cut-and-project sets: diffraction and harmonic analysis

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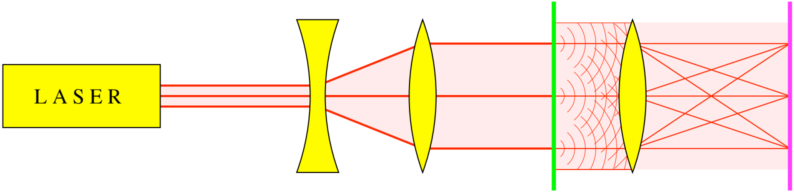
Seminaire Lotharingien de Combinatoire, March 2015

harmonic analysis?

- harmonic analysis of LCA groups
- heavy machinery, but quick proofs of fundamental results (density formula, pure point diffraction of regular model sets)
- standard tool for cut-and-project sets and Meyer sets

diffraction experiments



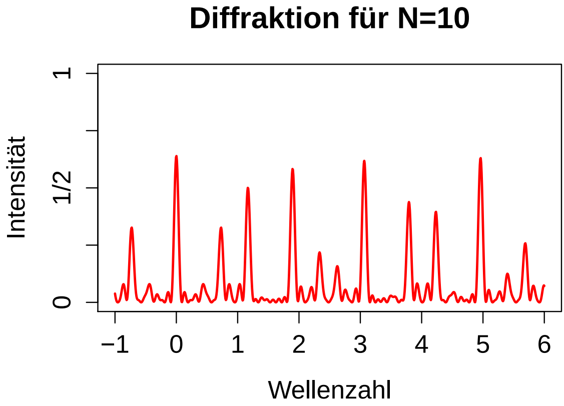
- laser or X-ray beam hits specimen (green)
- atoms emit diffraction waves (red)
- waves interfer and produce diffraction picture (purple)

Fraunhofer diffraction

optics: Kirchhoff's approximation

- atom in x emits diffraction wave, modelled by $e^{-2\pi i\, k\cdot x}$
- waves interfer additively (structure factor)
- observed intensity on screen at position k is absolute square

diffraction of the Fibonacci chain



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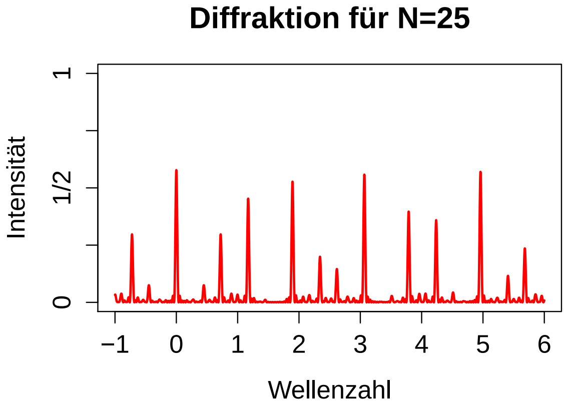

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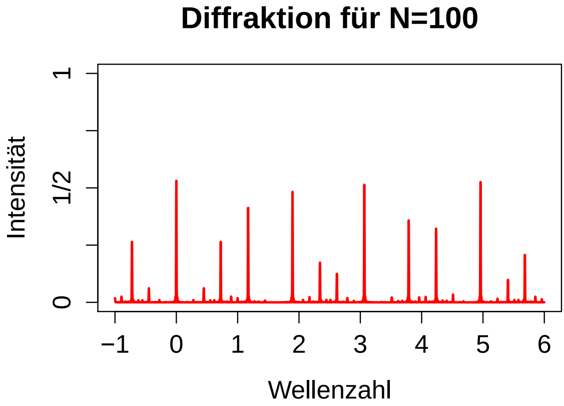

