural topology. This is shown in the following lemma taken from [6].

Lemma 0.1.4 *If (Ω, T) is a DDSF then a sequence (ω_n) converges to ω in the natural topology if and only if there exists a sequence (t_n) converging to 0 such that for every $L > 0$ there is an $n_0 \in \mathbb{N}$ with $(\omega_n + t_n) \cap B(0, L) = \omega \cap B(0, L)$ for $n \geq n_0$.*

0.1.3 ergodic Ergodic and combinatorial features of DDS

We start with a result that characterizes unique ergodicity of a Delone dynamical system in terms of the validity of a Banach space valued ergodic theorem. First, let us record the following notions of ergodic theory along with an equivalent "combinatorial" characterization available for Delone dynamical systems: (Ω, T) is called *non-periodic* if $T_t\omega \neq \Omega$ whenever $\omega \in \Omega$ and $t \in \mathbb{R}^d$ with $t \neq 0$. Is is called *minimal* if every orbit is dense. This is equivalent to $\mathcal{P}(\Omega) = \mathcal{P}(\omega)$ for every $\omega \in \Omega$. This latter property is called *local isomorphism property* in the tiling framework [12]. It is also referred to as repetitivity. Namely, it is equivalent to there existing an $R(P) > 0$ for every $P \in \mathcal{P}(\Omega)$ such that $B(p, R(P)) \wedge \omega$ contains a copy of P for every $p \in \mathbb{R}^d$ and every $\omega \in \Omega$. Note also that every minimal DDS is an (r, R)-system.

We are interested in ergodic averages. More precisely, we will take means of suitable functions along suitable sequences of patterns and pattern classes. These functions and sequences will be introduced next. Here and in the sequel we will use the following notation: For $Q \subset \mathbb{R}^d$ and $s > 0$ we define

$$Q_s \equiv \{x \in Q : \mathrm{dist}(x, \partial Q) \geq s\}, \;\; Q^s \equiv \{x \in \mathbb{R}^d : \mathrm{dist}(x, Q) \leq s\},$$

where, of course, dist denotes the usual distance and ∂Q is the boundary of Q. Moreover, we denote the Lebesgue measure of a measurable subset $Q \subset \mathbb{R}^d$ by $|Q|$. Then, a sequence (Q_n) of subsets in $\mathbb{R}^d$ is called a van Hove sequence if the sequence $(|Q_n|^{-1}|Q_n^s \setminus Q_{n,s}|)$ tends to zero for every $s \in (0, \infty)$. Similarly, a sequence (P_n) of pattern classes, (i.e. $P_n = [(\Lambda_n, Q_n)]$ with suitable Q_n, Λ_n) is called a van Hove sequence if Q_n is a van Hove sequence. (This is obviously well defined.) We can now discuss unique ergodicity. A dynamical system (Ω, T) is called *uniquely ergodic* if it admits only one T-invariant measure (up to normalization). For a Delone dynamical system, this is equivalent to the fact that for every pattern class P the frequency

$$f(P) \equiv \lim_{n\to\infty} |Q_n|^{-1} \sharp_P(\omega \wedge Q_n), \tag{1}$$

exists uniformly in $\omega \in \Omega$ for every van Hove sequence (Q_n). This equivalence was shown in Theorem 1.6 in [6] (see [9] as well). It goes back to [12], Theorem 3.3, in the tiling setting.

For patterns $X_i = (\Lambda_i, Q_i)$, $i = 1, \ldots, k$, and $X = (\Lambda, Q)$, we write $X = \oplus_{i=1}^k X_i$ if $\Lambda = \cup \Lambda_i$, $Q = \cup Q_i$ and the Q_i are disjoint up to their boundaries with the obvious extension to pattern classes.

