Beta-lattice multiresolution of quasicrystalline Bragg peaks*

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CRC701-Workshop
Aspects of Aperiodic Order
3-5 July 2008, University of Bielefeld

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* *Proceedings of SPIE Vol. 6701, Wavelets XII, (Optics & Photonics, San Diego, August 26-30 2007)*
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Some words about quasicrystals

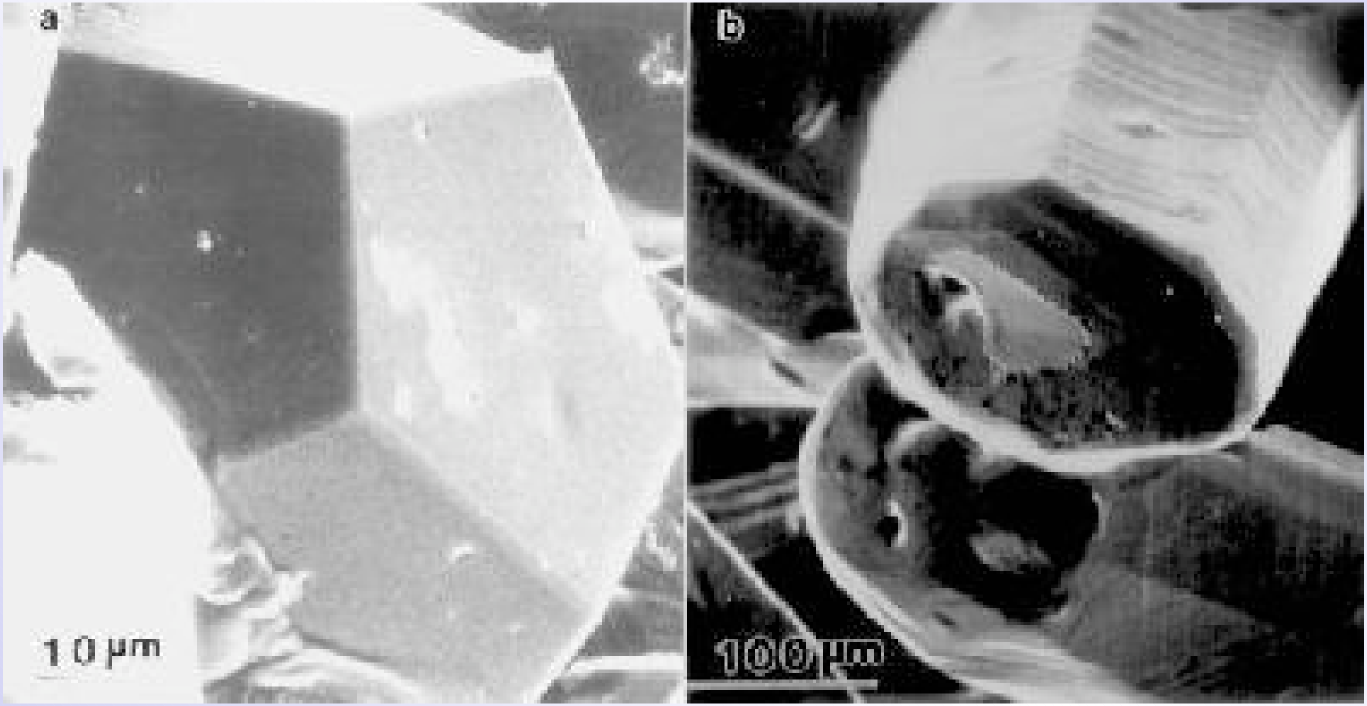
Quasicrystallography dates back to 1982 with the discovery, by Schechtman, Blech, Gratias, and Cahn[a], of an alloy, namely $Al_{0.86}Mn_{0.14}$, showing

i) diffraction pattern like a constellation of more-or-less bright spots $\longrightarrow$ long-distance order,