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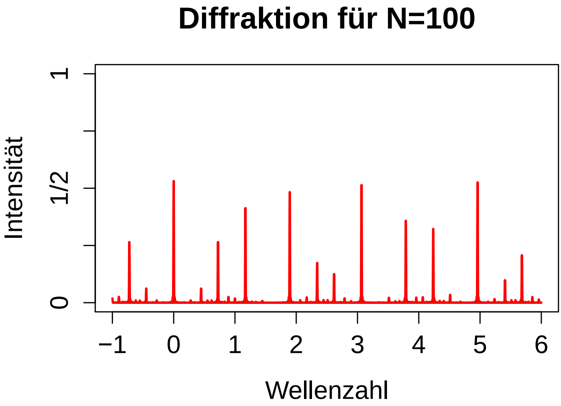
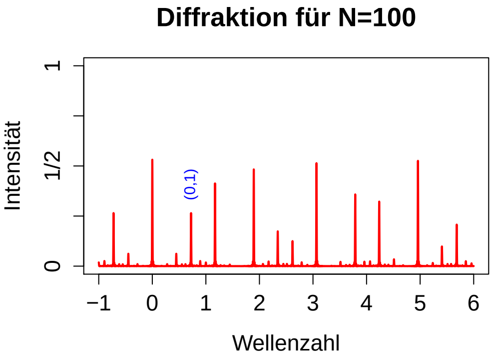


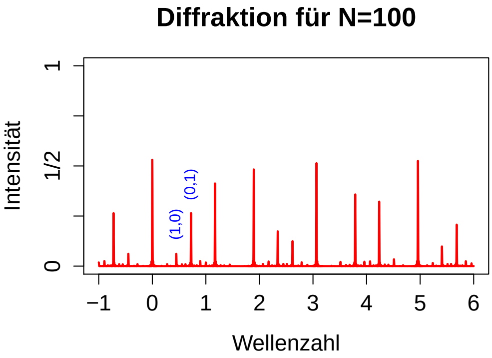
pure point diffractive?

Fibonacci chain diffraction: indexing Bragg peaks



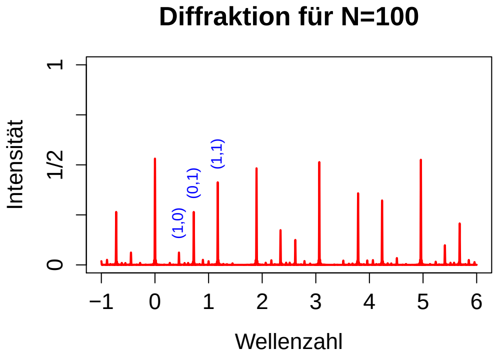
- position of peak $(0,1) \mathrel{\widehat{=}} 0.723606\ldots$

Fibonacci chain diffraction: indexing Bragg peaks



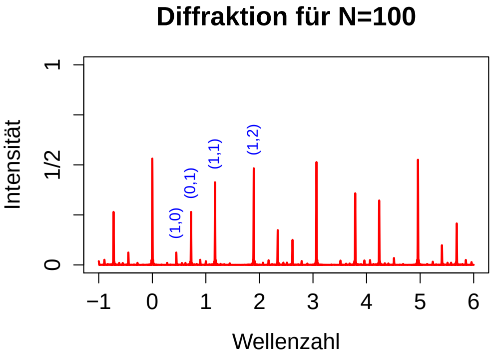
- positions of peaks: $(0,1)/(1,0) \mathrel{\widehat{=}} 1.618034\ldots =: \tau$

Fibonacci chain diffraction: indexing Bragg peaks



- peak positions: $(m,n) \mathrel{\widehat{=}} \frac{1}{c} \cdot (m + n\tau)$ where $c = 2.23606\ldots$

Fibonacci chain diffraction: indexing Bragg peaks



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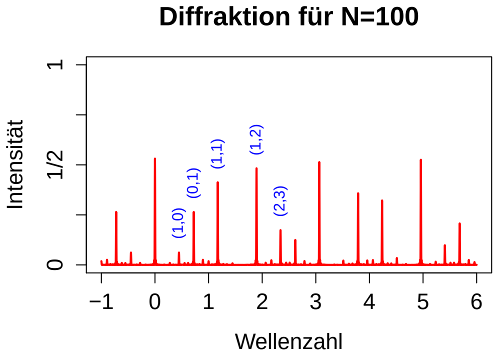