Definition 0.1.5 *Let Ω be a DDS and B be a vector space with seminorm $\| \cdot \|$). A function $F : \mathcal{P}(\Omega) :\longrightarrow B$ is called almost additive (with respect to $\| \cdot \|$) if there exists a function $b : \mathcal{P}(\Omega) \longrightarrow (0, \infty)$ with $\lim_{n\to\infty} |P_n|^{-1} b(P_n) = 0$ for every van Hove sequence (P_n) and a constant $D > 0$ such that*

(A1) $\|F(\oplus_{i=1}^k P_i) - \sum_{i=1}^k F(P_i)\| \leq \sum_{i=1}^k b(P_i)$,

(A2) $\|F(P)\| \leq D|P| + b(P)$.

(A3) $b(P_1) \leq b(P) + b(P_2)$ *whenever* $P = P_1 \oplus P_2$.

Now, our first result reads as follows.

Theorem 2 *For a minimal, aperiodic DDSF (Ω, T) the following are equivalent:*
(i) (Ω, T) is uniquely ergodic.
(ii) The limit $lim_{n\to\infty}|P_n|^{-1}F(P_n)$ exists for every van Hove sequence (P_n) and every almost additive F on (Ω, T) with values in a Banach space.

Remark 0.1.6 (a) The proof uses methods of Geerse/Hof [13] and ideas from Priebe [14]. In fact, Geerse/Hof established a similar result for a tiling associated to a primitive substitution.
(b) In the one dimensional case related results have been shown by one of the authors in [15].

The proof of the theorem makes use of completeness of the Banach space in crucial manner. However, it does not use the nondegeneracy of the norm. Thus, we get the following corollary (of its proof).

Corollary 0.1.7 *Let (Ω, T) be aperiodic and strictly ergodic. Let the vector space B be complete with respect to the topology induced by the seminorms $\|\cdot\|_\iota$, $\iota \in \mathcal{I}$. If $F : \mathcal{P} \longrightarrow B$ is almost additive with respect to every $\|\cdot\|_\iota$. $\iota \in \mathcal{I}$, then $\lim_{n\to\infty} |P_n|^{-1} F(P_n)$ exists for every van Hove sequence (P_n) in $\mathcal{P}(\Omega)$.*

The theorem and the corollary underline the strong averaging features of strictly ergodic DDS. Of course, quite some work has been devoted to studying local conditions ensuring unique ergodicity and minimality of a DDS. Two such conditions are *linear repetitiveity* and *dense repetitivity*. These conditions have recently been discussed and shown to imply strict ergodicity by Lagarias and Pleasants in [11] (for one-dimensional linearly repetitive systems see the work of Durand [16] as well). A DDSF is said to be linearly repetitive if there exists a constant C such that, for $r > 0$ given, every ball pattern of radius Cr contains every ball pattern of radius Cr. A DDSF is said to be densely repetitive if there exist a constant D sucht that every ball pattern of radius r is contained in every ball pattern of radius $CN(r)^{1/d}$, where $N(r)$ denotes the number of different ball patterns of radius r. As shown in [11] aperiodic linearly repetitive systems and aperiodic densely repetitive systems are in some sense closest to periodic systems among the non-periodic systems. The two concepts are related. In fact, as conjectured by Lagarias/Pleasants in [11] and recently shown in [17] by one of the authors the following holds.

Theorem 3 *Every aperiodic linearly repetitive DDS is densely repetitive.*

As far as uniform ergodic theorems go, linearly repetitive systems are rather special. Namely, they allow for a uniform subadditive ergodic theorem. As shown in [18, 19] the following holds. Let $\mathcal{C}(2)$ be the set of all cubes in $\mathbb{R}^d$ whose sidelengths $l_i(C)$, $i = 1, \ldots, d$ satisfy $1/2 \leq l_i(C)/l_j(C) \leq 2$ for all $i, j \in 1, \ldots, 2$.

Theorem 4 *Let (Ω, T) be a linearly repetititive DDS. Let $F : \mathcal{P}(\Omega) \longrightarrow \mathbb{R}$ be subadditive (i.e. $F(A \oplus B) \leq F(A) + F(B)$, whenever A and B are disjoint up to their boundary), then*

$$\lim_{n\to\infty} \frac{F(P_n)}{|P_n|}$$

exists for every van Hove sequence (P_n) with supports of P_n contained in $\mathcal{C}(2)$.

