Diffraction and discrete geometry

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The Plan

- Introduction

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- Periodic sets: Pure point diffraction via Poisson summation formula

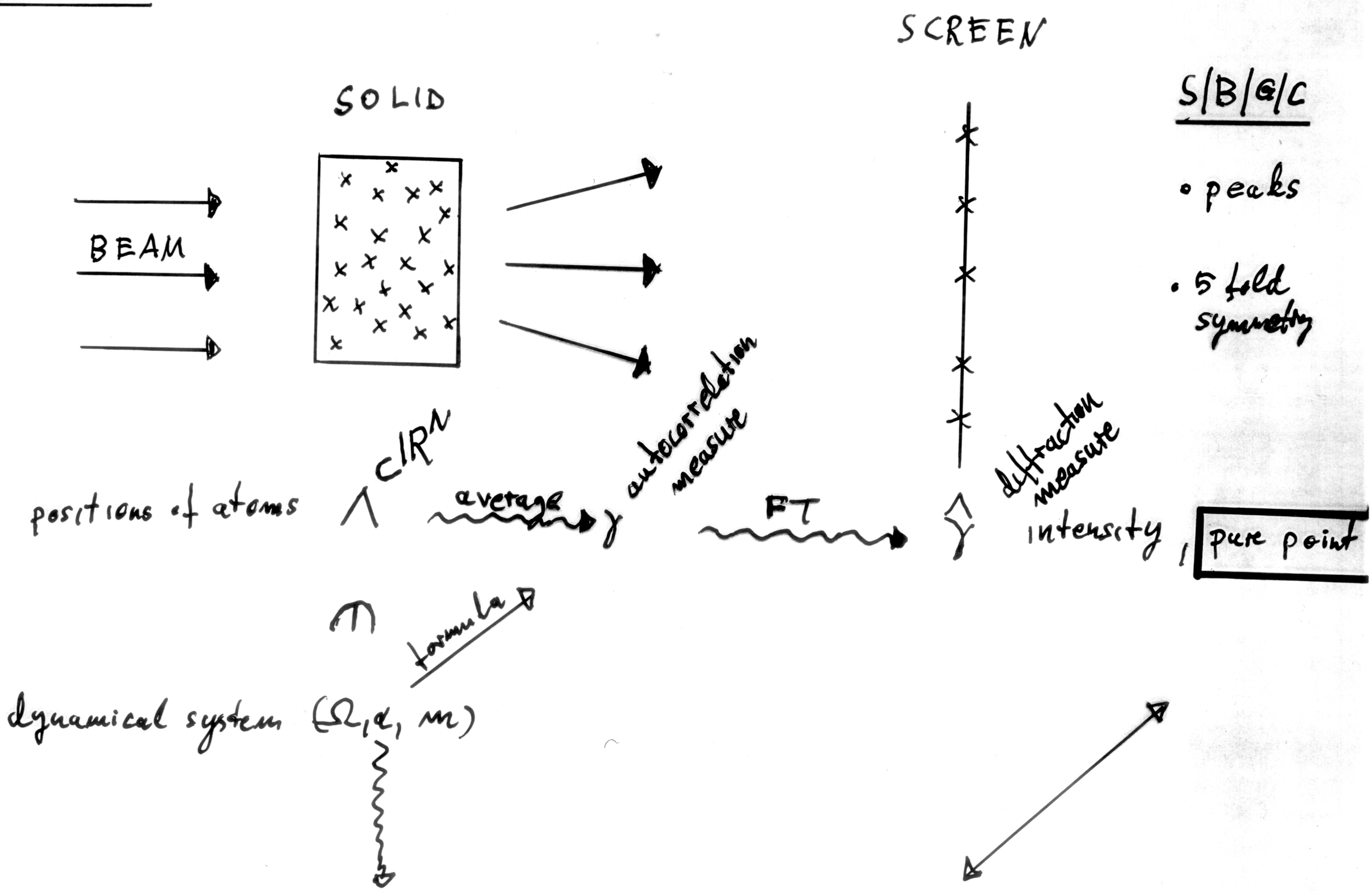
- Model sets: Pure point diffraction via almost periodicity

- Random sets: Appearance of an absolutely continuous component

- Difffraction and dynamical systems and all that....