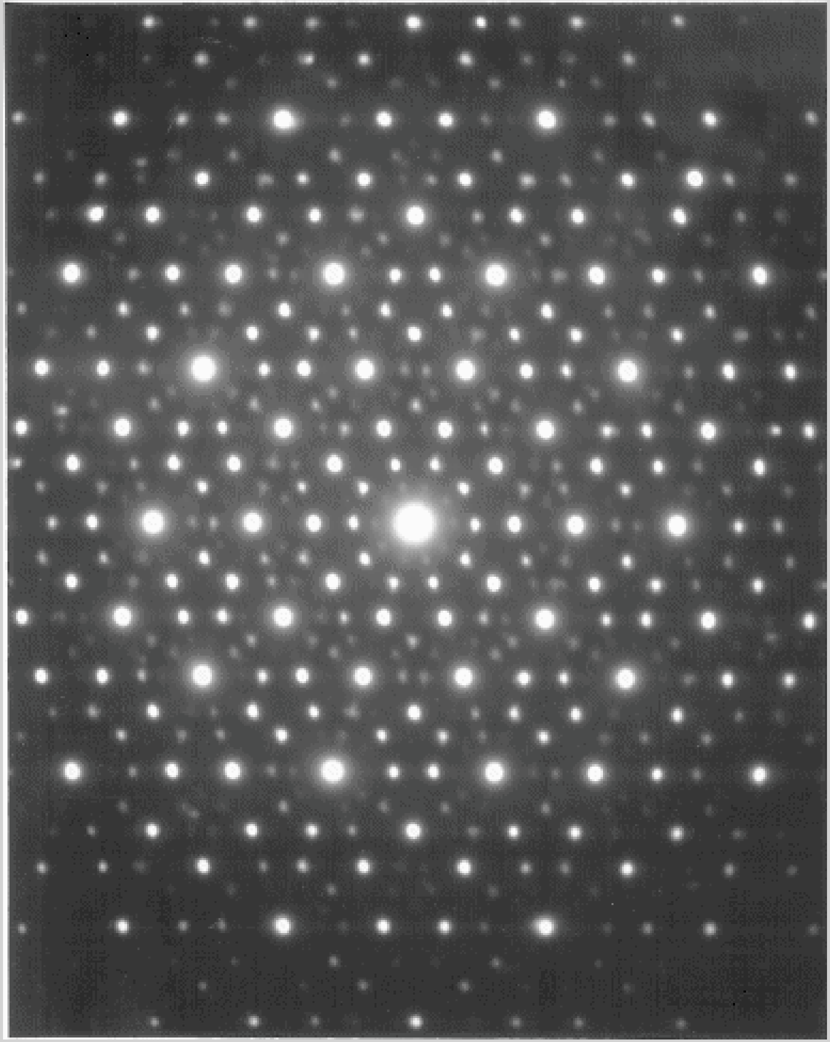
ii) spatial organisation of those Bragg peaks obeying five- or ten-fold symmetries, at least locally $\longrightarrow$ icosahedral organisation in real space with five-fold symmetries,

iii) spatial organisation of those Bragg peaks obeying specific scale invariance, more precisely invariance under dilations by a factor equal to some power of the golden mean $\tau = \frac{1+\sqrt{5}}{2} = 2\cos\frac{2\pi}{10}$.