Remark (1) The theorem gives a new proof of the uniquely ergodicity of linearly repetitive systems.
(2) The theorem holds also for functions which are subadditive up to a boundary term [18].

In $d = 1$ it is actually possible to characterize the subshifts for which the averages for arbitrary subadditive functions exist. They are those satisfying linear repetitivity on the average. More precisely, the following holds as shown by one of the authors in [15].

Theorem 5 *Let (Ω, T) be a minimal subshift over the finite alphabet A. Then, the following are equivalent:*
(i) $\lim_{|v|\to\infty} F(v)/|v|$ exists for arbitrary subadditive F on the associated set of finite words.
(ii) There exists a constant $C > 0$ with $\liminf_{|x|\to\infty} \frac{\sharp_v(x)}{|x|}|v| \geq C$ for arbitrary v in the associated set of words. Here, $\sharp_v(x)$ denotes the number of copies of v in x and $|x|$ is the length of x.

Generalizations of this one-dimensional result to DDS in arbitrary dimensions for an application to diffraction theory, are currently under investigation (see [20]). There also applications to computations of the eigenvalues of the DDS are given.

Let us close this section by emphasizing that the theorems on uniform existence of averages of subadditive functions have proven rather useful in recent works. They allow to prove Cantor spectrum of measure zero for large classes of one-dimensional quasicrystal Schrödinger operators [21, 22]. Moreover, they can also be used to study uniform existence of certain averages in lattice gas theory.

0.1.4 The associated algebras and operators

In this Section we introduce a C^*-algebra that had already been encountered in a different form in [10, 23]. Our presentation here is geared towards using the elements of the C^*-algebra as tight binding hamiltonians in a quantum mechanical description of disordered solids. We relate certain spectral properties of the members of such operator families to ergodic features of the underlying dynamical system. Moreover, we show that the eigenvalue counting functions of these operators are convergent. The limit, known as the integrated density of states, is an object of fundamental importance from the solid state physics point of view. Apart from proving its existence, we also relate it to the canonical trace on the von Neumann algebra $\mathcal{N}(\Omega, T, \mu)$ in case that the Delone dynamical system (Ω, T) uniquely ergodic. Results of this genre are known as Shubin's trace formula due to the celebrated results from [24].

Moreover, we review how noncommutative integration theory is used to construct the von Neumann algebra $\mathcal{N}(\Omega, T, \mu)$ of observables that reflects certain ergodic properties of the underlying DDS as well.

The results as well as the proofs can be found in [25]. First we study a 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 0.1.8 *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 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 in the following.

Remarks 0.1.9 (1) 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) $\Pi_{\omega \in \Omega} \mathcal{B}(\ell^2(\omega))$.

(2) Pointwise sum, the convolution (matrix) product

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

and the involution $k^*(p, \omega, q) := \overline{k}(q, \omega, p)$ make $\mathcal{A}^{fin}(\Omega, T)$ into a $*$-algebra.

(3) The mapping $\pi : \mathcal{K}^{fin}(\Omega, T) \to \Pi_{\omega \in \Omega} \mathcal{B}(\ell^2(\omega))$ defined in (1) 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*.

(4) We denote the completion of $\mathcal{A}^{fin}(\Omega, T)$ with respect to the norm $\|A\| := \sup_{\omega \in \Omega} \|A_\omega\|$ by $\mathcal{A}(\Omega, T)$.

(5) The mapping $\pi_\omega : \mathcal{A}^{fin}(\Omega, T) \to \mathcal{B}(\ell^2(\omega)), K \mapsto K_\omega$ with K_ω as in (1) is a representation that extends by continuity to a representation of $\mathcal{A}(\Omega, T)$ that we denote by the same symbol.

We get the following result that relates ergodicity properties of (Ω, T), spectral properties of the operator families from $\mathcal{A}(\Omega, T)$ and properties of the representations π_ω.

