APERIODIC ORDER – LECTURE 12 SUMMARY

1. Projection method — continuation (see [6, 2.6.1] and [1, 7.2]).

Recall some results and definitions from the last lecture.

Proposition 1.1. *Let* $\mathcal{L}$ *be an integral lattice in* $\mathbb{R}^n$ *and* $\mathcal{E} \subset \mathbb{R}^n$ *a linear subspace. Then the following are equivalent:*

(i) $\Pi(\mathcal{L})$ *is dense in* $\mathcal{E}$*;*

(ii) $\mathcal{E} \cap \mathcal{L} = \{0\}$*;*

(iii) $\Pi^{\perp}|_{\mathcal{L}}$ *is 1-to-1.*

Next we define the *cut and project scheme* (CPS). We restrict ourselves to Euclidean "internal space" for simplicity, but note that more general schemes (with LCAG internal spaces) are considered.

Definition 1.2. A *cut and project scheme* (CPS) is a triple $(\mathbb{R}^d, H, \mathcal{L})$, with the *internal space* $H \approx \mathbb{R}^{\ell}$ and $\mathcal{L} \subset \mathbb{R}^d \times H$ a lattice, with the two natural projections $\pi : \mathbb{R}^d \times H \to \mathbb{R}^d$ and $\pi_{\text{int}} : \mathbb{R}^d \times H \to H$ subject to the conditions that $\pi|_{\mathcal{L}}$ is injective and $\pi_{\text{int}}(\mathcal{L})$ is dense in H.

Definition 1.3. A subset $W \subset H$ is called a *window* or *acceptance domain* if W is bounded and has nonempty interior. It is called *regular* if the boundary ∂W has zero Lebesgue measure $\mathscr{L}^{\ell}$.

Definition 1.4. For $W \subset H$ consider

$$\Lambda(W) := \{\pi(\mathbf{x}) : \ \mathbf{x} \in \mathcal{L}, \ \pi_{\text{int}}(\mathbf{x}) \in W\}.$$

It is called a *model set* if W is a window. The model set is *generic* if $\pi_{\text{int}}(\mathcal{L}) \cap \partial W = \emptyset$, otherwise it is called *singular.*

Theorem 1.5. *Let* $(\mathbb{R}^d, H, \mathcal{L})$ *be a CPS and* $W \subset H$*.*

(i) *If* W *is bounded, then* $\Lambda(W)$ *has finite local complexity (FLC) and hence it is uniformly discrete;*

(ii) *if* W *has nonempty interior, then* $\Lambda(W)$ *is relatively dense in* $\mathbb{R}^d$*;*

(iii) *if* $\Lambda(W)$ *is a model set (i.e.* W *is bounded and* $W^{\circ} \neq \emptyset$*), then* $\Lambda(W)$ *is a Meyer set.*

Lemma 1.6. *Let* $(\mathbb{R}^d, H, \mathcal{L})$ *be a CPS and* W *a bounded window with nonempty interior. If* $\pi_{\text{int}}|_{\mathcal{L}}$ *is 1-to-1, then* $\Lambda(W)$ *is non-periodic.*

Remark 1.7. Recall that in the definition of CPS we required that $\pi|_{\mathcal{L}}$ be 1-to-1. Assuming that $\mathcal{L}$ is an integral lattice, we have, in view of Proposition 1.1:

$$\pi_{\text{int}}|_{\mathcal{L}} \text{ is 1-to-1} \iff (\mathbb{R}^d \times \{0\}) \cap \mathcal{L} = \{\mathbf{0}\};$$

$$\pi|_{\mathcal{L}} \text{ is 1-to-1} \iff (\{0\} \times H) \cap \mathcal{L} = \{\mathbf{0}\}.$$

Here the new stuff begins.

