# Aperiodic Order
## Part 5

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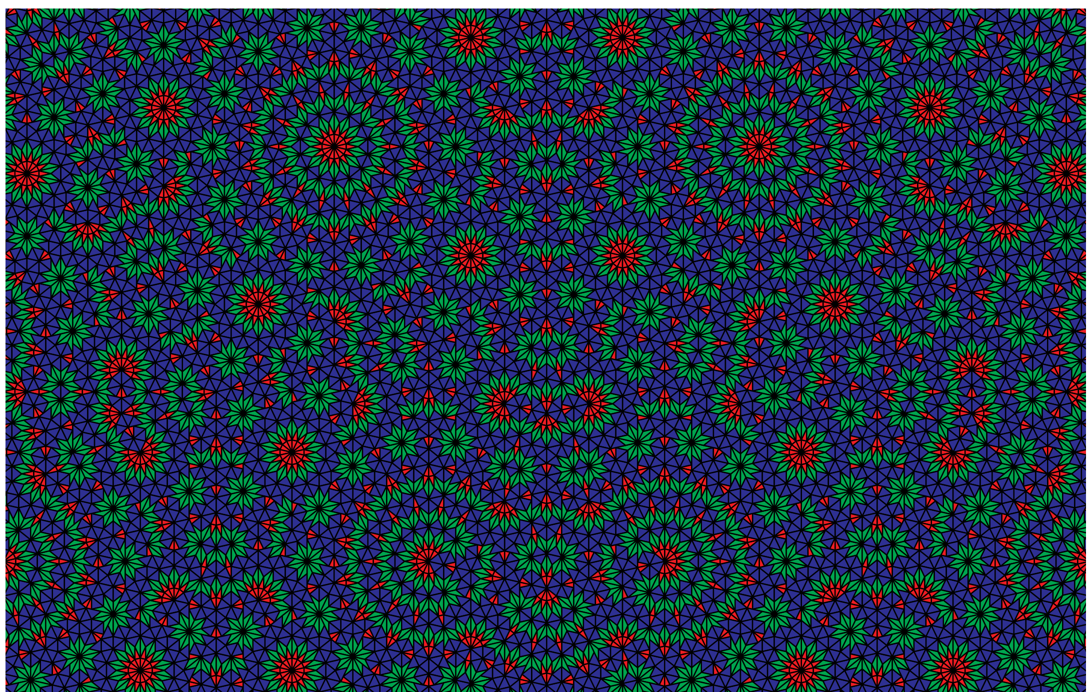
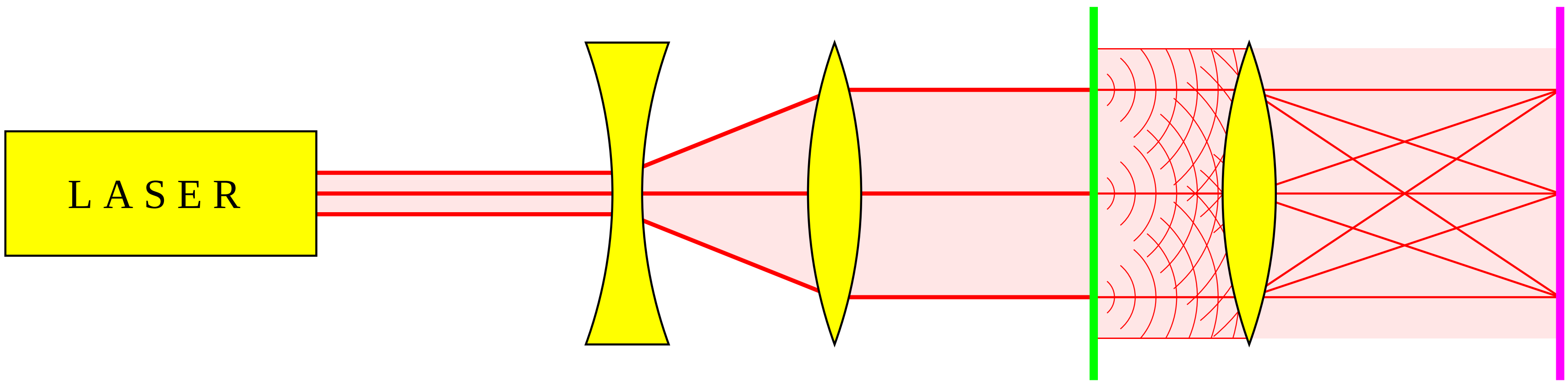
`http://mcs.open.ac.uk/ugg2/ltcc/`



# 5.1 Diffraction

## Optical diffraction




## Diffraction pattern

- interference of scattered waves
  → harmonic analysis
- structure analysis
- X-ray, electron or neutron diffraction
- information on order and symmetry