Introduction

DIFFRACTION



$T : \mathbb{R}^N \longrightarrow \mathcal{U}(L^2(\Omega, m))$, T pure point

$(T_x f)(w) = f(\alpha_{-x} w)$

<u>Simplest case</u> $\Lambda \subset \mathbb{R}^N$ finite $\rightsquigarrow$ Dirac comb $\delta_\Lambda = \sum_{x\in\Lambda} \delta_x$

$$
\begin{array}{ccc}
\sum_{x\in\Lambda}\delta_x = \delta_\Lambda & \xrightarrow{\quad * \quad} & \delta_\Lambda * \delta_{-\Lambda} = \sum_{x,y\in\Lambda} \delta_{x-y} \\
\Big\downarrow \text{FT} & & \Big\downarrow \text{FT} \\
\sum_{x\in\Lambda} e^{-2\pi i x\xi} = F(\delta_\Lambda) & \xrightarrow{\quad |\cdot|^2 \quad} & I_\Lambda = \sum_{x,y\in\Lambda} e^{-2\pi i (x-y)\xi}
\end{array}
$$

Prerequisites

Measures and convolutions

G locally compact Abelian group, e.g. $\mathbb{R}^N$, $\mathbb{Z}^N$, $\mathbb{T}^N := \mathbb{R}^N/\mathbb{Z}^N$.

Definition 1. *A (positive) measure on G is a linear map*

$$\mu : C_c(G) \longrightarrow \mathbb{C}$$

satisfying $\mu(\varphi) \geq 0$, whenever $\varphi \geq 0$.

Notation: $\int \varphi d\mu = \int \varphi(x) d\mu(x) = \mu(\varphi)$.

Example. Lebesgue measure on $\mathbb{R}^N$ $\varphi \mapsto \int \varphi(x) dx$.

Example. $\delta_x : C_c(G) \longrightarrow \mathbb{C}$, $\varphi \mapsto \varphi(x)$ for $x \in G$.

Example. $\Lambda \in G$ finite. $\delta_\Lambda = \sum_{x \in \Lambda} \delta_x$, i. e.

$$\delta_\Lambda : C_c(G) \longrightarrow \mathbb{C}, \ \ \delta_\Lambda(\varphi) = \sum_{x \in \Lambda} \varphi(x).$$

Example. $G = \mathbb{R}^N$. $\delta_{\mathbb{Z}^N} = \sum_{x \in \mathbb{Z}^N}$, i. e.

$$\delta_{\mathbb{Z}^N} : C_c(\mathbb{R}^N) \longrightarrow \mathbb{C}, \ \delta_{\mathbb{Z}^N}(\varphi) := \sum_{x \in \mathbb{Z}^N} \varphi(x).$$

Definition 2. *A measure is called bounded or finite if it can be extended to $C_b(G)$. (" $\mu(1) < \infty$").*

Example. $G = \mathbb{R}$, $c_n \geq 0$, with $\sum_{n=1}^{\infty} c_n < \infty$. Then $\sum_{n \in \mathbb{N}} c_n \delta_n$ is a finite measure.

Definition 3. *A measure μ on G is called translation bounded if for one (all) $\varphi \in C_c(G)$ with $\varphi \geq 0$, $\varphi \neq 0$, there exists an $C_\varphi \geq 0$ with*

$$\mu(\varphi(\cdot - x)) \leq C_\varphi$$

for all $x \in G$.

Example. $\Lambda \subset \mathbb{R}^N$ uniformly discrete (i.e. exists an $r > 0$ with $\|x - y\| \geq 2r$ for all $x, y \in \Lambda$ with $x \neq y$). Then,

$$\delta_\Lambda : C_c(\mathbb{R}^N) \longrightarrow \mathbb{C}, \ \varphi \mapsto \sum_{x \in \Lambda} \varphi(x),$$

is a translation bounded measure.

Example. $G = \mathbb{R}^N$. $\delta_{\mathbb{Z}^N}$.

Definition 4. *For measures* μ *and* ν *the convolution* $\mu * \nu$ *is the measure defined by*

$$\mu * \nu(\varphi) = \int \int \varphi(x+y) d\mu(x) d\nu(y).$$

Example. $\delta_x * \delta_y = \delta_{x+y}$.