1.1. **Uniform distribution.**

Theorem 1.8. *Let $(\mathbb{R}^d, H, \mathcal{L})$ be a CPS. Let W be a regular window. Then the model set $\Lambda(W)$ is uniformly distributed in $\mathbb{R}^d$ in the following sense. For any $x \in R^d$,*

$$\lim_{R\to\infty} \frac{\#(\Lambda(W) \cap B_R(x))}{\mathscr{L}^d(B_R)} = \delta(\mathcal{L}) \cdot \mathscr{L}^\ell(W), \quad \text{as} \quad R \to \infty,$$

where $\delta(\mathcal{L}) = \mathscr{L}(\mathbb{R}^d \times H/\mathcal{L})$ is the volume of the fundamental domain of the lattice $\mathcal{L}$.

We will not prove this in class; see e.g. [4, Prop. 3.2] for a recent exposition.

1.2. **Pure discrete spectrum.**

Theorem 1.9. *Suppose that $(\mathbb{R}^d, H, \mathcal{L})$ is a CPS and W a regular window. Consider the model set $\Lambda(W)$. Then the associated Delone set dynamical system $(X_{\Lambda(W)}, \mathbb{R}^d)$ is uniquely ergodic and has pure discrete spectrum. If $\Lambda(W)$ is generic, then the dynamical system is minimal.*

Proof sketch. It is more convenient to change the view a little bit. Instead of $\mathbb{R}^d \times H$ consider the isomorphic Euclidean space $\mathbb{R}^n$, and suppose, for simplicity, that the lattice $\mathcal{L}$ is the standard integer lattice $\mathbb{Z}^n$. The “physical space” will be denoted by E; it is isomorphic to $\mathbb{R}^d$, so let $\mathbf{i} : \mathbb{R}^d \to E$ denote this isomorphism. The “internal space” is then $E^\perp$; this is H in the previous notation. We will keep the notation for projections: $\pi := \Pi_E$ and $\pi_{\text{int}} = \Pi_{E^\perp}$. The model set $\Lambda(W)$ can be expressed as

$$\Lambda := \Lambda(W) = (\mathbf{i}^{-1}\pi)((W + E) \cap \mathbb{Z}^n)$$

(indeed, $W + E = \{\mathbf{x} \in \mathbb{R}^n : \ \pi_{\text{int}}(\mathbf{x}) \in W\}$). Together with this, we consider the *model sets family*

$$\Lambda_{\mathbf{s}} := (\mathbf{i}^{-1}\pi)((W + E) \cap (\mathbb{Z}^n + \mathbf{s})) \ \text{ for } \mathbf{s} \in \mathbb{R}^d.$$

It is clear that

$$\Lambda_{\mathbf{s}} = \Lambda(W - \pi_{\text{int}}\mathbf{s}) + \pi\mathbf{s},$$

so the elements of the model set family are Delone (even Meyer) sets. Note that $\Lambda_{\mathbf{s}} = \Lambda_{\mathbf{s}+\mathbf{g}}$ for $\mathbf{g} \in \mathbb{Z}^n$, so the model set family is naturally parametrized by the torus $\mathbb{R}^n/\mathbb{Z}^n$. On the torus $\mathbb{T}^n$ we consider the $\mathbb{R}^d$-action obtained by translations along E:

$$T_{\mathbf{s}} : \ \mathbf{x} \mapsto \mathbf{x} + \mathbf{s} \pmod{\mathbb{Z}^n} \ \text{ for } \mathbf{s} \in E \approx \mathbb{R}^d.$$