# 5.1 Diffraction

**Wiener diagram**

$$\begin{array}{ccc} g & \xrightarrow{\;\;*\;\;} & g * \widetilde{g} \\ {\scriptstyle\mathcal{F}}\big\downarrow & & \big\downarrow{\scriptstyle\mathcal{F}} \\ \widehat{g} & \xrightarrow{\;|.|^2\;} & |\widehat{g}|^2 \end{array}$$

commutative for integrable function $g$ (with $\widetilde{g}(x) := \overline{g(-x)}$ )

**Kinematic diffraction:**

diagonal map $g \mapsto |\widehat{g}|^2$

**Mathematical diffraction theory:**

use path via autocorrelation

for translation bounded measures

# 5.2 Why measures?

**Measures**

- are natural mathematical objects to describe distributions (of scatterers or radiation) is space
- provide a unified generalisation of continuous (density) and discrete (tiling) approaches
- ensure that quantities are mathematically well-defined

**Absolutely continuous measure** $\mu$ (with density $\varrho$) on $\mathbb{R}^d$

$$\mu(f) = \int_{\mathbb{R}^d} f(x)\, \mathrm{d}\mu(x) = \int_{\mathbb{R}^d} f(x)\, \varrho(x)\, \mathrm{d}x$$

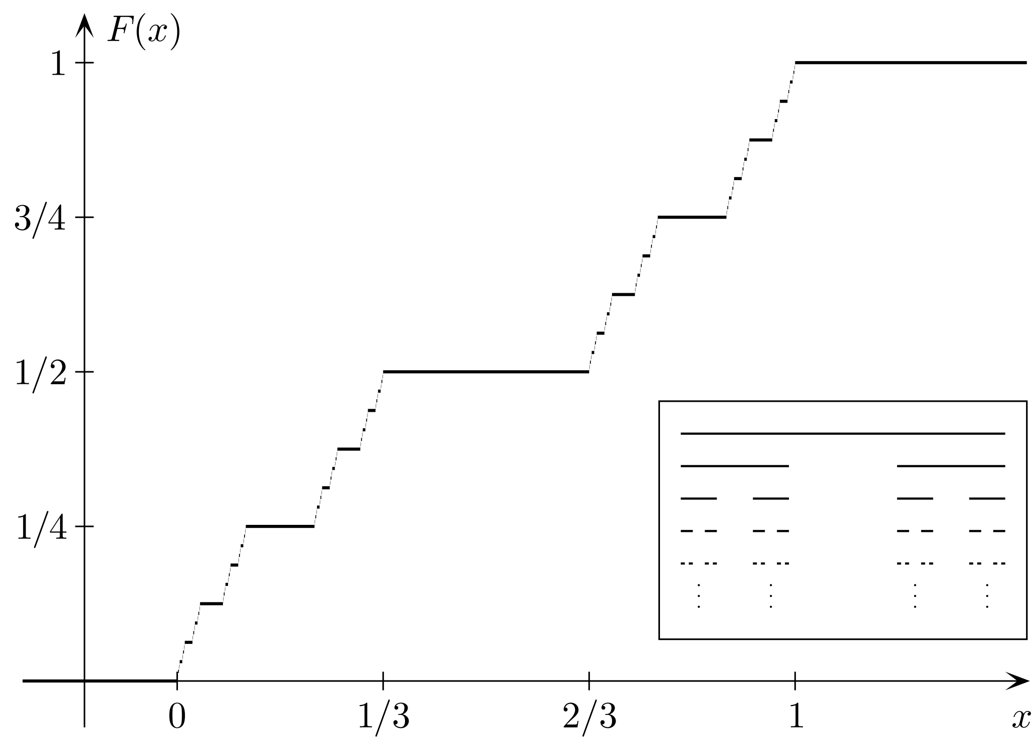
**Pure point measure** $\mu$ on $\mathbb{R}^d$

$$\mu(f) = \Big(\sum_{i \in I} w_i\, \delta_{x_i}\Big)(f) = \sum_{i \in I} w_i\, f(x_i)$$

# 5.2 Why measures?

**Singular continuous measure**

- gives no weight to any single point
- support is uncountable set of zero Lebesgue measure
- ‘trivial’ cases (e.g. measures on lines in the plane)
- probability measure $\mu$ for middle-thirds Cantor set with continuous distribution function $F(x) = \mu([0, x])$



# 5.3 Measures

Using the Riesz–Markov representation theorem, we can introduce measures on $\mathbb{R}^d$ (in one-to-one correspondence with regular Borel measures) via linear functionals in the following way.