Theorem 6 *The following conditions on a DDS (Ω, T) are equivalent:*

(i) *(Ω, T) is minimal.*

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

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

Now we introduce algebras of observables that extend the C*-algebra considered above.

Definition 0.1.10 *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.

As is clear from the definition, the elements of $\mathcal{N}(\Omega, T, \mu)$ are classes of families of operators. However, we will not distinguish too pedantically between classes and their representatives in the sequel.

Remark 0.1.11 It is possible to define $\mathcal{N}(\Omega, T, \mu)$ by requiring seemingly weaker conditions. Namely, one can consider families (A_ω) that are essentially bounded and satisfy the covariance condition almost everywhere. However, by standard procedures (see [26, 27]), it is possible to show that each of these families agrees almost everywhere with a family satisfying the stronger conditions discussed above.

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 case has been considered in [28, 6].

Apparently, $\mathcal{N}(\Omega, T, \mu)$ is an involutive algebra under the obvious operations. To see that it has a predual, i.e., that it is a weak-*-algebra is not obvious. We prove this in [25] by identifying $\mathcal{N}(\Omega, T, \mu)$ with the algebra of random operators for a suitable random Hilbert space, as will be outlined now. For details we refer to [6, 25] where we use the following concepts from Connes non-commutative integration theory [26]: We introduced

- a suitable *groupoid* $\mathcal{G}(\Omega, T)$,
- a *transversal measure* $\Lambda = \Lambda_\mu$ for a given invariant measure μ on (Ω, T)
- and a Λ-*random Hilbert space* $\mathcal{H} = (\mathcal{H}_\omega)_{\omega\in\Omega}$

leading to the von Neumann algebra

$$\mathcal{N}(\Omega, T, \mu) := \mathrm{End}_\Lambda(\mathcal{H})$$

of *random operators*, all in the terminology of [26]. When everything is put together, this gives:

Theorem 7 *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. More precisely,*

$$\mathcal{N}(\Omega, T, \mu) = \mathrm{End}_\Lambda(\mathcal{H}),$$

where $\Lambda = \Lambda_\nu$ and $\mathcal{H} = (\ell^2(\mathcal{X}^\omega, \alpha^\omega))_{\omega\in\Omega}$ are defined as above.

We can use the measurable structure to identify $L^2(\mathcal{X}, m)$, where $m = \int_\Omega \alpha^\omega \mu(\omega)$ with $\int_\Omega^\oplus \ell^2(\mathcal{X}^\omega, \alpha^\omega)\, d\mu(\omega)$. This gives the faithful representation

$$\pi : \mathcal{N}(\Omega, T, \mu) \longrightarrow B(L^2(\mathcal{X}, m)), \pi(A)f((\omega, x)) = (A_\omega f_\omega)((\omega, x))$$

and the following immediate consequence.

Corollary 0.1.12 $\pi(\mathcal{N}(\Omega,T,\mu)) \subset B(L^2(\mathcal{X},m))$ *is a von Neumann algebra.*

Next we want to identify conditions under which $\pi(\mathcal{N}(\Omega,T,\mu))$ is a factor. Recall that a Delone set ω is said to be *non-periodic* if $\omega + t = \omega$ implies that $t = 0$.

Theorem 8 *Let (Ω,T) be an (r,R)-system and let μ be an ergodic invariant measure on Ω. If ω is non-periodic for μ-a.e. $\omega \in \Omega$ then $\mathcal{N}(\Omega,T,\mu)$ is a factor.*

Remark 0.1.13 Since μ is ergodic, the assumption of non-periodicity in the Theorem can be replaced by assuming that there is a set of positive measure consisting of non-periodic ω.

The following theorem is a consequence of [29]. It deals with almost sure constancy of spectral features of random operators.