Example. $\Lambda \subset \mathbb{R}^N$ finite:

$$\delta_\Lambda * \delta_{-\Lambda} = \left(\sum_{x \in \Lambda} \delta_x \right) * \left(\sum_{y \in \Lambda} \delta_{-y} \right) = \sum_{x,y \in \Lambda} \delta_{x-y}.$$

The Fourier transform on $\mathcal{S}$

The Schwartz space $\mathcal{S} := \mathcal{S}(\mathbb{R}^N)$ is defined by

$$\{\varphi \in C^\infty(\mathbb{R}^N) : p_k(\varphi) < \infty \text{ for all } k \in \mathbb{N}\},$$

where

$$p_k(\varphi) := \sup_{x\in\mathbb{R}^N, \alpha_1+\cdots\alpha_N\leq k} \{(1+|x|^k)|\partial_{x_1}^{\alpha_1}\cdots\partial_{x_N}^{\alpha_N}\varphi(x)|\}.$$

For $\varphi, \psi \in \mathcal{S}$, we define

$$\mathcal{F}(\varphi)(\xi) := \widehat{\varphi}(\xi) := \int e^{-2\pi i\xi\cdot x}\varphi(x)dx$$

$$\check{\mathcal{F}}(\psi)(x) := \check{\psi}(x) := \int e^{2\pi i\xi\cdot x}\psi(\xi)d\xi.$$

and

$$\varphi * \psi(x) := \int \varphi(x-y)\psi(y)dy.$$

Theorem 5. *$\mathcal{F} : \mathcal{S} \longrightarrow \mathcal{S}$ is bijective with inverse $\check{\mathcal{F}}$. Moreover,*

$$\mathcal{F}(\varphi * \psi) = \mathcal{F}(\varphi)\mathcal{F}(\psi), \ \ \mathcal{F}(\mathrm{e}^{2\pi i\eta\cdot}\varphi)(\xi) = \mathcal{F}(\varphi)(\xi-\eta).$$

$\mathcal{S}(\mathbb{T}^N) := C^\infty(\mathbb{T}^N) \simeq \{\varphi \in C^\infty(\mathbb{R}^N) :\ \mathbb{Z}^N\text{−periodic}\}$,

$\mathcal{S}(\mathbb{Z}^N) := \{\varphi : \mathbb{Z}^N \longrightarrow \mathbb{C} : \sup(1+|n|^k)|\varphi(n)| < \infty \ all\ k \in \mathbb{N}\}$.

Define

$$(\mathcal{F}_{\mathbb{T}^N}\varphi)(k) := \int_{\mathbb{T}^N} e^{-2\pi i k\cdot q}\varphi(q)dq$$

$$(\mathcal{F}_{\mathbb{Z}^N}\psi)(q) := \sum_{k\in\mathbb{Z}^N} e^{2\pi i k\cdot q}\psi(k).$$

Theorem 6. *$\mathcal{F}_{\mathbb{T}^N} : \mathcal{S}(\mathbb{T}^N) \longrightarrow \mathcal{S}(\mathbb{Z}^N)$ is bijective with inverse $\mathcal{F}_{\mathbb{Z}^N}$.*

Two useful formulae:

For $\varphi \in \mathcal{S}$, define $\widetilde{\varphi}$ by $\widetilde{\varphi}(x) := \overline{\varphi}(-x)$. Then, $\mathcal{F}(\widetilde{\varphi}) = \overline{\mathcal{F}(\varphi)}$. In particular,

$$\mathcal{F}(\varphi * \widetilde{\varphi}) = |\mathcal{F}(\varphi)|^2$$

and

$$\mathcal{F}(\psi * \widetilde{\psi})(\xi) = |\mathcal{F}(\varphi)|^2(\xi - \eta)$$

for $\psi = e^{2\pi i\eta\cdot}\varphi$.

Distributions and measures

Definition 7. *A linear map*

$$\phi : \mathcal{S} \longrightarrow \mathbb{C}$$

is called a tempered distribution if $\phi(\varphi_n) \longrightarrow \phi(\varphi)$ *whenever* $p_k(\varphi_n - \varphi) \longrightarrow 0$*,* $n \to \infty$*, for every* $k \in \mathbb{N}$*. The set of all tempered distributions is denoted by* $\mathcal{S}'$*.*

Example. If g is a bounded function on $\mathbb{R}^N$, then ϕ_g with

$$\phi_g(\varphi) := \int \varphi(x) g(x) dx$$

belongs to $\mathcal{S}'$.