Let $C_{\mathsf{c}}(\mathbb{R}^d)$ be the space of complex-valued continuous functions on $\mathbb{R}^d$ with compact support. A (complex) *measure* $\mu$ on $\mathbb{R}^d$ is a linear functional on $C_{\mathsf{c}}(\mathbb{R}^d)$ with the extra condition that, for every compact set $K \subseteq \mathbb{R}^d$, there is a constant $a_K$ such that

$$|\mu(g)| \;\leq\; a_K \, \|g\|_\infty$$

holds for all $g \in C_{\mathsf{c}}(\mathbb{R}^d)$ with support in $K$. Here, $\|g\|_\infty := \sup_{x \in K} |g(x)|$ is the supremum norm of $g$.

# 5.3 Measures

If $\mu$ is a measure, the *conjugate* of $\mu$ is defined by the mapping $g \mapsto \overline{\mu(\bar{g})}$. It is again a measure and denoted by $\bar{\mu}$.

A measure $\mu$ is called *real* (or signed) if $\bar{\mu} = \mu$, or (equivalently) if $\mu(g)$ is real for all real-valued $g \in C_{\mathsf{c}}(\mathbb{R}^d)$.

A real measure $\mu$ is called *positive* if $\mu(g) \geq 0$ for all $g \geq 0$.

For every measure $\mu$, there is a smallest positive measure, called its *total variation* $|\mu|$, such that $|\mu(g)| \leq |\mu|(g)$ holds for all non-negative $g \in C_{\mathsf{c}}(\mathbb{R}^d)$.

$\mu(A)$ (measure of a set) and $\mu(f)$ (measure of a function), related via characteristic function $1_A$ of a (relatively compact) Borel set $A$ via $\mu(1_A) = \mu(A)$

# 5.3 Measures

Point measure $\delta_x$ defined as

$$\delta_x(A) = \begin{cases} 1, & \text{if } x \in A, \\ 0, & \text{otherwise,} \end{cases}$$

for an arbitrary Borel set $A \subseteq \mathbb{R}^d$.

The Lebesgue measure of an integrable function $g$ is $\lambda(g) = \int_{\mathbb{R}^d} g \,\mathrm{d}\lambda = \int_{\mathbb{R}^d} g(x)\,\mathrm{d}x$, while the measure of a Borel set $A$ is $\lambda(A) = \int_{\mathbb{R}^d} 1_A \,\mathrm{d}\lambda$.

The measures $\delta_0$ and $\lambda$ are related by

$$\widehat{\delta_0} = \lambda \quad \text{and} \quad \widehat{\lambda} = \delta_0 .$$

A measure $\mu$ on $\mathbb{R}^d$ is called *translation bounded* if $\sup_{x\in\mathbb{R}^d} |\mu|(x+K) < \infty$ holds for every compact $K \subseteq \mathbb{R}^d$.

# 5.3 Measures

**Lebesgue decomposition theorem:**

Any positive, regular Borel measure $\mu$ on $\mathbb{R}^d$ has a unique decomposition

$$\mu \;=\; \mu_{\mathsf{pp}} + \mu_{\mathsf{sc}} + \mu_{\mathsf{ac}}$$

relative to Lebesgue measure $\lambda$, where $\mu_{\mathsf{sc}}$ is the unique part of $\mu$ that is both continuous and singular relative to $\lambda$.

A complex measure $\mu$ on $\mathbb{R}^d$ is called *positive definite* if $\mu(g * \widetilde{g}) \geq 0$ holds for all $g \in C_{\mathsf{c}}(\mathbb{R}^d)$.

If $\mu$ is a positive definite measure on $\mathbb{R}^d$, its Fourier transform $\widehat{\mu}$ exists and is a translation bounded positive measure on $\mathbb{R}^d$.

# 5.3 Measures

The convolution of two finite measures on $\mathbb{R}^d$, or of a finite with a translation bounded measure, is well-defined. This is no longer the case if both measures are unbounded, but you may attempt to define a volume averaged convolution as

$$\mu \circledast \nu \; := \lim_{R \to \infty} \frac{\mu_R * \nu_R}{\mathrm{vol}(B_R)},$$

where $\mu_R$ and $\nu_R$ are the restrictions of $\mu$ and $\nu$ to the (open) ball $B_R(0)$.

We call two measures $\mu$ and $\nu$ *mutually amenable* when this limit exists for balls as well as for arbitrary nested van Hove sequences. The resulting measure is called the *Eberlein convolution* of $\mu$ and $\nu$.

# 5.4 Fourier transform

Let $\mathcal{S}(\mathbb{R}^d)$ be the space of rapidly decreasing $C^\infty$-functions on $\mathbb{R}^d$, also known as Schwartz functions.