This is a *Kronecker dynamical system*, which has pure discrete spectrum (we proved a similar statement for a single translation on the torus; this case is similar). We can identify $\mathbf{s} \longleftrightarrow \Lambda_{\mathbf{s}}$. We want to relate this system to the space of Delone set X_Λ. It is clear that $\Lambda + \mathbf{s} = \Lambda_{\mathbf{s}}$ when $\mathbf{s} \in E$, so the translation orbit of Λ belongs to our model set family. The problem is with *singular* elements $\Lambda_{\mathbf{s}}$ (when $\pi(\mathbb{Z}^n + \mathbf{s}) \cap \partial W \neq \emptyset$). However, such elements form a set of zero Lebesgue measure and 1st category topologically by our assumptions. Notice also, assuming $\Lambda_{\mathbf{s}}$ is nonsingular, $\Lambda_{\mathbf{t}}$ is close to $\Lambda_{\mathbf{s}}$ in the "local" topology of Delone set spaces, whenever $\mathbf{t}$ is close to $\mathbf{s}$. To make sure that the dynamical systems $(\mathbb{T}^n, T_{\mathbf{s}})_{\mathbf{s} \in E}$ and $(X_\Lambda, \mathbb{R}^d)$ are (measurably) isomorphic, we assume that $E^\perp \cap \mathbb{Z}^n = \emptyset$. Then the Kronecker system is minimal, in particular, the subspace E, after factoring modulo $\mathbb{Z}^n$, forms a dense subset of the torus $\mathbb{T}^n$, and hence every element of X_Λ corresponds to some $\Lambda_{\mathbf{s}}$ (this requires an argument). We thus obtain an "almost topological conjugacy" between the systems, and the result follows. □

1.3. **Tilings from projection method.** In order to get a tiling of $\mathbb{R}^d$ by tiles which are d-dimensional parallelepipeds (like Penrose rhombi in the 2-dimensional case), we can choose the *"canonical window"*

$$W := \pi_{\text{int}}(\mathcal{V}(\mathbf{0})),$$

where $\mathcal{V}(\mathbf{0})$ is the Voronoi cell of the origin $\mathbf{0}$ in the lattice $\mathcal{L}$. Then we consider the Voronoi tiling $\mathcal{V}$ of $\mathcal{L} + \mathbf{s}$ in $\mathbb{R}^n$ and those cells which are "cut" (intersected) by the subspace E. We then consider the *dual* tiling of V, which is called the *Delone tiling* $\mathcal{D}$. The rule is that we project a j-face of the tiling $\mathcal{D}$ by π to the subspace E if the corresponding dual $(n-j)$-face of the tiling V is cut by E, for $j \leq d$. The shift vector $\mathbf{s}$ is called "generic" if E does not intersect any $(n-d-1)$-faces of $\mathcal{V}$. This ensures that we really do get a tiling $\mathcal{T}$ of E. Its vertices are projections of vertices of $\mathcal{D}$, corresponding to the centers of $\mathcal{V}$-tiles cut by E, and these are exactly the elements of the Delone set

$$\Lambda_{\mathbf{s}} := \{\pi(\mathbf{x}) : \ \mathbf{x} \in \mathcal{L} + \mathbf{s}, \ \pi_{\text{int}}(\mathbf{x}) \in W\}.$$

On the other hand, the tiles of $\mathcal{T}$ are projections of d-faces of $\mathcal{D}$, which correspond to $(n-d)$-faces of $\mathcal{V}$. If $\mathcal{L} = \mathbb{Z}^n$, then $\mathcal{V}$ is the standard periodic tiling by grid cubes, shifted by $(\frac{1}{2}, \dots, \frac{1}{2})$, and $\mathcal{D}$ is the original tiling by grid cubes.

If E is chose to be a subspace that is stable under some subgroup of the symmetry group of $\mathcal{L}$, then the projected tilings will exhibit some "traces of symmetry". It will be appear locally, but not globally; however, the global symmetry will reappear in diffraction spectrum.