Example. If μ is a translation bounded measure on $\mathbb{R}^N$, then ϕ with

$$\phi_\mu(\varphi) := \int \varphi d\mu$$

belongs to $\mathcal{S}'$ and satisfies $\phi_\mu(|\varphi|^2) \geq 0$ for every $\varphi \in \mathcal{S}$.

Proposition 8. *Let* $\phi \in \mathcal{S}'$ *be given with* $\phi(|\varphi|^2) \geq 0$ *for every* $\varphi \in \mathcal{S}$*. Then* $\phi = \phi_\mu$ *for a suitable measure* μ*.*

On $\mathcal{S}'$ we define the Fourier transform $\mathcal{F}$ by

$$\mathcal{F} : \mathcal{S}' \longrightarrow \mathcal{S}', \ \ \mathcal{F}(\phi)(\varphi) := \phi(\widehat{\varphi}).$$

Example. μ finite measure. Then,

$$\mathcal{F}(\mu)(\xi) = \int e^{-2\pi i \xi \cdot x} d\mu(x).$$

In particular, $\mathcal{F}(\delta_x)(\xi) = e^{-2\pi i \xi \cdot x}$.

Proposition 9. *μ, ν finite measures. Then,*

$$\mathcal{F}(\mu * \nu) = \mathcal{F}(\mu)\mathcal{F}(\nu).$$

Proposition 10. *$\varphi \in C_c^\infty(\mathbb{R}^N)$, γ translation bounded measure,*

$$(\varphi * \gamma)(x) := \int \varphi(x - y) d\gamma(y).$$

Then,

$$\mathcal{F}(\varphi * \gamma) = \widehat{\varphi}\widehat{\gamma}.$$

Poisson summation formula and diffraction for crystallographic sets

Theorem 11. *(PSF) Let Γ be a lattice in $\mathbb{R}^N$ with dual lattice Γ^* and density dens(Γ). Then,*

$$\widehat{\delta_\Gamma} = \textit{dens}(\Gamma)\, \delta_{\Gamma^*}.$$

Definition 12. $\Lambda \subset \mathbb{R}^N$ *is called crystallographic if it is uniformly discrete and invariant under a lattice Γ. Thus, $\Lambda = F + \Gamma$ with a lattice Γ and F finite.*

Theorem 13. $\Lambda = F + \Gamma$ *crystallographic. Then,*

$$\widehat{\delta_\Lambda} = \sum_{k \in \Gamma^*} c_k \delta_k$$

with $c_k = \textit{dens}(\Gamma)\, \widehat{\delta_F}(k)$.

Note: In the situation of the theorem it is natural to define

$$I := I_\Lambda := \sum_{k \in \Gamma^*} |c_k|^2 \delta_k.$$

Diffraction for infinite sets: General framework

(following Hof '95 a, see Cowley '95 as well)

For $n \in \mathbb{N}$ let C_n be the cube in $\mathbb{R}^N$ with side length $2n$ centred in the origin.

The autocorrelation measure

Definition 14. *$\Lambda \subset \mathbb{R}^N$ uniformly discrete. Then, the autocorrelation γ of Λ is defined by*

$$\gamma := \gamma_\Lambda := vague - \lim_{n\to\infty} \frac{1}{|C_n|} \delta_{\Lambda\cap C_n} * \delta_{-\Lambda\cap C_n}$$

(if the limit exists).

Notation and note:

$$\begin{aligned}\gamma_n : &= \frac{1}{|C_n|}\delta_{\Lambda\cap C_n} * \delta_{-\Lambda\cap C_n} = \frac{1}{|C_n|}\sum_{x,y\in\Lambda\cap C_n}\delta_{x-y}\\ &= \sum_{z\in\Lambda-\Lambda}\frac{\left(\sum_{x,y\in\Lambda\cap C_n, x-y=z} 1\right)}{|C_n|}\delta_z.\end{aligned}$$

Proposition 15. *Λ uniformly discrete with minimal distance $2r$. Then,*

$$\gamma(B_s(0)) = dens(\Lambda)$$

for every $s < r$.