The *Fourier transform* of a Schwartz function $\phi \in \mathcal{S}(\mathbb{R}^d)$, we mean

$$(\mathcal{F}\phi)(k) \;=\; \widehat{\phi}(k) \;:=\; \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi \mathrm{i} kx}\, \phi(x)\, \mathrm{d}x,$$

which is well-defined and again a Schwartz function, with $k \in \mathbb{R}^d$.

The mapping $\mathcal{F}\colon\; \mathcal{S}(\mathbb{R}^d) \longrightarrow \mathcal{S}(\mathbb{R}^d)$ is a homeomorphism, with inverse

$$(\mathcal{F}^{-1}\psi)(x) \;=\; \check{\psi}(x) \;=\; \int_{\mathbb{R}^d} \mathrm{e}^{2\pi \mathrm{i} kx}\, \psi(k)\, \mathrm{d}k$$

# 5.4 Fourier transform

A *tempered distribution* is a continuous linear functional $T\colon \mathcal{S}(\mathbb{R}^d) \longrightarrow \mathbb{C}$ on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$.

$(T, \phi) := T(\phi)$ denotes the evaluation of $T$ with a function $\phi \in \mathcal{S}(\mathbb{R}^d)$, called a *test function*.

Each continuous function $g$ of at most polynomial growth defines a tempered distribution $T_g$ via

$$T_g(\phi) \; := \int_{\mathbb{R}^d} \phi(x)\, g(x)\, \mathrm{d}x \, .$$

Such distributions are also called *regular* .

The Fourier transform of a tempered distribution $T \in \mathcal{S}'(\mathbb{R}^d)$ is given by

$$\widehat{T}(\phi) \; := \; T\big(\widehat{\phi}\,\big)$$

for all test functions $\phi \in \mathcal{S}(\mathbb{R}^d)$.

# 5.4 Fourier transform

If $\mu$ is a *finite* measure on $\mathbb{R}^d$, its Fourier transform (or Fourier–Stieltjes transform) can directly be defined as

$$\widehat{\mu}(k) \;=\; \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi \mathrm{i} k x} \, \mathrm{d}\mu(x),$$

which is a bounded and uniformly continuous function on $\mathbb{R}^d$.

If $\mu$ and $\nu$ are finite measures on $\mathbb{R}^d$, their *convolution* $\mu * \nu$ is defined by

$$\big(\mu * \nu\big)(g) \;=\; \int_{\mathbb{R}^d \times \mathbb{R}^d} g(x+y) \, \mathrm{d}\mu(x) \, \mathrm{d}\nu(y),$$

with $g \in C_{\mathsf{c}}(\mathbb{R}^d)$.

**Proposition:** The convolution $\mu * \nu$ of two finite measures on $\mathbb{R}^d$ satisfies $\widehat{\mu * \nu} \;=\; \widehat{\mu}\,\widehat{\nu}$.

# 5.4 Fourier transform

**Theorem:** Let $\mu$ be a finite and $\nu$ a translation bounded measure on $\mathbb{R}^d$. Then, the convolution $\mu * \nu$ exists and is a translation bounded measure.

**Proposition:** If $\mu$ is a positive definite measure on $\mathbb{R}^d$, its Fourier transform $\widehat{\mu}$ exists, and is a translation bounded positive measure on $\mathbb{R}^d$.

**Useful relations:**

$\widehat{\delta_x} = \mathrm{e}^{-2\pi \mathrm{i} xy}$ (in the sense of tempered distributions,

so $\widehat{\delta_x}(\phi) = \delta_x(\widehat{\phi}) = \widehat{\phi}(x) = \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi \mathrm{i} xy}\, \phi(y)\, \mathrm{d}y$)

⟶ as measures $\widehat{\delta_0} = \lambda$ and $\widehat{\lambda} = \delta_0$

Finite measure $\nu$ on $\mathbb{R}^d$

⟶ $\widehat{\nu * \lambda} = c\delta_0$ with $c = \widehat{\nu}(0) = \nu(\mathbb{R}^d)$.

# 5.5 Autocorrelation measure

For a locally finite point set $\varLambda$, define its *Dirac comb* as

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

For a measure $\mu$ on $\mathbb{R}^d$, define $\widetilde{\mu}$ by $\widetilde{\mu}(g) := \overline{\mu(\widetilde{g})}$, with $g \in C_{\mathsf{c}}(\mathbb{R}^d)$.

For a translation bounded measure $\mu$ on $\mathbb{R}^d$, we define the *natural autocorrelation* $\gamma$ by

$$\gamma \; = \; \mu \circledast \widetilde{\mu} \; = \; \lim_{R \to \infty} \frac{\mu_R * \widetilde{\mu}_R}{\mathrm{vol}(B_R)},$$

if the limit exists. In this case, $\gamma$ is a translation bounded, positive definite measure on $\mathbb{R}^d$.