[a] D. Shechtman, I. Blech, D. Gratias, and J.W. Cahn, *prl* **53**(1984), 1951

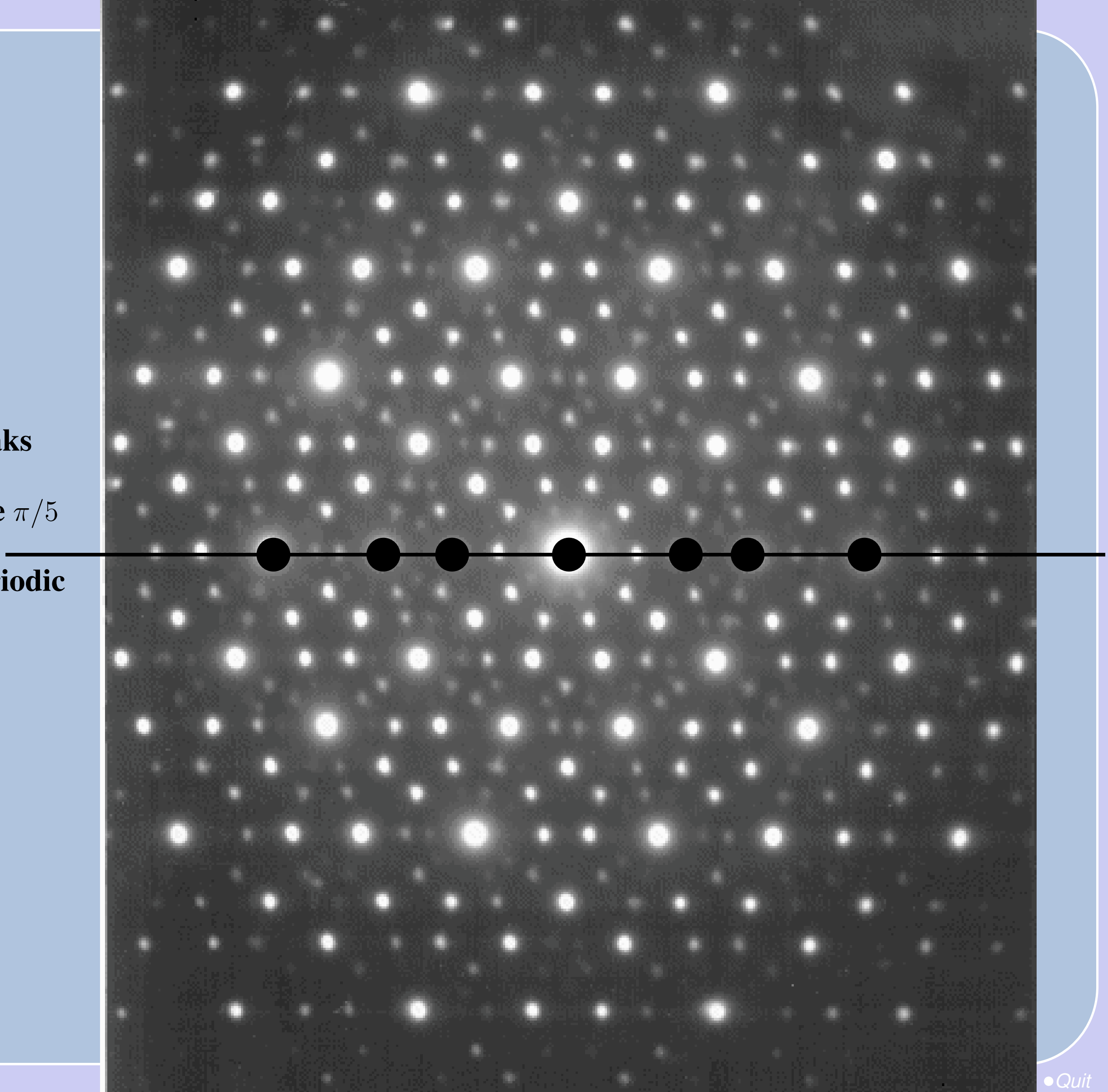


Tsai et al.



Lifshitz

- ♣ **Bragg peaks**
- ♣ **invariance** $\pi/5$
- ♣ **quasi- periodic**
- ♣ **density**



Bragg peak in $\mathbb{R}^n$

- A Bragg peak in $\mathbb{R}^n$ is a pair

$$p = (\mathbf{x}, I_{\mathbf{x}}),$$

  where $\mathbf{x}$ is a point in $\mathbb{R}^n$, called the (geometrical) support of p, and $I_{\mathbf{x}} > 0$ is a positive real number called the intensity of p .

- The support of all Bragg peaks in a given pure-point diffraction spectrum is a point set $\mathcal{Z} \subset \mathbb{R}^n$ (a lattice for crystals) with Lebesgue measure 0 in $\mathbb{R}^n$ and the range of their intensities is a bounded subset $\mathcal{I}$ of the positive real line (constant for periodic crystals). So the corresponding pp diffraction spectrum Π is the set of Bragg peaks which reads as :

$$\Pi = \{p = (\mathbf{x}, I_{\mathbf{x}}) \,|\, \mathbf{x} \in \mathcal{Z},\, I_{\mathbf{x}} \in \mathcal{I}\}\,.$$

- Moreover, there exists a maximal intensity, $I_{\max} \in \mathcal{I} \subset (0, I_{\max}]$, lowest upper bound of $\mathcal{I}$, and all points supporting it are symmetry center for $\mathcal{Z}$ with respect to space inversion. One of them will be chosen as the origin of $\mathbb{R}^n$.

Cyclotomic Pisot-Vijayaraghavan Pure-Point Diffraction Spectrum

A k-fold cyclotomic Pisot–Vijayaraghavan (PV) pure-point diffraction spectrum is a 2d pure-point diffraction spectrum which is supported by the (generically dense) point set of cyclotomic integers

$$\mathbb{Z}[\zeta] = \sum_{q=0}^{k-1} \mathbb{Z}\zeta^q = \mathbb{Z}[\beta] + \mathbb{Z}[\beta]\zeta,$$

with

- $\zeta = e^{i\frac{2\pi}{k}}$
- β is a *cyclotomic Pisot-Vijayaraghavan number*[a], *i.e.*

$$\mathbb{Z}[\beta] = \mathbb{Z}\left[2\cos\frac{2\pi}{k}\right]$$

  such that as a scaling invariance factor it is relevant to the pure-point diffractive properties

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[a] A *Pisot-Vijayaraghavan*, or PV, number $\beta > 1$ is an algebraic integer, dominant root of the polynomial $P(X) = X^n - a_{n-1}X^{n-1} - \cdots - a_1 X - a_0$, with $a_0, \cdots, a_{n-1} \in \mathbb{Z}$, such that the other roots of $P(X)$, are strictly smaller than 1. It is said to be a *unit* if $a_0 = \pm 1$.