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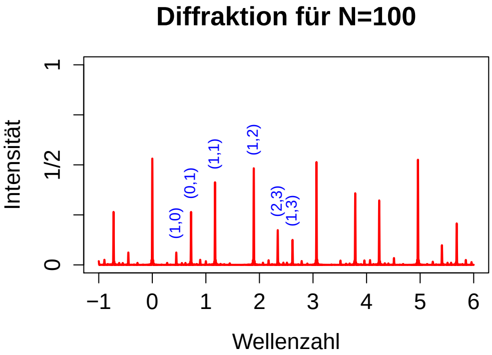

- peak positions: $(m, n) \,\widehat{=}\, \frac{1}{c} \cdot (m + n\tau)$ where $c = 2.23606\ldots$

mathematical diffraction theory

Let Λ uniformly discrete such that even $\Lambda\Lambda^{-1}$ is uniformly discrete

- $\omega = \sum_{p\in\Lambda} \delta_p$ Dirac comb of Λ
- infer diffraction of Λ from finite samples $\omega_n = \omega|_{B_n}$
- convolution theorem yields Wiener diagram

$$\begin{array}{ccc} \omega_n & \xrightarrow{\;*\;} & \omega_n * \widetilde{\omega_n} \\ \mathcal{F}\big\downarrow & & \big\downarrow\mathcal{F} \\ \widehat{\omega_n} & \xrightarrow{\;|\cdot|^2\;} & \widehat{\omega_n}\cdot\overline{\widehat{\omega_n}} \end{array}$$

$\widetilde{\omega}(f) = \omega(\widetilde{f})$ with $\widetilde{f}(x) = \overline{f(x^{-1})}$

- identify Bragg peaks and continous components from the Lebesgue decomposition of the limiting measure of $\widehat{\omega_n}\cdot\overline{\widehat{\omega_n}}$
- Fourier analysis of unbounded measures!

mathematical diffraction theory

$$\begin{array}{ccc} \omega_n & \xrightarrow{\;\;*\;\;} & \omega_n * \widetilde{\omega_n} \\ \mathcal{F}\Big\downarrow & & \Big\downarrow\mathcal{F} \\ \widehat{\omega_n} & \xrightarrow{\;|\cdot|^2\;} & \widehat{\omega_n}\cdot\overline{\widehat{\omega_n}} \end{array}$$

- Assume that the *autocorrelation* γ of ω exists as a vague limit

$$\gamma = \lim_{n\to\infty} \frac{1}{\theta(B_n)} \omega_n * \widetilde{\omega_n}$$

- Since γ is positive definite, it is transformable, and by continuity of the Fourier transform we have

$$\mathcal{F}\left(\lim_{n\to\infty} \frac{1}{\theta(B_n)} \omega_n * \widetilde{\omega_n}\right) = \lim_{n\to\infty} \mathcal{F}\left(\frac{1}{\theta(B_n)} \omega_n * \widetilde{\omega_n}\right) = \lim_{n\to\infty} \frac{1}{\theta(B_n)} \widehat{\omega_n}\cdot\overline{\widehat{\omega_n}}$$

- We work with the autocorrelation as $\widehat{\omega}$ may not be a measure.
- This is in contrast to the case Λ a lattice.

Fourier analysis on LCA groups: setup

- σ–compact LCA group G with Haar measure θ_G
- inverse function: $\widetilde{f}(x) = \overline{f(x^{-1})}$
- convolution: for $f, g \in L^1(G)$ define $f * g \in L^1(G)$ by

$$f * g(x) = \int f(y) g(y^{-1}x) \, \mathrm{d}\theta_G(y)$$

- character $\chi : G \to \mathbb{U}(1)$ continuous group homomorphism

Pontryagin dual $\widehat{G}$ and Fourier transform

- $\widehat{G}$ set of all characters with topology induced by

$$N(K,\varepsilon) = \{\chi \in \widehat{G} \mid \forall k \in K : |\chi(k) - 1| < \varepsilon\}$$

for non-empty compact $K \subset G$ and $\varepsilon > 0$

- $\widehat{G}$ LCA group with Haar measure $\theta_{\widehat{G}}$
- Fourier transforms $\widehat{f}, \check{f} : \widehat{G} \to \mathbb{C}$ of $f \in L^1(G)$

$$\widehat{f}(\chi) = \int_G f(x)\overline{\chi(x)}\,\mathrm{d}\theta_G(x), \qquad \check{f}(\chi) = \int_G f(x)\chi(x)\,\mathrm{d}\theta_G(x)$$

- Normalise $\theta_{\widehat{G}}$ such that Plancherel's formula

$$||f||_2 = ||\widehat{f}||_2$$

is satisfied for all $f \in L^1(G) \cap L^2(G)$.