Example. $\Lambda = \Gamma$ lattice in $\mathbb{R}^N$. Then,

$$\gamma_\Gamma = \text{dens}(\Gamma)\delta_\Gamma.$$

In particular, $\gamma_{\mathbb{Z}^N} = \delta_{\mathbb{Z}^N}$.

Example. $\Lambda = F + \Gamma$ crystallographic. Then,

$$\gamma_\Lambda = \text{dens}(\Gamma)\delta_F * \delta_{-F} * \delta_\Gamma.$$

Recall: A measure μ is called positive definite if $\mu(\varphi * \widetilde{\varphi}) \geq 0$ for all $\varphi \in C_c(G)$. $\check{\mu}$ is the measure defined by

$$\int \varphi(x) d\check{\mu}(x) = \int \varphi(-x) d\mu(x).$$

Proposition 16. *Let γ be the autocorrelation of Λ.*

(a) $\gamma = \check{\gamma}$.

(b) γ is translation bounded.

(c) γ is positive definite.

The autocorrelation and finite local complexity

Question: $\gamma = \gamma_\Lambda$. Is

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

with suitable $\eta(z) \geq 0$?

Example. Let $\Lambda \subset \mathbb{R}$ be given by

$$\Lambda = \{0\} \cup \{n + \frac{1}{n+1} : n \in \mathbb{N}\} \cup \{-n - \frac{1}{1+n} : n \in \mathbb{N}\}.$$

Then, $\gamma_\Lambda = \gamma_\mathbb{Z} = \delta_\mathbb{Z}$.

Proposition 17. *If* $\sharp(\Lambda - \Lambda) \cap B_R(0) < \infty$ *for every* $R > 0$*, then* $\gamma = \sum_{z \in \Lambda - \Lambda} \eta(z) \delta_z$ *(if* γ *exists).*

Lemma 18. *For* $\Lambda \subset \mathbb{R}^N$ *uniformly discrete the following assertions are equivalent:*

(i) $\sharp(\Lambda - \Lambda) \cap B_R(0) < \infty$ *for every* $R > 0$*.*

(ii) $\Lambda - \Lambda$ *is discrete and closed.*

(iii) Λ *is of finite local complexity i.e.*

$$\sharp\{(\Lambda - x) \cap B_R(0) : x \in \Lambda\} < \infty$$

for all $R > 0$*.*

The diffraction measure

Theorem 19. *Let γ be the autocorrelation of $\varLambda$. Then, $\widehat{\gamma}$ is a translation bounded measure and*

$$\widehat{\gamma} = vague - \lim_{n\to\infty} \frac{1}{|C_n|} I_{\varLambda\cap C_n},$$

where $I_{\varLambda\cap C_n} = \mathcal{F}(\delta_{\varLambda\cap C_n} * \delta_{-\varLambda\cap C_n}) = |\mathcal{F}(\delta_{\varLambda\cap C_n})|^2$.

Definition 20. *$\varLambda \subset \mathbb{R}^N$ uniformly discrete with autocorrelation γ. Then, $\widehat{\gamma}$ is called the diffraction measure of $\varLambda$.*

Example. $\varLambda = \varGamma$ lattice. Then,

$$\widehat{\gamma} = (\mathrm{dens}(\varGamma))^2\, \delta_{\varGamma^*}.$$

Example. $\varLambda = F + \varGamma$ crystallographic. Then,

$$\widehat{\gamma} = \sum_{k\in\varGamma^*} m_k \delta_k$$

with $m_k = (\mathrm{dens}(\varGamma))^2 |\widehat{\delta_F}|^2(k)$.

Cut and project schemes and model sets

(going back to Meyer '72, see e.g. Moody '00 and Schlottmann '00 as well).

A *cut and project scheme* $(\mathbb{R}^N, H, \widetilde{L})$ is given by:

$$\begin{array}{ccccc}
\mathbb{R}^N & \xleftarrow{\ \pi\ } & \mathbb{R}^N \times H & \xrightarrow{\ \pi_{\text{int}}\ } & H \\
\cup & & \cup & & \cup \text{dense} \\
L & \xleftarrow{\ 1-1\ } & \tilde{L} & \longrightarrow & L^\star \\
\| & & & & \| \\
L & & \xrightarrow{\qquad \star \qquad} & & L^\star
\end{array}$$

where

- H is a locally compact, σ-compact group, called the *internal space*,
- $\tilde{L}$ is a *lattice* in $\mathbb{R}^N \times H$,
- π and π_{int} are the canonical projections.
- π is one-to-one and π_{int} has dense range.