# 5.6 Diffraction measure

Let $\mu$ be a translation bounded complex measure whose natural autocorrelation $\gamma_\mu$ exists. The Fourier transform $\widehat{\gamma_\mu}$ is then called the *diffraction measure* of $\mu$.

**Proposition:** Let $\varLambda$ be a locally finite point set with natural autocorrelation $\gamma$. Its diffraction measure $\widehat{\gamma}$ comprises a Dirac measure at $0$, with $\widehat{\gamma}(\{0\}) = \bigl(\mathrm{dens}(\varLambda)\bigr)^2$.

# 5.7 Poisson's summation formula

**Proposition:** For all $\phi \in \mathcal{S}(\mathbb{R}^d)$, one has

$$\sum_{m\in\mathbb{Z}^d} \phi(m) = \sum_{m\in\mathbb{Z}^d} \widehat{\phi}(m)\,.$$

**Proof:** Define $g(x) = \sum_{\ell\in\mathbb{Z}^d} \phi(x+\ell)$, uniformly convergent

uniformly convergent Fourier series $g(x) = \sum_{m\in\mathbb{Z}^d} c_m \,\mathrm{e}^{2\pi \mathrm{i} m x}$

with $c_m = \int_{\mathbb{T}^d} \mathrm{e}^{-2\pi\mathrm{i} m x}\, g(x)\,\mathrm{d}x \implies g(0) = \sum_{m\in\mathbb{Z}^d} c_m = \sum_{m\in\mathbb{Z}^d} \phi(m)$

$$c_m = \int_{\mathbb{T}^d} \sum_{\ell\in\mathbb{Z}^d} \mathrm{e}^{-2\pi\mathrm{i} m x}\,\phi(x+\ell)\,\mathrm{d}x = \sum_{\ell\in\mathbb{Z}^d} \int_{\ell+\mathbb{T}^d} \mathrm{e}^{-2\pi\mathrm{i} m x}\,\phi(x)\,\mathrm{d}x$$

$$= \int_{\mathbb{R}^d} \mathrm{e}^{-2\pi\mathrm{i} m x}\,\phi(x)\,\mathrm{d}x = \widehat{\phi}(m)$$

■

# 5.7 Poisson's summation formula

**Proposition:** Interpreted as an equation for tempered distributions, one has the identity $\widehat{\delta_{\mathbb{Z}^d}} = \delta_{\mathbb{Z}^d}$.

**Proof:**

$\widehat{\delta_{\mathbb{Z}^d}} = \delta_{\mathbb{Z}^d}$ means that $\widehat{\delta_{\mathbb{Z}^d}}(\phi) = \delta_{\mathbb{Z}^d}(\phi)$ for all $\phi \in \mathcal{S}(\mathbb{R}^d)$

Now

$$\widehat{\delta_{\mathbb{Z}^d}}(\phi) = \left(\widehat{\delta_{\mathbb{Z}^d}}, \phi\right) = \left(\delta_{\mathbb{Z}^d}, \widehat{\phi}\right)$$

$$= \sum_{m \in \mathbb{Z}^d} \widehat{\phi}(m) = \sum_{m \in \mathbb{Z}^d} \phi(m)$$

$$= \left(\delta_{\mathbb{Z}^d}, \phi\right) = \delta_{\mathbb{Z}^d}(\phi) \qquad \blacksquare$$

# 5.7 Poisson's summation formula

**Theorem:** If $\mathit{\Gamma}$ is a lattice in $\mathbb{R}^d$, with dual lattice $\mathit{\Gamma}^*$, and if $\phi \in \mathcal{S}(\mathbb{R}^d)$ is an arbitrary Schwartz function, one has

$$\sum_{m \in \mathit{\Gamma}} \phi(m) \; = \; \mathrm{dens}(\mathit{\Gamma}) \sum_{\ell \in \mathit{\Gamma}^*} \widehat{\phi}(\ell).$$

Moreover one has the following identity of lattice Dirac combs,

$$\widehat{\delta_{\mathit{\Gamma}}} \; = \; \mathrm{dens}(\mathit{\Gamma}) \, \delta_{\mathit{\Gamma}^*},$$

which simultaneously is an identity between tempered distributions and translation bounded measures.