Theorem 9 *Let (Ω,T) be an (r,R)-system and μ be T-invariant. Let μ be ergodic and $(A_\omega) \in \mathcal{N}(\Omega,T,\mu)$ be selfadjoint. Then there exist sets $\Sigma, \Sigma_{ac}, \Sigma_{sc}, \Sigma_{pp}, \Sigma_{ess} \subset \mathbb{R}$ and a subset $\widetilde{\Omega}$ of Ω of full measure such that $\Sigma = \sigma(A_\omega)$ and $\sigma_\bullet(A_\omega) = \Sigma_\bullet$ for $\bullet = ac, sc, pp, ess$ and $\sigma_{disc}(A_\omega) = \emptyset$ for every $\omega \in \widetilde{\Omega}$.*

0.1.5 The integrated density of states and Shubins trace formula

We now define a particular trace on $\mathcal{N}(\Omega,T,\mu)$. To this end, choose a nonnegative $u \in C_c(\mathbb{R}^d)$ with $\int_{\mathbb{R}^d} u(x)dx = 1$. Let M_u be the operator of multiplication by u. It can be shown that

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

does not depend on the choice of u as long as the integral is one [6, 25]. Important features of τ are given in the following lemma.

Lemma 0.1.14 *Let (Ω,T) be an (r,R)-system and μ be T-invariant. Then the map $\tau : \mathcal{N}(\Omega,T,\mu) \longrightarrow \mathbb{C}$ is continuous, faithful, nonegative on $\mathcal{N}(\Omega,T,\mu)^+$ and satisfies $\tau(A) = \tau(U^*AU)$ for every unitary $U \in \mathcal{N}(\Omega,T,\mu)$ and arbitrary $A \in \mathcal{N}(\Omega,T,\mu)$, i.e., τ is a trace.*

Having defined τ, we can now associate a canonical measure ρ_A to every selfadjoint $A \in \mathcal{N}(\Omega,T,\mu)$.

Definition 0.1.15 *For $A \in \mathcal{N}(\Omega,T,\mu)$ selfadjoint, and $B \subset \mathbb{R}$ Borel measurable, we set $\rho_A(B) \equiv \tau(\chi_B(A))$, where χ_B is the characteristic function of B.*

For the next result we refer to [29].

Lemma 0.1.16 *Let (Ω,T) be an (r,R)-system and μ be T-invariant. Let $A \in \mathcal{N}(\Omega,T,\mu)$ selfadjoint be given. Then ρ_A is a spectral measure for A. In particular, the support of ρ_A agrees with the spectrum Σ of A and the equality $\rho_A(F) = \tau(F(A))$ holds for every bounded measurable F on $\mathbb{R}$.*

We now come to relate the abstract trace τ defined above with the mean trace per unit volume. The latter object is quite often considered by physicists and bears the name *integrated density of states*. Its proper definition rests on ergodicity.

Proposition 0.1.17 *Assume that (Ω, T) is a uniquely ergodic (r, R)-system with invariant probability measure μ and $A \in \mathcal{A}(\Omega, T)$. Then, for any van Hove sequence (Q_n) it follows that*

$$\lim_{n \in \mathbb{N}} \frac{1}{|Q_n|} \mathrm{tr}(A_\omega|_{Q_n}) = \tau(A)$$

for all $\omega \in \Omega$.

Clearly, $A_\omega|_Q$ denotes the restriction of A_ω to the finite dimensional subspace $\ell^2(\omega \cap Q)$, whenever $Q \subset \mathbb{R}^d$ is bounded.

The following result finally 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 per volume below E (counting multiplicities).

Theorem 10 *Let (Ω, T) be a uniquely ergodic (r, R)-system and μ its invariant probability measure. Then for selfadjoint $A \in \mathcal{A}(\Omega, T)$ and any van Hove sequence (Q_n) we get that for every $\varphi \in C(\mathbb{R})$ and every ω*

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

Consequently, the measures $\rho_\omega^{Q_n}$ converge weakly to the measure ρ_A defined above by $\langle \rho_A, \varphi \rangle := \tau(\varphi(A))$.