Then, $L := \pi(\widetilde{L})$ and $L^\star := \pi_{\text{int}}(\widetilde{L})$ are groups. As π is one-to-one, there is a uniquely defined group homomorphism

$$\star : L \longrightarrow L^\star$$

such that $(x,h) \in \widetilde{L}$ if and only if $h = x^\star$.

Given an cut and project scheme and a so called window $W \subset H$ we define

$$\curlywedge(W) \;:=\; \{x \in L : x^\star \in W\}.$$

Example. Fibonacci chain.

Example. Penrose tiling.

Let a cut and project scheme $(\mathbb{R}^N, H, \widetilde{L})$ be given and

$$\curlywedge(W) := \{x \in L : x^\star \in W\}.$$

Proposition 21. *$\emptyset \neq V \subset H$ open. Then, $\curlywedge(V)$ is relatively dense.*

Proposition 22. *$K \subset H$ compact. Then, $\curlywedge(K)$ is uniformly discrete.*

Definition 23. *If W is a non-empty compact subset of H, which is the closure of its interior, then $\curlywedge(W)$ is called a model set. A model set is called* regular *if ∂W has Haar measure* 0 *in H,*

Theorem 24. *Let Λ be a model set. Then, Λ is uniformly discrete and relatively dense. Moreover, $\Lambda - \Lambda$ is uniformly discrete as well. In particular, Λ has finite local complexity.*

Definition 25. *A set $\Lambda \subset \mathbb{R}^N$ is called a Meyer set if $\Lambda - \Lambda$ is uniformly discrete.*

Theorem 26. *(Meyer) Any Meyer set is a subset of a model set.*

See Lagarias '96, Moody ' 97, Moody '00 for further discussion as well.

Uniform distribution

Recall: $f : H \longrightarrow \mathbb{R}$ is called Riemann-integrable if for every $\varepsilon > 0$, there exist $\varphi, \psi \in C_c(H)$ with

$$\varphi \leq f \leq \psi \text{ and } \int (\psi - \varphi) dh \leq \varepsilon.$$

Note:

- Any Riemann-integrable function vanishes outside a compact set.

- The characteristic function χ_W of a compact set W is Riemann-integrable if and only if the boundary ∂W of W has Haar measure zero.

Theorem 27. *(Uniform distribution) Let* $(\mathbb{R}^N, H, \widetilde{L})$ *be a cut and project scheme. Then, there exists a* $c > 0$ *such that*

$$\lim_{n\to\infty} \frac{1}{|C_n|} \sum_{x\in C_n\cap L} f(x^\star) = c \int_H f(h)dh$$

for every Riemann-integrable $f : H \longrightarrow \mathbb{R}$.

Going back to Weyl '16, see Schlottmann '98, Baake/Moody '00, Moody '02.

Almost periodic functions and a result of Wiener

Lemma 28. *For $a \in C_b(\mathbb{R}^N)$ the following assertions are equivalent:*

(i) $\overline{\{a(\cdot - t) : t \in \mathbb{R}^n\}}$ *is compact in* $(C_b(\mathbb{R}^N), \|\cdot\|_\infty)$.

(ii) For each $\varepsilon > 0$, the set

$$\{t \in \mathbb{R}^N : \|a(\cdot - t) - a\|_\infty \le \varepsilon\}$$

is relatively dense in $\mathbb{R}^N$.

Definition 29. *A function satisfying the conditions of the previous lemma is called almost periodic.*

Notation: The set of ε-almost-periods appearing in (ii) is denoted by AP(ε).

Example. For each $\xi \in \mathbb{R}^N$ the function $y \mapsto e^{-2\pi i \xi \cdot y}$ is almost periodic.