# 5.8 Lattice periodic case

**Proposition:** If $\varGamma \subseteq \mathbb{R}^d$ is a lattice, with fundamental domain $\mathrm{FD}(\varGamma)$, and if $\mu$ is a $\varGamma$-periodic measure on $\mathbb{R}^d$, there is a *finite* measure $\varrho$ that is concentrated on $\mathrm{FD}(\varGamma)$, or on a subset of $\mathrm{FD}(\varGamma)$, so that $\mu = \varrho * \delta_{\varGamma}$.

**Theorem:** Let $\varGamma$ be a lattice in $\mathbb{R}^d$, and $\omega$ a $\varGamma$-invariant measure, represented as $\omega = \varrho * \delta_{\varGamma}$ with $\varrho$ a finite measure. Then, the autocorrelation $\gamma_{\omega}$ of $\omega$ is given by

$$\gamma_{\omega} = (\varrho * \widetilde{\varrho}\,) * \gamma_{\varGamma} \;=\; \mathrm{dens}(\varGamma)\,(\varrho * \widetilde{\varrho}\,) * \delta_{\varGamma},$$

with the diffraction measure

$$\widehat{\gamma_{\omega}} = \bigl(\mathrm{dens}(\varGamma)\bigr)^{2}\, |\widehat{\varrho}\,|^{2}\, \delta_{\varGamma^{*}}$$

In particular, $\widehat{\gamma_{\omega}}$ is a positive pure point measure, with $\mathrm{supp}(\widehat{\gamma}) \subseteq \varGamma^{*}$ and $\widehat{\gamma_{\omega}}\bigl(\{0\}\bigr) = \bigl(\mathrm{dens}(\varGamma)\bigr)^{2}\, |\widehat{\varrho}(0)|^{2}$.

# 5.8 Lattice periodic case

**Example:** Consider the $\mathbb{Z}^2$-periodic weighted Dirac comb

$$\omega \;=\; \varrho * \delta_{\mathbb{Z}^2} \quad \text{with} \quad \varrho \;=\; \delta_{(0,0)} + \delta_{(a,b)}\,.$$

The autocorrelation is $\gamma_\omega = (\varrho * \widetilde{\varrho}\,) * \delta_{\mathbb{Z}^2}$, with

$$\begin{aligned} \varrho * \widetilde{\varrho} \;&=\; \big(\delta_{(0,0)} + \delta_{(a,b)}\big) * \big(\delta_{(0,0)} + \delta_{-(a,b)}\big) \\ &=\; 2\,\delta_{(0,0)} + \delta_{(a,b)} + \delta_{-(a,b)}\,. \end{aligned}$$

The corresponding diffraction measure is $\widehat{\gamma_\omega} = |\widehat{\varrho}\,|^2 \delta_{\mathbb{Z}^2}$ with

$$\begin{aligned} |\widehat{\varrho}\,|^2(k,\ell) \;&=\; 2 + 2\,\mathrm{Re}\big(\mathrm{e}^{-2\pi \mathrm{i}(ka+\ell b)}\big) \\ &=\; 2 + 2\cos\big(2\pi(ka+\ell b)\big) \\ &=\; \big(2\cos\big(\pi(ka+\ell b)\big)\big)^2 \qquad \text{for } k,\ell \in \mathbb{Z}. \end{aligned}$$

# 5.9 Incommensurate structures

**Example:**

Let $\alpha > 0$ be an irrational number and consider the Dirac comb

$$\omega_\alpha := \delta_{\mathbb{Z}} + \delta_{\alpha\mathbb{Z}}.$$

The corresponding autocorrelation $\gamma_\alpha = \omega_\alpha \circledast \widetilde{\omega_\alpha}$ exists and reads

$$\gamma_\alpha = \delta_{\mathbb{Z}} + \frac{1}{\alpha}\delta_{\alpha\mathbb{Z}} + \frac{2}{\alpha}\lambda.$$

The diffraction measure is

$$\widehat{\gamma_\alpha} = \delta_{\mathbb{Z}} + \frac{1}{\alpha^2}\,\delta_{\mathbb{Z}/\alpha} + \frac{2}{\alpha}\,\delta_0.$$

# 5.10 Model sets

**Theorem:** Let $\varLambda = \curlywedge(W)$ be a regular model set for the CPS $(\mathbb{R}^d, H, \mathcal{L})$, with compact window $W = \overline{W^{\circ}}$. The diffraction measure $\widehat{\gamma_{\varLambda}}$ is a positive and positive definite, translation bounded, pure point measure. It is explicitly given by