Fourier analysis of unbounded measures

$\mathcal{M}(G)$ set of Borel measures on G

Definition (cf. Argabright–de Lamadrid 74)

$\mu \in \mathcal{M}(G)$ is transformable if there exists $\widehat{\mu} \in \mathcal{M}(\widehat{G})$ such that for all $f \in C_c(G)$ such that $\check{f} \in L^1(\widehat{G})$ we have

$$\check{f} \in L^1(\widehat{\mu}), \qquad \langle \mu, f \rangle = \langle \widehat{\mu}, \check{f} \rangle .$$

- Poisson summation formula
- $\widehat{\mu}$ uniquely determined by μ
- $\widehat{\mu}$ *translation bounded*, i.e., for every compact $K \subset G$

$$\sup\{|\mu|(tK) \mid t \in G\} < \infty,$$

with $|\mu| \in \mathcal{M}(G)$ the total variation measure of μ

examples of transformable measures

- μ positive definite, i.e., for all $f \in C_c(G)$

$$\int_G f * \widetilde{f}(x)\, \mathrm{d}\mu(x) \geqslant 0$$

- for example: δ_Λ Dirac comb of a lattice $\Lambda \subset G$

$$\widehat{\delta_\Lambda} = \mathrm{dens}(\Lambda) \cdot \delta_{\Lambda^0}$$

with dual lattice $\Lambda^0 = \{\chi \in \widehat{G} \mid \chi(p) = 1 \forall p \in \Lambda\}$

classical examples

- finite measures, positive definite fctns, L^p-fctns for $p \in [1, 2]$

The function space $KL(G)$

$$KL(G) := \{f \in C_c(G) \mid \widehat{f} \in L^1(\widehat{G})\}$$

Such functions are not rare:

- If $f, g \in L^2(G)$ have compact support, then $f * g \in KL(G)$.
- example: $1_W * \widetilde{1_W}$ for relatively cpct measurable $W \subset G$.
- In fact $KL(G)$ is dense in $C_c(G)$.

character averages

Lemma

Let $\chi \in \widehat{G}$. Then for every van Hove sequence $(A_n)_{n\in\mathbb{N}}$ in G

$$\lim_{n\to\infty} \frac{1}{\theta(A_n)} \int_{A_n} \chi(x)\,\mathrm{d}\theta(x) = \delta_{\chi,e}.$$

This is obvious for $\chi = e$. Consider $\chi \neq e$ for the following proof.

- By left invariance of the Haar measure and $\chi(xy) = \chi(x)\chi(y)$

$$\int_{A_n} \chi(y)\,\mathrm{d}\theta(y) = \int_G 1_{A_n}(xy)\chi(xy)\,\mathrm{d}\theta(y) = \chi(x)\int_{x^{-1}A_n} \chi(y)\,\mathrm{d}\theta(y)$$

  Due to the van Hove property of $(A_n)_{n\in\mathbb{N}}$, we have

$$\left|\int_{x^{-1}A_n} \chi(y)\,\mathrm{d}\theta(y) - \int_{A_n} \chi(y)\,\mathrm{d}\theta(y)\right| \leqslant \theta((x^{-1}A_n)\Delta A_n) = o(\theta(A_n))$$

- Combining the above properties yields

$$|1-\chi(x)|\cdot\left|\frac{1}{\theta(A_n)}\int_{A_n} \chi(y)\,\mathrm{d}\theta(y)\right| = o(1)$$

- Lemma follows with $x \in G$ such that $\chi(x) \neq 1$. □

The discrete part of $\widehat{\mu}$ can be computed by averaging over μ:

Proposition

Let $\mu \in \mathcal{M}(G)$ be transformable and translation bounded and consider $\chi \in \widehat{G}$. Then for every van Hove sequence $(A_n)_{n\in\mathbb{N}}$ in G we have

$$\widehat{\mu}(\{\chi\}) = \lim_{n\to\infty} \frac{1}{\theta(A_n)} \int_{A_n} \overline{\chi}(x)\,\mathrm{d}\mu(x)$$

history

- Argabright–de Lamadrid 90 for $\widehat{\mu}$ transformable
- Hof 95 for euclidean G
- Lenz 09 for μ the autocorrelation measure

- w.l.o.g. for $\chi = e$ since $\widehat{\mu}(\{\chi\}) = (\delta_{\chi^{-1}} * \widehat{\mu})(\{e\}) = \widehat{\overline{\chi}\mu}(\{e\})$
- smoothing of characteristic functions:

$$f_n = \frac{1}{\theta(A_n)} \cdot 1_{A_n}, \qquad (f_n)_\varphi = \varphi * f_n,$$

where $\varphi = \psi * \widetilde{\psi}$ with $\psi \in C_c(G)$ and $\int \psi = 1$.

- Then $(f_n)_\varphi \in KL(G)$ by the above lemma, and PSF yields

$$\mu((f_n)_\varphi) = \widehat{\mu}\left(\widetilde{(f_n)_\varphi}\right)$$

- Consider the limit $n \to \infty$ on the rhs: Since

$$\widetilde{(f_n)_\varphi}(\chi) \to \delta_{\chi,e}, \qquad \left|\widetilde{(f_n)_\varphi}\right| = |\check{\varphi}| \cdot \left|\check{f_n}\right| \leqslant |\check{\varphi}|,$$

we can use dominated convergence to infer

$$\lim_{n\to\infty} \widehat{\mu}\left(\widetilde{(f_n)_\varphi}\right) = \widehat{\mu}(\delta_{\chi,e}) = \widehat{\mu}(\{e\})$$

- Indeed by the previous lemma for $\chi \neq e$ we have

$$\left|\widetilde{(f_n)_\varphi}(\chi)\right| = |\check{\varphi}(\chi)| \cdot \left|\check{f_n}(\chi)\right| \leqslant ||\varphi||_1 \cdot \left|\check{f_n}(\chi)\right| \to 0$$

Consider the limit $n \to \infty$ on the lhs of

$$\mu((f_n)_\varphi) = \widehat{\mu}\left(\widecheck{(f_n)_\varphi}\right)$$

- f_n and $(f_n)_\varphi$ differ only near the boundary of A_n, i.e.,

  $$f_n(x) \neq (f_n)_\varphi(x) \Longrightarrow x \in \partial^K A_n$$

  where $K = \mathrm{supp}(\varphi)$
- Hence by a standard estimate

  $$|\mu(f_n) - \mu((f_n)_\varphi)| \leqslant ||1 - \varphi||_\infty \cdot \frac{|\mu|(\partial^K A_n)}{\theta(A_n)}$$

- rhs vanishes by translation boundedness of μ and by the van Hove property of $(A_n)_{n\in\mathbb{N}}$. □

reminder: model sets

assumptions: G, H σ-cpct LCA groups, H metrisable

cut-and-project scheme with *star map* $()^\star : L \to L^\star$

$$\begin{array}{ccccc} G & \xleftarrow{\pi_G} & G \times H & \xrightarrow{\pi_H} & H \\ \cup & & \cup & & \cup \\ L & \xleftarrow{1\text{–}1} & \text{lattice } \mathcal{L} & \xrightarrow{\text{dense}} & L^\star \end{array}$$

projection set via *window* $W \subset H$

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

regular model set: W relatively cpct measurable, $\mathrm{vol}(\partial W) = 0$ $(\mathring{W} \neq \varnothing)$

We normalise Haar measure of H such that $\mathrm{dens}(\mathcal{L}) = 1$.

dual cut-and-project schemes

duality theory for LCA groups leads to dual cut-and-project scheme

Theorem (dual cut-and-project scheme)

Let $(G, H, \mathcal{L})$ be a cut-and-project scheme and let $\mathcal{L}^0 \in \widehat{G} \times \widehat{H}$ be the lattice dual to $\mathcal{L}$. Then $(\widehat{G}, \widehat{H}, \mathcal{L}^0)$ is also a cut-and-project scheme.