1.4. **Penrose tiling.** The Penrose tiling can be obtained by projection from $\mathbb{R}^4$ or from $\mathbb{R}^5$, but it is easier to describe the 5-dimensional set-up. Let A be the matrix of the linear operator which cyclically permutes the basis vectors of $\mathbb{R}^5$:

$$A: \ \mathbf{e}_1 \to \mathbf{e}_2 \to \mathbf{e}_3 \to \mathbf{e}_4 \to \mathbf{e}_5 \to \mathbf{e}_1.$$

The matrix A has eigenvalues $\{1, \xi, \xi^2, \xi^3, \xi^4\}$, where $\xi = e^{2\pi i/5}$. It has an eigenvector $\mathbf{w} = [1, \dots, 1]^t$ and two real invariant planes: E and E', such that $A|_E$ is a rotation by $2\pi/5$, with eigenvalues $\zeta, \overline{\zeta} = \zeta^4$, and $A|_{E'}$ is a rotation by $4\pi/5$, with eigenvalues $\zeta^2, \overline{\zeta^2} = \zeta^3$. We take $\mathcal{L} = \mathbb{Z}^5$ and the canonical window W. The complication is that

$$E^\perp = E' \oplus \mathrm{Span}(\mathbf{w})$$

is not totally irrational. This complicates the analysis of Section 1.2. Taking (generic) model sets $\Lambda_{\mathbf{s}}$ and $\Lambda_{\mathbf{s}'}$, we will be in the same space if and only if $\pi_{\mathrm{int}}(\mathbf{s}) = \pi_{\mathrm{int}}(\mathbf{s}')$ mod 1. It is known that Penrose tilings are obtained by specifying

$$\pi_{\mathrm{int}}(\mathbf{s}) = \gamma \mathbf{w}, \quad \text{with } \gamma = 1/2 \mod 1.$$

Proving this is too complicated; this is due to [DeBruijn, 1981]. For other values of $\mathbf{s}$ we get what is called *generalized Penrose tilings.*

2. MATHEMATICAL DIFFRACTION (SEE [7, Section 7])

A sharp diffraction picture has been the hallmark of aperiodic order. How do we describe it mathematically? In our idealized world, when atoms are replaced by points, we consider the so-called *Dirac comb* of Λ,

$$\delta_\Lambda := \sum_{x \in \Lambda} \delta_x.$$

For $r > 0$ we calculate the *autocorrelation* of δ_Λ restricted to the ball $B_r = B_r(0)$:

$$\delta_{\Lambda \cap B_r} * \widetilde{\delta}_{\Lambda \cap B_r} = \sum_{x,y \in \Lambda \cap B_r} \delta_{x-y}.$$

Here the over-tilde indicates changing the sign of the argument. The absolute value of the Fourier transform of the last expression represents the scattering intensity of the diffraction pattern of the *finite* set of scatterers in the ball B_r. In order to consider the diffraction of the entire Λ, we need to let $r \to \infty$, after normalizing by the volume:

$$\gamma = \lim_{r \to \infty} \frac{1}{\mathrm{Vol}(B_r)} \sum_{x,y \in \Lambda \cap B_r} \delta_{x-y}.$$

We will assume that the limit distribution exists in the *vague topology*, i.e., this limit exists when taken against rapidly decreasing test functions. One can show that if Λ has Uniform Cluster Frequencies, then

$$\gamma = \sum_{z \in \Lambda - \Lambda} \nu(z) \delta_z,$$

where $\nu(z)$ is the frequency of the cluster $\{x, x+z\}$ in Λ. The distribution γ is called the *auto-correlation measure* of Λ. It is positive-definite, hence its Fourier transform $\widehat{\gamma}$ is a positive measure by Bochner's Theorem. **The measure $\widehat{\gamma}$ gives the diffraction pattern of Λ.** It can be decomposed into the discrete (or pure point) part, called the *Bragg spectrum*, and continuous part.

2.1. Connection of the diffraction spectrum to the dynamical spectrum.

To relate the autocorrelation of δ_Λ to spectral measures we need to do some "smoothing." Let $\omega \in \mathcal{C}_0(\mathbb{R}^d)$, that is, ω is continuous and has compact support. Denote

$$\rho_{\omega,\Lambda'} := \omega * \delta_{\Lambda'}$$

and let

$$f_\omega(\Lambda') := \rho_{\omega,\Lambda'}(0) \quad \text{for} \quad \Lambda' \in X_\Lambda.$$