Examples of Cyclotomic Pisot-Vijayaraghavan numbers

They appear in quasi-crystallographic structures in the plane :

$$k = 5 \qquad \beta = \tau = \frac{1+\sqrt{5}}{2} = 1 + 2\cos\frac{2\pi}{5} \text{ (pentagonal)},$$

$$k = 10 \qquad \beta = 1 + \tau = \tau^2 = \frac{1+\sqrt{5}}{2} = 1 + 2\cos\frac{\pi}{5} \text{ (decagonal)},$$

$$k = 10 \qquad \beta = \tau^2 = \frac{3+\sqrt{5}}{2} = 1 + 2\cos\frac{\pi}{5} \text{ (decagonal)},$$

$$k = 8 \qquad \beta = \delta = 1 + \sqrt{2} = 1 + 2\cos\frac{\pi}{4} \text{ (octogonal)},$$

$$k = 12 \qquad \beta = \theta = 2 + \sqrt{3} = 2 + 2\cos\frac{\pi}{6} \text{ (dodecagonal)}.$$

Note that in the case $k = 7$, we have $\beta = 1 + 2\cos\frac{2\pi}{7}$ which is solution to the cubic equation $X^3 - 2X^2 - X + 1 = 0$.

The set of β-integers

- Every one is familiar with the binary system used to express real numbers as series in powers of 2 :

$$x = \pm(x_j 2^j + x_{j-1} 2^{j-1} + \cdots + x_l 2^l + \cdots),$$

$j = j(x) \in \mathbb{N}$: highest power of 2 such that $2^j \leq |x| < 2^{j+1}$, $x_j =$ integral part of $|x|/2^j \equiv \lfloor |x|/2^j \rfloor \in \{0, 1\}$.

- The same algorithm, called greedy algorithm, can be employed to represent real numbers in a system based on an arbitrary real number $\beta > 1$:

$$x = \pm(x_j \beta^j + x_{j-1} \beta^{j-1} + \cdots + x_l \beta^l + \cdots) \equiv \pm x_j x_{j-1} \ldots x_1 x_0 \cdot x_{-1} x_{-2} \ldots$$

where the "letters" assume their values in the alphabet $\{0, 1, \ldots, \beta - 1\}$ if β is natural , and $\lfloor \beta \rfloor$ if β is not $\}$. But if β is not natural, all words are not allowed.

- For instance, the first positive τ-integers are given by

$$\underset{(0)}{0} \overbrace{}^{1} \underset{(1)}{1} \overbrace{}^{\frac{1}{\tau}} \underset{(10)}{\tau} \overbrace{}^{1} \underset{(100)}{\tau^2} \overbrace{}^{1} \underset{(101)}{\tau^2+1} \overbrace{}^{\frac{1}{\tau}} \underset{(1000)}{\tau^3} \overbrace{}^{1} \underset{(1001).}{\tau^3+1}$$

Beta-lattices

- $\mathbb{Z}_\beta$: set of beta-integers *i.e.* set of real numbers such that their beta-expansion is polynomial,
$$\mathbb{Z}_\beta = \{x \in \mathbb{R} \mid |x| = x_k \cdots x_0\}$$
- $\mathbb{Z}_\beta$ is relatively dense, self-similar and symmetrical with respect to the origin,
- If β is a Pisot-Vijayaraghavan number, then the set $\mathbb{Z}_\beta$ is uniformly discrete and hence is Delaunay.

Let $(\mathbf{e}_i)$ be a base of $\mathbb{R}^n$ and β a a Pisot-Vijayaraghavan (and more generally a Parry number). The corresponding beta-lattice is the Delaunay set in $\mathbb{R}^n$:

$$\Gamma = \sum_{i=1}^{d} \mathbb{Z}_\beta \mathbf{e}_i.$$

This set is obviously self-similar and symmetrical with respect to the origin :