Theorem 30. *The almost periodic functions form a closed sub algebra of* $(C_b(\mathbb{R}^N), \|\cdot\|_\infty)$, *which is closed under taking complex conjugates.*

Recall: μ measure on $\mathbb{R}^N$. Then,

$$\mu = \mu_c + \mu_{pp},$$

where $\mu_c(\{x\}) = 0$ for every $x \in \mathbb{R}^N$ and

$$\mu_{pp} = \sum_{n=1}^{\infty} c_n \delta_{x_n}$$

with suitable $x_n \in \mathbb{R}^N$ $c_n \geq 0$, $n \in \mathbb{N}$. If μ is finite, then $\sum_{n=1}^{\infty} c_n < \infty$.

Theorem 31. *(Wiener) Let μ be a finite measure on $\mathbb{R}^N$. Then,*

$$\lim_{n\to\infty} \frac{1}{|C_n|} \int_{C_n} |\widehat{\mu}(\xi)|^2 d\xi = \sum_{x\in\mathbb{R}^N} |\mu(\{x\})|^2.$$

Theorem 32. *(Wiener) Let μ be a finite measure on $\mathbb{R}^N$. Then, μ is a pure point measure if and only if $\widehat{\mu}$ is almost periodic.*

Diffraction for model sets

(following Baake/Moody '04)

Let a cut and project scheme $(\mathbb{R}^N, H, \widetilde{L})$ be given.

Proposition 33. *Let $W \subset H$ be given such that χ_W is Riemann-integrable and set $\varLambda := \curlywedge(W)$. Then,*

$$\gamma_\varLambda = \sum_{z \in \varLambda - \varLambda} \eta(z)\delta_z$$

with $\eta(z) = \int_H \chi_W(h)\chi_W(h - z^\star)dh = \chi_W * \chi_{-W}(z^\star)$.

Note: If we define $\eta(z) = \chi_W * \chi_{-W}(z^\star)$ for arbitrary $z \in L$, then $\eta(z) = 0$ for $z \notin \varLambda - \varLambda$. In particular, we have

$$\gamma_\varLambda = \sum_{z \in L} \eta(z)\delta_z.$$

Lemma 34. *Let $W \subset H$ be given such that χ_W is Riemann-integrable and set $\varLambda := \curlywedge(W)$. Let $\gamma_\varLambda = \sum_{x \in L} \eta(z)\delta_z$ be the associated autocorrelation. Then, for every $\varepsilon > 0$, the set*

$$\{z \in L : |\eta(x - z) - \eta(x)| \leq \varepsilon \text{ for all } x \in L\}$$

is relatively dense in $\mathbb{R}^N$.

We can now state the main result on diffraction for model sets.

Theorem 35. *Let $W \subset H$ be compact with non-empty interior and boundary of Haar measure zero. Set $\varLambda := \curlywedge(W)$. Then, $\varLambda$ is pure point diffractive i.e. $\widehat{\gamma}$ is a pure point measure.*

Note: Proof shows: $\widehat{\gamma}$ pure point if and only if $\gamma * \varphi * \widetilde{\varphi}$ almost periodic for all $\varphi \in C_c^\infty$.

(At least implicitly) formulated soon after discovery of quasicrystals. Proven in Hof '98, (see Hof '95 a) as well), Schlottmann '00. Proof given here follows Baake/Moody '04.

Calculating $\widehat{\gamma}$ (following Hof '95 a).

Assume the situation of the previous theorem.

Define

$\widetilde{L}^{\perp} := \{(\xi,\sigma) \in \mathbb{R}^N \times \widehat{H} : \forall (l,l^*) \in \widetilde{L}\; e^{-2\pi i \xi l}\sigma(l^\star) = 1\}$.

Then, $\star$ induces a map

$$\star : \pi_{\mathbb{R}^N}(\widetilde{L}^{\perp}) \longrightarrow \pi_{\widehat{H}}(\widetilde{L}^{\perp})$$

such that $(\xi,\sigma) \in \widetilde{L}^{\perp}$ if and only if $\sigma = \xi^\star$.

Proposition 36. *(a) Let $\xi \in \pi_{\mathbb{R}^N}(\widetilde{L}^{\perp})$ be given and $\sigma := \xi^\star$. Then,*

$$c_\xi := \lim_{n\to\infty} \frac{1}{|C_n|} \sum_{x \in (t+C_n)\cap \varLambda} e^{-2\pi i \xi \cdot x} = \int_W \sigma(h)dh$$

uniformly in $t \in \mathbb{R}^N$.