Lemma 2.1. *$f_\omega \in \mathcal{C}(X_\Lambda)$.*

Proof. We have

$$f_\omega(\Lambda') = \int \omega(-x)\, d\delta_{\Lambda'}(x) = \sum_{x \in -\mathrm{supp}(\omega) \cap \Lambda'} \omega(-x).$$

The continuity of f_ω follows from the continuity of ω and the definition of topology on X_Λ. □

Denote by $\gamma_{\omega,\Lambda}$ the autocorrelation of $\rho_{\omega,\Lambda}$. Assuming that there is a unique autocorrelation measure γ, we have

$$\gamma_{\omega,\Lambda} = (\omega * \widetilde{\omega}) * \gamma.$$

Lemma 2.2. ([Dworkin '93], see also [2]) *The spectral measure of f_ω satisfies*

$$\sigma_{f_\omega} = \widehat{\gamma_{\omega,\Lambda}}.$$

Proof. By definition, $f_\omega(-x+\Lambda) = \rho_{\omega,\Lambda}(x)$. Therefore,

$$\begin{aligned} \gamma_{\omega,\Lambda}(x) &= \lim_{r\to\infty} \frac{1}{\mathrm{Vol}(B_r)} \int_{B_r} \rho_{\omega,\Lambda}(x+y)\overline{\rho_{\omega,\Lambda}(y)}\,dy \\ &= \lim_{r\to\infty} \frac{1}{\mathrm{Vol}(B_r)} \int_{B_r} f_\omega(-x-y+\Lambda)\overline{f_\omega(-y+\Lambda)}\,dy \\ &= \int_{X_\Lambda} f_\omega(-x+\Lambda')\overline{f_\omega(\Lambda')}\,d\mu(\Lambda') \\ &= \langle U_x f_\omega, f_\omega\rangle\,, \end{aligned} \tag{2.1}$$

where $U_x f(\Lambda') = f(\Lambda' - x)$ is the unitary (Koopman) operator on $L^2(X_\Lambda, \mu)$ associated with the shift by x. Here the third equality is the main step; it follows from unique ergodicity and the continuity of f_ω. Thus,

$$\widehat{\gamma_{\omega,\Lambda}} = \widehat{(U_{(\cdot)} f_\omega, f_\omega)} = \sigma_{f_\omega},$$

and the proof is finished. □

The introduction of the function f_ω and the series of equations (2.1) is often called "Dworkin's argument".

Lemma 2.2 implies, essentially, that the diffraction spectrum is always a "part" of the dynamical spectrum. In particular, (a) if the dynamical spectrum is pure discrete, then the diffraction spectrum is pure discrete and (b) every Bragg peak must be an eigenvalue. The latter implies that if the dynamical system has no nontrivial eigenvalues, then there are no Bragg peaks except at the origin. The following was proved in [3].

Theorem 2.3. *Suppose that the Delone set Λ has FLC and Uniform Cluster Frequencies. Then the following are equivalent:*

(i) *Λ has pure discrete dynamical spectrum;*

(ii) *δ_Λ has pure point diffraction spectrum.*

About the proof. (i) ⇒ (ii) This is essentially proved by [Dworkin '93], see also [2]. By Lemma 2.2, pure point dynamical spectrum implies that $\widehat{\gamma_{\omega,\Lambda}}$ is pure point for any $\omega \in \mathcal{C}_0(\mathbb{R}^d)$. Note that

$$\widehat{\gamma_{\omega,\Lambda}} = |\widehat{\omega}|^2 \widehat{\gamma}.$$

Choosing a sequence $\omega_n \in \mathcal{C}_0(\mathbb{R}^d)$ converging to the delta measure δ_0 in the vague topology, we can conclude that $\widehat{\gamma}$ is pure point as well, as desired. This approximation step requires some care.

(ii) ⇒ (i) This is proved using the group property of the point spectrum, i.e., the product of eigenfunctions is an eigenfunction. It is largely a generalization of an argument in [Queffelec, Prop. IV.21], see [3] for details. □

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