- diffraction is described within the dual cut-and-project scheme
- for euclidean groups $\widehat{G} \simeq G$ and $\widehat{H} \simeq H$

weighted model sets and transformability

for cp scheme $(G, H, \mathcal{L})$ and $h : H \to \mathbb{C}$ define *weighted model set*

$$\omega_h = \sum_{x \in L} h(x^\star)\delta_x$$

Theorem (R-Strungaru)

Let $(G, H, \mathcal{L})$ be a cut-and-project scheme and let $h \in KL(H)$. Then ω_h is a transformable measure with

$$\widehat{\omega_h} = \omega_{\check{h}}$$

Here $\omega_{\check{h}}$ is the weighted model set of the dual cut-and-project scheme $(\widehat{G}, \widehat{H}, \mathcal{L}^0)$ with weight function $\check{h} \in L^1(\widehat{H})$.

proof of transformability

for arbitrary $g \in KL(G)$ we have

$$\langle \omega_h, g \rangle = \langle \delta_{\mathcal{L}}, g \cdot h \rangle = \langle \delta_{\mathcal{L}^0}, \check{g} \cdot \check{h} \rangle = \langle \omega_{\check{h}}, \check{g} \rangle$$

- first equation: $\pi_G|_{\mathcal{L}}$ one-to-one
- second equation: PSF and $g \cdot h \in KL(G \times H)$.
- third equation: $\pi_{\widehat{G}}\big|_{\mathcal{L}^0}$ one-to-one
- equations also imply $\omega_h \in \mathcal{M}(G)$ and $\check{g} \in L^1(\omega_{\check{h}})$
- hence $\widehat{\omega_h} = \omega_{\check{h}}$ by definition

weighted model sets and density formula

Theorem (density formula)

Let $h \in C_c(H)$. Then for every van Hove sequence $(A_n)_{n\in\mathbb{N}}$

$$\lim_{n\to\infty} \frac{\omega_h(A_n)}{\theta_G(A_n)} = \int_H h(x)\mathrm{d}\theta_H(x).$$

history

- Meyer 70's for euclidean G, H via PSF (see also Matei–Meyer 10, Lev–Orlevskii 13)
- Schlottmann 98, geometric proof
- Moody 02 via dynamical systems
- Lenz–R 07 for "admissible" $h \in L^1_{bc}(H)$ via dynamical systems

weighted model sets and density formula

an immediate consequence:

Corollary

The density formula also holds for $h = 1_W$ where $W \subset H$ is relatively cpct measurable with almost no boundary $\theta_H(\partial W) = 0$.

Consider arbitrary $\varepsilon > 0$.

- Since h is Riemann integrable, we find $\varphi, \psi \in C_c(H)$ such that

$$\varphi \leqslant h \leqslant \psi, \qquad \int_H (\psi(x) - \varphi(x)) \mathrm{d}\theta_H(x) \leqslant \varepsilon/2$$

- The density formula yields for sufficiently large n the estimate

$$-\varepsilon \leqslant -\varepsilon/2 + \int \psi - \frac{\omega_\psi(A_n)}{\theta_G(A_n)} \leqslant \int h - \frac{\omega_h(A_n)}{\theta_G(A_n)} \leqslant \varepsilon/2 + \int \varphi - \frac{\omega_\varphi(A_n)}{\theta_G(A_n)} \leqslant \varepsilon$$

proof for $h \in C_c(H)$

first step: proof for $h \in KL(H)$ by PSF

- Assume that $h \in KL(H)$. Then $\widehat{\omega}_h = \omega_{\check{h}}$ and

$$\int_H h(x) \mathrm{d}\theta_H(x) = \check{h}(e) = \omega_{\check{h}}(\{e\}) = \widehat{\omega_h}(\{e\}) = \lim_{n\to\infty} \frac{\omega_h(A_n)}{\theta(A_n)}$$

second step: extension to $C_c(H)$ by approximation

- Use that $KL(H)$ is dense in $C_c(H)$.
- consider the uniformly discrete $\Lambda = \mathrm{supp}(\omega_h) \subseteq G$ and note

$$\overline{\mathrm{dens}}(\Lambda) = \limsup_{n\to\infty} \frac{1}{\theta_G(A_n)} |\Lambda \cap A_n| < \infty$$

- Take $h \in C_c(H)$, write $K = \mathrm{supp}(h)$ and fix some compact unit neighborhood U in H.