(b) Let $\xi \notin \pi_{\mathbb{R}^N}(\widetilde{L}^{\perp})$ be given. Then,

$$c_\xi := \lim_{n\to\infty} \frac{1}{|C_n|} \sum_{x \in (t+C_n)\cap \varLambda} e^{-2\pi i \xi \cdot x} = 0$$

uniformly in $t \in \mathbb{R}^N$.

Theorem 37. $\widehat{\gamma} = \sum_{(\xi,\sigma)\in\widetilde{L}^{\perp}} |c_\xi|^2 \delta_\xi$.

Note: $\widetilde{L}^{\perp}$ is canonically isomorphic to $(\mathbb{R}^N \times H)/\widetilde{L}$.

See Bombieri/Taylor '86 as well.

Diffraction for random sets

Bernoulli model

Choose $k \in \mathbb{Z}^N$ with probability 1/2. This yields a random set $\omega \subset \mathbb{Z}^N$. Then, for typical ω:

$$\begin{aligned} \eta(z) &= \lim_{n\to\infty} \frac{1}{|C_n|} \sharp\{x, y \in \omega \cap C_n : x - y = z\} \\ &= \begin{cases} \frac{1}{2} & : \quad z = 0 \\ & : \\ \frac{1}{4} & : \quad z \neq 0. \end{cases} \end{aligned}$$

Thus

$$\gamma = \frac{1}{4}\delta_{\mathbb{Z}^N} + \frac{1}{4}\delta_0.$$

In particular,

$$\widehat{\gamma} = \frac{1}{4}\delta_{\mathbb{Z}^N} + \frac{1}{4}.$$

Appearance of an absolutely continuous component in the spectrum!

Lattice system with disorder (following Baake/Sing '04)

Let $\omega \subset \mathbb{Z}^N$ be given such that

$$\eta(z) := \lim_{n\to\infty} \frac{1}{|C_n|} \sharp\{x, y \in \omega \cap C_n : x - y = z\}$$

exists for every $z \in \mathbb{Z}^N$. Then,

$$\gamma_\omega = \sum_{z\in\mathbb{Z}^N} \eta(z)\delta_z.$$

For Gibbsian models it turns out that (in certain energy regions)

$$\eta(z) = \frac{1}{4} + s(z)$$

with $s(z)$ rapidly decaying. Then, $\mathcal{F}_{\mathbb{Z}^N}(s)$ exists and we have

$$\widehat{\gamma} = \frac{1}{4}\delta_{\mathbb{Z}^N} + \widehat{s}.$$

Random displacement model (following Hof 95 b).

Situation: Let $\Lambda \subset \mathbb{R}^N$ be given with

- finite local complexity,

- existence of pattern frequencies, i.e.

$$\lim_{n\to\infty} \frac{1}{|C_n|} \sharp\{x \in \Lambda \cap C_n : x + P \subset \Lambda\}$$

exists for all $P \subset \mathbb{R}^N$ finite.

Let γ be the autocorrelation of Λ and

$$n_0 = \gamma(\{0\}) = \text{dens}(\Lambda).$$

Let $\{s_x\}_{x\in\Lambda}$ be independent, identically distributed random variables with values in $\mathbb{R}^N$. Denote their common distribution by ν. Set

$$\mu := \delta_\Lambda, \quad \mu' := \sum_{x\in\Lambda} \delta_{x+s_x}.$$

Theorem 38. *Assume the above situation. Then, with probability one the autocorrelation*

$$\gamma' := \lim_{n\to\infty} \frac{1}{|C_n|} \mu'|_{C_n} * \widetilde{\mu'|_{C_n}}$$

exists and

$$\gamma' = \gamma * \nu * \widetilde{\nu} + n_0(\delta_0 - \nu * \widetilde{\nu})$$

holds. In particular,

$$\widehat{\gamma'} = |\widehat{\nu}|^2 \widehat{\gamma} + n_0(1 - |\widehat{\nu}|^2).$$

Summary and warning

We have confirmed the "meta theorem"

- Order $\equiv$ pure point diffraction.
- Disorder $\equiv$ absolutely continuous diffraction component.

for three classes of examples: Periodic sets, Model sets and (certain) random sets.

However, the Bernoulli model and the Rudin-Shapiro substitution (with suitable weights) yield the same diffraction measure.

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