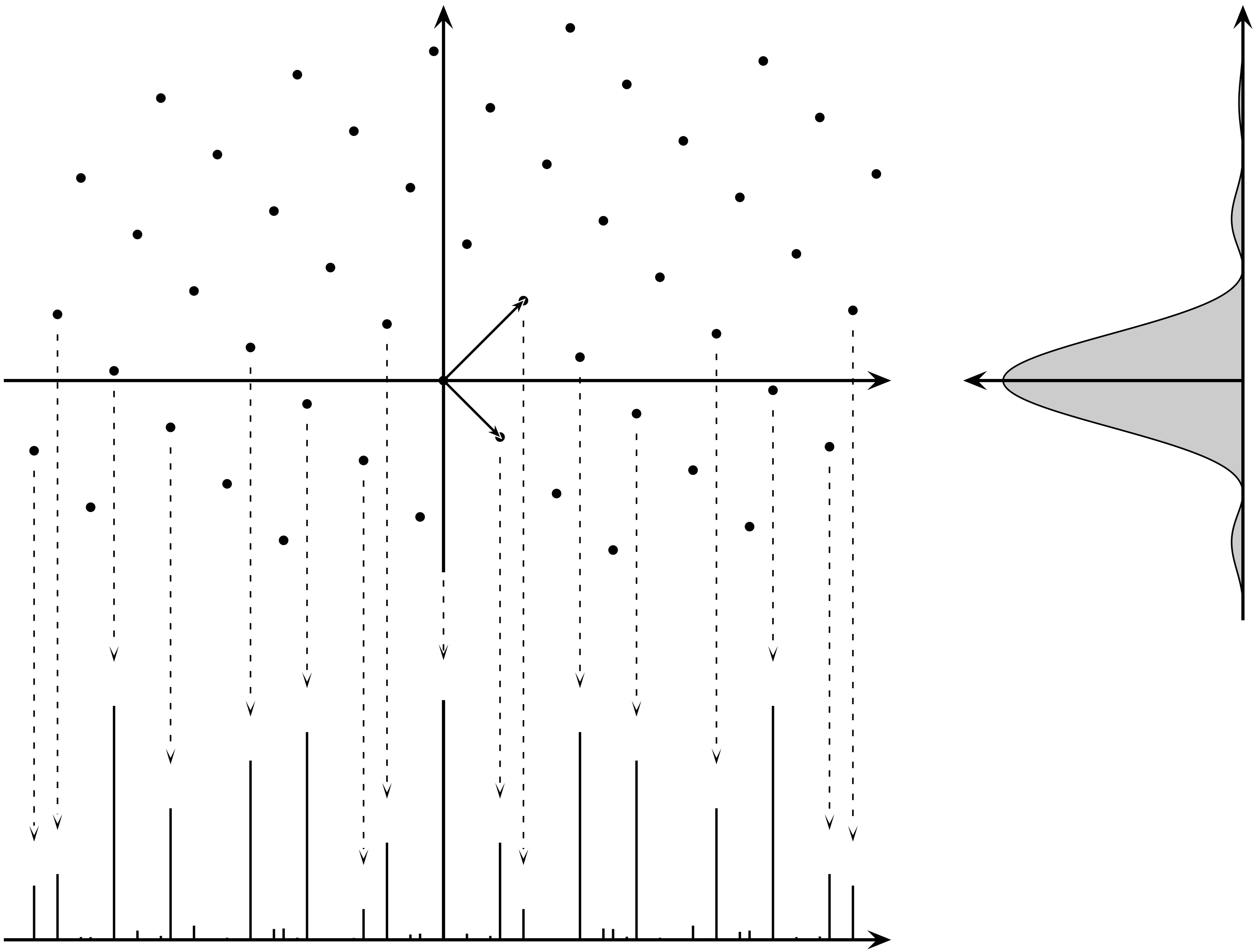
$$\widehat{\gamma_{\varLambda}} = \sum_{k \in L^{\circledast}} I(k)\, \delta_k ,$$

where $L^{\circledast} := \pi(\mathcal{L}^{*})$. The diffraction intensities are $I(k) = |A(k)|^2$ with the amplitudes

$$A(k) \;=\; \frac{\mathrm{dens}(\varLambda)}{\mu_H(W)}\, \widehat{1_W}(-k^{\star}) \;=\; \frac{\mathrm{dens}(\varLambda)}{\mu_H(W)} \int_W \langle k^{\star}, y\rangle \,\mathrm{d}\mu_H(y).$$