For any $g \in KL(H)$ such that $\mathrm{supp}(g) \subseteq KU$ we then have for n sufficiently large the estimate

$$\left|\int_H h(x)\mathrm{d}\theta_H(x) - \frac{\omega_h(A_n)}{\theta_G(A_n)}\right| \leqslant \left|\int_H h(x)\mathrm{d}\theta_H(x) - \int_H g(x)\mathrm{d}\theta_H(x)\right| + \\ + \left|\int_H g(x)\mathrm{d}\theta_H(x) - \frac{\omega_g(A_n)}{\theta_G(A_n)}\right| + \left|\frac{\omega_g(A_n)}{\theta_G(A_n)} - \frac{\omega_h(A_n)}{\theta_G(A_n)}\right| \\ \leqslant ||h-g||_\infty \left(\theta_H(KU) + 2\cdot\overline{\mathrm{dens}}(\Lambda)\right) + \left|\int_H g(x)\mathrm{d}\theta_H(x) - \frac{\omega_g(A_n)}{\theta_G(A_n)}\right|.$$

- Since $KL(H)$ is dense in $C_c(H)$ we find $g \in KL(H)$ (of support contained in KU) such that the first term in the above estimate does not exceed $\varepsilon/2$.
- by the density formula for $KL(H)$ the second term is also smaller than $\varepsilon/2$ if n is sufficiently large.

regular model sets are pure point diffractive

Theorem

Let $(G, H, \mathcal{L})$ be a cut-and-project scheme, and let $h = 1_W$ for $W \subset H$ relatively cpct measurable and $\theta_H(\partial W) = 0$. Then the weighted model set ω_h has autocorrelation γ and diffraction $\widehat{\gamma}$ given by

$$\gamma = \omega_{h * \widetilde{h}}, \qquad \widehat{\gamma} = \omega_{|\check{h}|^2}$$

history

- Hof 95 via harmonic analysis (euclidean G, H)
- Schlottmann 00 via dynamical systems
- Baake–Moody 04 via almost periodic measures
- R–Strungaru via PSF

proof

- autocorrelation γ of ω_h vague limit of finite ac measures

$$\gamma_n = \frac{1}{\theta(A_n)} \, \omega_h\big|_{B_n} * \widetilde{\omega_h\big|_{B_n}} = \sum_{z \in L} \eta_n(z) \delta_z ,$$

where $|_{A_n}$ denotes restriction w.r.t. any van Hove $(A_n)_{n\in\mathbb{N}}$ and

$$\eta_n(z) = \frac{1}{\theta_G(A_n)} \sum_{x \in \curlywedge(W \cap (W + z^\star)) \cap A_n} h(x^\star) \overline{h(x^\star - z^\star)}$$

- $\lim_{n\to\infty} \eta_n(z) = h * \widetilde{h}(z^\star)$ for all $z \in L$ by density formula
- as $\operatorname{supp}(\gamma)$ uniformly discrete, γ_n converges to $\omega_{h*\widetilde{h}}$
- since $h * \widetilde{h} \in KL(H)$, transform follows from PSF

diffraction of the Fibonacci chain

$$\widehat{\gamma} = \sum_{k \in \mathbb{Z}[\tau]/\sqrt{5}} \left(\frac{\tau}{\sqrt{5}}\right)^2 \left(\frac{\sin(\pi\tau k^\star)}{\pi\tau k^\star}\right)^2 \delta_k$$

- $\mathbb{Z}[\tau] = \{m + n\tau \mid m, n \in \mathbb{Z}\} = L$
- peaks dense in $\widehat{G} = \mathbb{R}$!
- star map: $(m + n\tau)^\star = m - n/\tau$
- note that $\widehat{\omega}$ does not exist as a measure since $\sin(x)/x$ is not an L^1 function.

references

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