The above statement has many precursors: [30, 31, 32, 2, 24] in the context of almost periodic, random or almost random operators on $\ell^2(\mathbb{Z}^d)$ or $L^2(\mathbb{R}^d)$. It generalizes results by Kellendonk [23] on tilings associated with primitive substitutions. Its proof relies on ideas from [30, 31, 32, 23] and [33]. Nevertheless, it is new in the present context.

The primary object from the physicists point of view is the finite volume limit:

$$N[A](E) := \lim_{n \to \infty} n[A_\omega, Q_n](E)$$

known as the integrated density of states. It has a striking relevance as the number of energy levels below E per unit volume, once its existence and independence of ω are settled.

The last theorem provides the mathematically rigorous version. Namely, the distribution function $N_A(E) := \rho_A(-\infty, E]$ of ρ_A is the right choice. It gives a limit of finite volume counting measures since

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

Therefore, the desired independence of ω is also clear. Moreover, by standard arguments we get that the distribution functions of the finite volume counting functions converge to N_A at points of continuity of the latter.

A better convergence result can be deduced from the strong ergodic result Theorem 2 presented in the Section 0.1.3. To do so we proceed as follows.

The spectral counting functions appearing as approximants of the integrated density of states are obviously elements of the vector space $\mathcal{D}$ consisting of all bounded right continuous functions $f : \mathbb{R} \longrightarrow \mathbb{R}$ equipped for which $\lim_{x\to-\infty} f(x) = 0$ and $\lim_{x\to\infty} f(x)$ exists. Equipped withe the supremum norm $\|f\|_\infty \equiv \sup_{x\in\mathbb{R}} |f(x)|$ this vector space is a Banach space. It turns out that the spectral counting function is essentially an almost additive function. More precisely the following holds [34].

Theorem 11 *Let (Ω, T) be a DDS. Let A be an operator of finite range. Then $F^A : \mathcal{P}(\Omega) \longrightarrow \mathcal{D}$, defined by $F^A(P) \equiv n(A_\omega, Q_{R^A})$ for $P = [(\omega \wedge Q)]$ is a well defined almost additive function.*

Remark 0.1.18 The theorem seems to be new even in the one-dimensional case. (There, of course, it is very easy to prove.)

Now, our results on convergence of the integrated density of states reads as follows.

Theorem 12 *Let (Ω, T) be an aperiodic strictly ergodic DDSF. Let A be a selfadjoint operator of finite range and (Q_n) be an arbitrary van Hove sequence. Then the measures $\rho_{Q_n}^{A_\omega}$ converge in distribution to the measure ρ^A and this convergence is uniform in $\omega \in \Omega$.*

As a consequence of this stronger convergence we can explain the occurrence of discontinuities of the integrated density of states. Namely such discontinuities are always due to finitely supported eigenfunctions, i.e., to very strongly localized states. This has been worked out in [35].

Theorem 13 *Let (Ω, T) be a strictly ergodic DDSF. Let A be a selfajoint random operator of finite range. 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) $\omega \in \Omega$.*

It is rather straightforward to see that locally supported eigenfunctions lead to a discontinuity of the IDS. Moreover one can show easily that every DDS can be changed in such a way that the original and the new system are "more or less the same" and such that the new system exhibits locally supported eigenfunctions. The idea is to replace points in the original system by a "small" graph that allows an eigenfunction. The equivalence of the two systems can be phrased in the notion of *mutually locally derivable* (MLD), going back to [36]. For a thorough discussion, see [35]. Here we only give the result and a picture of the small graph that one can choose to implement. Here the little squares mark the vertices of the graph and the straight lines are the edges of the graph. Next to each vertex we indicate the value of a locally supported eigenfunction of the nearest neighbor laplacian.