$$\beta\Gamma \subset \Gamma, \quad \Gamma = -\Gamma.$$

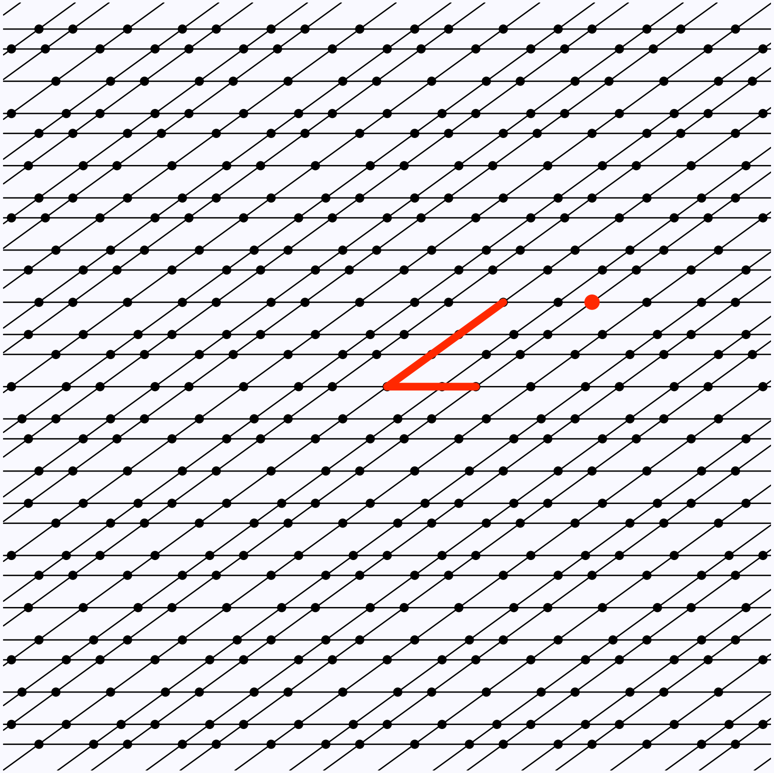
A Tau-lattice in $\mathbb{R}^2$

$$\zeta = e^{\frac{i\pi}{5}}$$

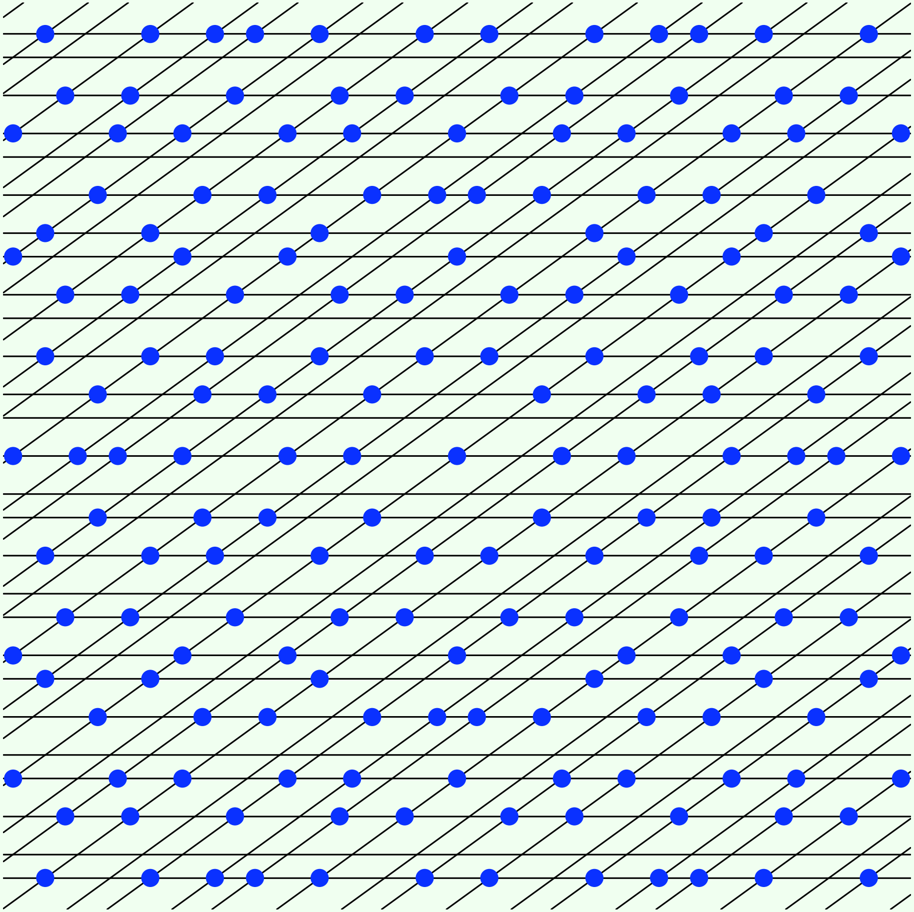
$$\Gamma(\tau) = \mathbb{Z}_\tau + \mathbb{Z}_\tau \zeta$$