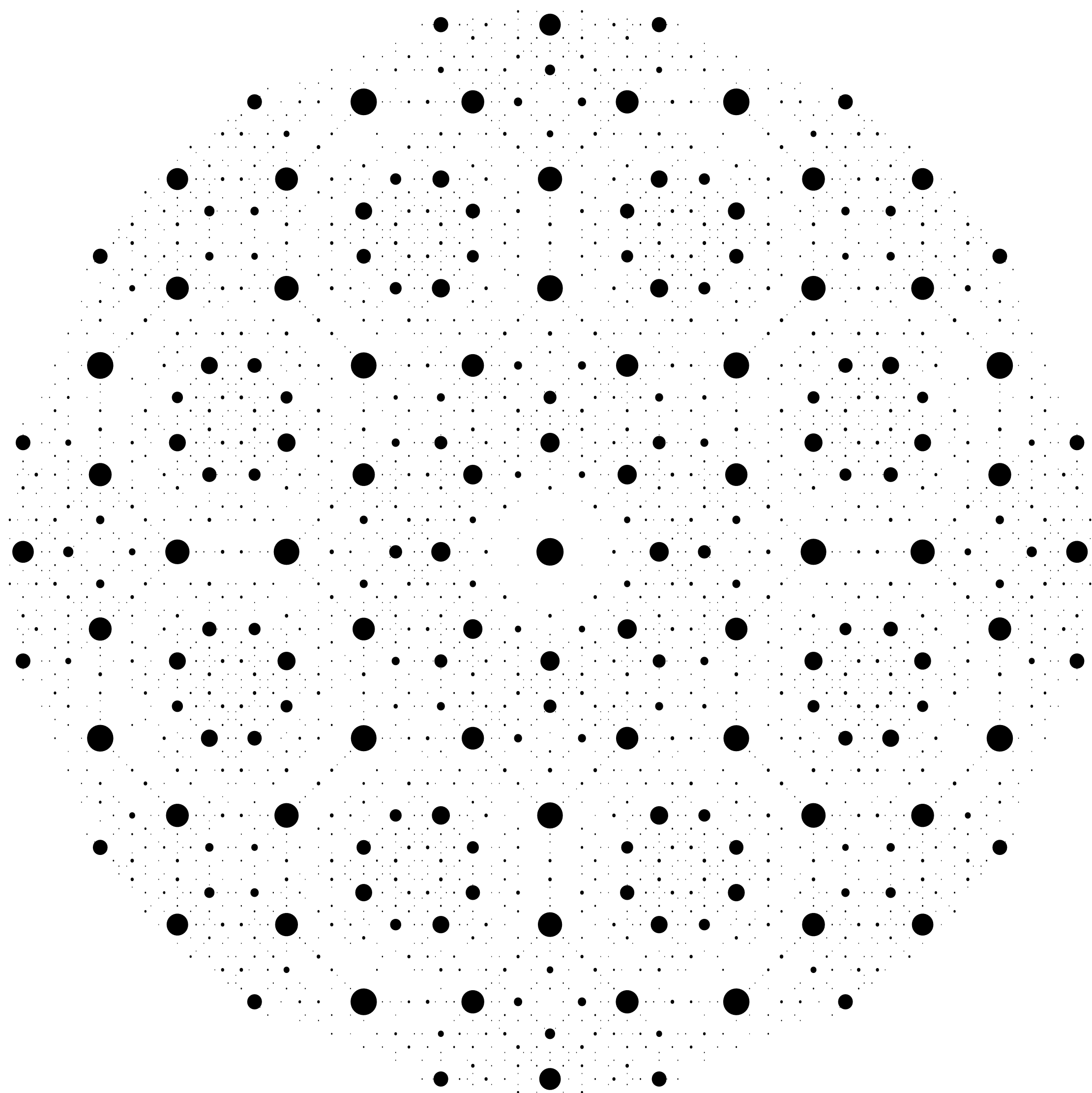
# 5.10 Model sets

**Example:**



# 5.10 Model sets

## Ammann–Beenker diffraction:



# 5.10 Model sets

**Diffraction intensity for Ammann–Beenker case:**

Bragg peaks at positions $k_1 + k_2\xi^2 \in \frac{1}{2}\mathbb{Z}[\xi] \subseteq \mathbb{C}$ (where $\xi = \exp(2\pi\mathrm{i}/8)$) with intensities

$$
\begin{aligned}
I\big((k_1,k_2)\big) = \frac{1}{\big(4\pi^2(k_2'+k_1')(k_2'-k_1')\big)^2} \Big(&\cos(k_2'\pi)\cos(\lambda k_1'\pi) \\
&- \cos(k_1'\pi)\cos(\lambda k_2'\pi) - \frac{k_1'}{k_2'}\sin(k_2'\pi)\sin(\lambda k_1'\pi) \\
&+ \frac{k_2'}{k_1'}\sin(k_1'\pi)\sin(\lambda k_2'\pi)\Big)^2
\end{aligned}
$$

with $\lambda = 1 + \sqrt{2}$ and algebraic conjugation $\;' \colon \sqrt{2} \mapsto -\sqrt{2}$

# 5.11 Experiment

**Diffraction of icosahedral quasicrystal:**