Theorem 14 *Let (Ω, T) be a arbitrary DDSF. Then there exists a DDSF (Ω^b, T) and a random operator of finite range (A_w^b) such that (Ω, T) and (Ω^b, T) are mutually locally derivable and (A_w^b) has locally supported eigenfunctions with eigenvalue E for every $\omega \in \Omega^b$. Moreover, (A_w^b) can be chosen to be the nearest neighbor laplacian of suitable graph.*

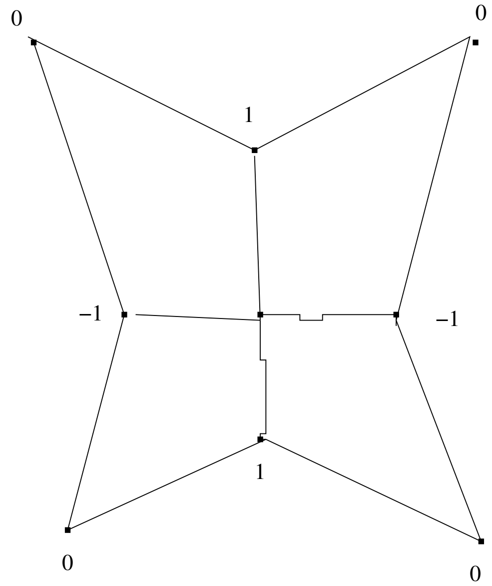

Figure 1: The finite graph G_{fin}.

The starting point is a small graph $G_{fin} = (V_{fin}, E_{fin})$ and an eigenfunction u_{fin} of the associated nearest neighbor laplacian. For definiteness sake consider Figure 1. The values of u_{fin} are indicated near the corresponding vertices. Here the eigenvalue is $E = 0$.

It is clear that whatever edges reach out of the four corners in a larger graph extending G_{fin}, the extension of u_{fin} by 0 to the larger vertex set will still constitute an eigenfunction of the laplacian on the large graph. It is now easy to implement this picture into a given DDSF.

For those who prefer tiling examples we now indicate how to view the construction above in this framework. Take a tiling dynamical system (see [6, 5]) and replace one given tile T by a suitable homeomorphic image of T^b indicated in Figure 2 by the full lines. We also indicated the next neighbor relations, showing that the resulting graph is just G_{fin} above.

0.1.6 Conclusion

To sum up, using Delone sets one can define natural tight binding hamiltonians for quasicrystals. These hamiltonians have many aspects in common with the hamiltonians of disordered systems. They can be considered as families indexed by the points of a Delone dynamical system.

However, the complex geometry of Delone sets can lead to effects like discontinuities of the integrated density of states. Moreover, these models exhibit a striking uniformity as far as their ergodic properties are concerned. Thus, despite all analogies, there are important differences to disordered systems.

ergodic Ergodic properties of the Delone dynamical system in question are of central im-

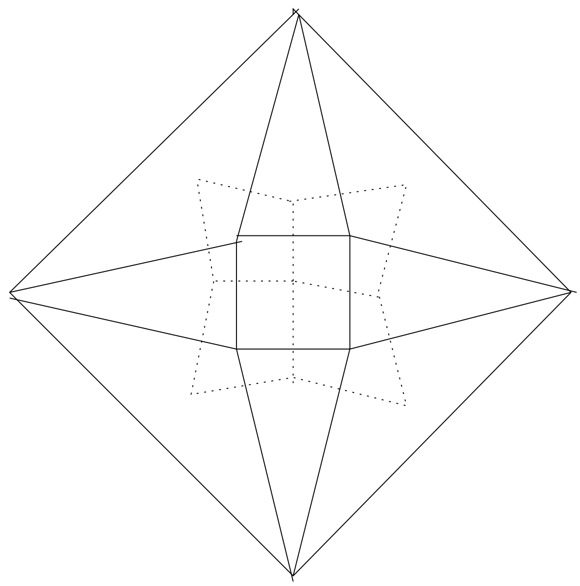

Figure 2: The tiling of G_{fin}.

portance in different aspects as well and they can be deduced to questions concerning the complexity of the individual Delone sets that belong to the DDS. Certain spectral information concerning the hamiltonian for a quasicrystal can be deduced from ergodic information. Moreover, the hamiltonians can be regarded as elements of certain operator algebras and the latter reflect ergodic features of the underlying DDS.

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