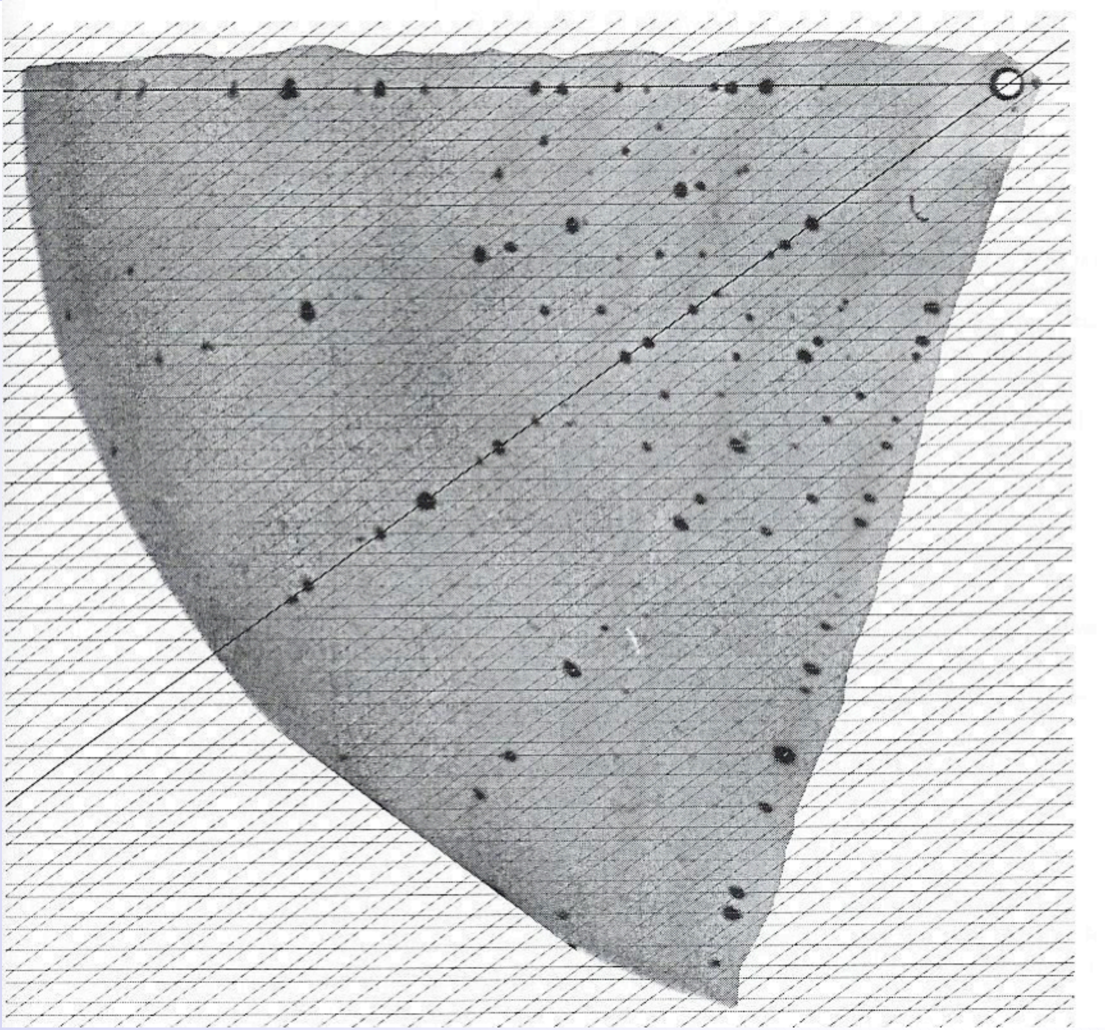
$$z_{2,3} = b_2 + b_3\zeta$$
$$\equiv (2, 3)$$

$$z_{m,n} = b_m + b_n\zeta$$



2D QC embedded in a Tau-lattice
or Tau-lattice as a counting background for QC





Monochromatic X*-ray diffraction pattern (*$Al_{63}Cu_{17.5}Co_{17.5}Si_2$*, synchrotron LURE, Orsay) inplanted in a* τ*-lattice at a suitable scale.*

On the use of beta-lattices as nested sequences - Proposition I

Let β be a Pisot-Vijayaraghavan unit of degree d and $\mathbb{Z}_\beta$ its corresponding set of β-integers. Let $\Gamma = \sum_{i=1}^n \mathbb{Z}_\beta \mathbf{e}_i$ be the corresponding beta-lattice in $\mathbb{R}^n$, and $\widetilde{\Gamma}_\infty = \sum_{i=1}^n \mathbb{Z}[\beta]\mathbf{e}_i$ the $\mathbb{Z}$-module built from the basis $\mathbf{e}_i$ and the algebraic β. Suppose that all integers have finite β-expansion.

(ι) Suppose that there exists a finite l such that $\mathbb{Z}_\beta + \mathbb{Z}_\beta \subset \mathbb{Z}_\beta/\beta^l$. Let $\Gamma_j = \Gamma/\beta^j$ be the scaled beta-lattices issued from $\Gamma \equiv \Gamma_0$. Then we have the infinite nested sequence of Delaunay sets and the inductive limit :

$$\cdots \subset \Gamma_{j-1} \subset \Gamma_j \subset \Gamma_{j+1} \subset \cdots \text{ and } \widetilde{\Gamma}_\infty = \operatorname{ind}\lim_{j\to\infty} \Gamma_j .$$

($\iota\iota$) Let F_d be a finite set in $\mathbb{Z}[\beta]$ such that $\underbrace{\mathbb{Z}_\beta + \cdots \mathbb{Z}_\beta}_{d \text{ times}} \subset \mathbb{Z}_\beta + F_d$.

Suppose that there exists a finite k such that $\beta^k F_d \subset \mathbb{Z}_\beta$. Let Γ^{F_d} (resp. $\Gamma^{F_d}_{kj}$) be the decorated (resp. scaled&decorated) beta-lattice defined by $\Gamma^{F_d} := \Gamma + \sum_{i=1}^n F_d \mathbf{e}_i$ (resp. $\Gamma^{F_d}_{kj} = \Gamma^{F_d}/\beta^{kj}$). Then we have the infinite nested sequence of Delaunay sets and the inductive limit :

$$\cdots \subset \Gamma^{F_d}_{k(j-1)} \subset \Gamma^{F_d}_{jk} \subset \Gamma^{F_d}_{k(j+1)} \subset \cdots$$
$$\text{and } \widetilde{\Gamma}_\infty = \operatorname{ind}\lim_{j\to\infty} \Gamma^{F_d}_j .$$

On the use of beta-lattices as nested sequences - Proposition II

Let β be a Pisot-Vijayaraghavan unit of degree d and $\mathbb{Z}_\beta$ its corresponding set of β-integers. Let $\Gamma = \sum_{i=1}^{n} \mathbb{Z}_\beta \mathbf{e}_i$ be the corresponding beta-lattice in $\mathbb{R}^n$, and $\widetilde{\Gamma}_\infty = \sum_{i=1}^{n} \mathbb{Z}[\beta]\mathbf{e}_i$ the $\mathbb{Z}$-module built from the basis $\mathbf{e}_i$ and the algebraic β.
Suppose that there exist integers which do not have finite β-expansion.
There exists a finite set $F_\mathbb{N} \subset \mathbb{Z}[\beta]$ such that all integers have finite β-expansion $\bmod\ F_\mathbb{N}$. Define the finite set $G_d = F_\mathbb{N} + F_\mathbb{N}\beta + \cdots + F_\mathbb{N}\beta^{d-1} \subset \mathbb{Z}[\beta]$ and the corresponding finite point set in $\mathbb{R}^n$, $\mathcal{G}_d = \sum_{i=1}^{n} G_d \mathbf{e}_i$. Let F_d be a finite set in $\mathbb{Z}[\beta]$ such that $\underbrace{\mathbb{Z}_\beta + \cdots \mathbb{Z}_\beta}_{d \text{ times}} \subset \mathbb{Z}_\beta + F_d$. Suppose there exists a finite k such that $\beta^k F_d \subset \mathbb{Z}_\beta$. Let Γ^{F_d} and $\Gamma^{F_d}_{jk}$ be like in Prop. I.
Then we have the infinite nested sequence of Delaunay sets and the inductive limit :

$$\cdots \subset \Gamma^{F_d}_{k(j-1)} + \mathcal{G}_d \subset \Gamma^{F_d}_{kj} + \mathcal{G}_d \subset \Gamma^{F_d}_{k(j+1)} + \mathcal{G}_d \subset \cdots$$
$$\text{and } \widetilde{\Gamma}_\infty = \operatorname{ind}\lim_{j\to\infty} \Gamma^{F_d}_{kj} + \mathcal{G}_d.$$

Multiresolution analysis of Bragg spectra

- Here is a method of analysing and classifying Bragg spectra in $\mathbb{R}^n$ given some (infinite) nested sequence $\left(\widetilde{\Gamma}_j\right)_{j\in\mathbb{Z}}$ having the support $\mathcal{Z}$ of Bragg peaks as inductive limit :

$$\cdots \subset \widetilde{\Gamma}_{j-1} \subset \widetilde{\Gamma}_j \subset \widetilde{\Gamma}_{j+1} \subset \cdots \quad \text{and} \quad \mathcal{Z} = \text{ind}\lim_{j\to\infty} \widetilde{\Gamma}_j .$$

- The supports of most quasi-crystalline Bragg peaks with k-fold symmetry are precisely the dense rings of cyclotomic integers built from $\zeta = e^{i\frac{2\pi}{k}}$ (up to an irrelevant scale factor).

- Precisely, for β-lattices $\Gamma = \sum_{i=1}^{n} \mathbb{Z}_\beta \mathbf{e}_i$ or some decorated versions $\widetilde{\Gamma}$ of them, where β is Pisot unit, we have

$$\cdots \subset \widetilde{\Gamma}_{j-1} \subset \widetilde{\Gamma}_j \stackrel{\text{def}}{=} \widetilde{\Gamma}/\beta^j \subset \widetilde{\Gamma}_{j+1} \subset \cdots \text{ and } \widetilde{\Gamma}_\infty = \text{ind}\lim_{j\to\infty} \widetilde{\Gamma}_j .$$

with $\widetilde{\Gamma}_\infty = \sum_{i=1}^{n} \mathbb{Z}[\beta]\mathbf{e}_i$.

Multiresolution of Bragg Peaks - I

- Introduce the diffraction spectrum with "cut-off" $X > 0$:
  The subset of Bragg peaks $\Pi(X) \subset \Pi$ is defined by :

$$\Pi(X) = \{p = (\mathbf{x}, I_{\mathbf{x}}) \in \Pi \mid I_{\mathbf{x}} \geq X\} \,.$$

- Clearly the set-valued function $X \to \Pi(X)$ is decreasing till reaching the empty set value :

$$X \geq Y \Rightarrow \Pi(X) \subset \Pi(Y),$$
$$\text{and } \forall X > I_{\max},\ \Pi(X) = \emptyset.$$

Multiresolution of Bragg Peaks - II : "Model Set" Assumption

- In order to put in relation the nested continuously indexed family $(\Pi(X))_{X\in\mathcal{I}}$ and the nested discretely indexed sequence $\left(\widetilde{\Gamma}_j\right)_{j\in\mathbb{Z}}$ we need the :

  Assumption 1 *For any $X > 0$ there exists $j \in \mathbb{Z}$ such that $\Pi(X)$ is supported by $\widetilde{\Gamma}_j$*

  $$\mathrm{Supp}(\Pi(X)) \subset \widetilde{\Gamma}_j.$$

- One next proceed to a discretization of the intensity interval $\mathcal{I}$ based on

  Assumption 2 *To any $j \in \mathbb{Z}$ there corresponds the positive real X_j defined by*

  $$X_j = \min\left\{X \mid \mathrm{Supp}(\Pi(X)) \subset \widetilde{\Gamma}_j\right\}.$$

- Concretely, if $X \geq X_j$, then $\Pi(X)$ is supported by $\widetilde{\Gamma}_j$, whereas if $X < X_j$, there exists $p \in \Pi(X)$ such that $\mathbf{x}(p) \notin \widetilde{\Gamma}_j$.

Multiresolution of Bragg Peaks - III :
***Multiresolving Filter* and Partition**

Definition 1 *Given the nested sequence* $\left(\widetilde{\Gamma}_j\right)_{j\in\mathbb{Z}}$ *such that Assumptions 1 and 2 hold true, two nested sequences of subsets of the spectrum are relevant :*

$$P_i = \Pi(X_i)\,, \tag{1}$$

$$G_j = \{p = (\mathbf{x}, I_{\mathbf{x}}) \in \Pi \mid \mathbf{x} \in \Gamma_j\} \tag{2}$$

Note that (2) depends more on the geometrical disposal of the spectrum whereas (1) is more centered on intensity features. Clearly, both increasing sequences have the pp diffraction spectrum Π as inductive limit :

$$\cdots \subset P_{i-1} \subset P_i \subset P_{i+1} \subset \cdots \subset \Pi\,,$$

$$\cdots \subset G_{j-1} \subset G_j \subset G_{j+1} \subset \cdots \subset \Pi\,.$$

Multiresolution of Bragg Peaks - IV : *Multiresolving Filter* and Partition

Of course, if we make explicit one of the approximation sets in each sequence, say P_i (resp. G_j), and if we wish to be more precise by dealing with the next approximation, P_{i+1} (resp. G_{j+1}), it is not needed to reboot all the analysis : it is enough to add “detail” set D_i^P (resp. D_j^G) along the following partitions :

$$
\begin{aligned}
P_{i+1} &= P_i \cup D_{i+1}^P, \\
D_{i+1}^P &:= \left\{p = (\mathbf{x}, I_{\mathbf{x}}) \in \Pi \;\mid\; X_{i+1} \leq I_{\mathbf{x}} < X_i\right\}, \\
G_{j+1} &= G_j \cup D_{j+1}^G, \\
D_{j+1}^G &:= \left\{p = (\mathbf{x}, I_{\mathbf{x}}) \in \Pi \;\mid\; \mathbf{x} \in \widetilde{\Gamma}_{j+1} \setminus \widetilde{\Gamma}_j\right\}.
\end{aligned}
$$

In the language of wavelets and multiresolution analysis, the sets P_i and G_j are referred to as the tendency *at scale i and j, respectively, and the sets D_{i+1}^P and D_{j+1}^G as the sets of* details.

Multiresolution of Bragg Peaks - IV : The Fingerprint

Hence we get the two partitions of the pp diffraction spectrum :

$$\Pi = \bigcup_{i=-\infty}^{\infty} D_i^P \ , \quad \text{and} \quad \Pi = \bigcup_{j=-\infty}^{\infty} D_j^G \ .$$

These two partitions are not identical and each one presents its own advantages in carrying out a classification of the Bragg peaks based on multiresolution . Obvious refinement is based on the intersection of the two partitions.

Multiresolution of Bragg Peaks - V : The Fingerprint

Proposition 1 *With the above definitions and supposing that Assumptions 1 and 2 are fulfilled, the most refined partition of the pp-diffraction spectrum* Π *reads as :*

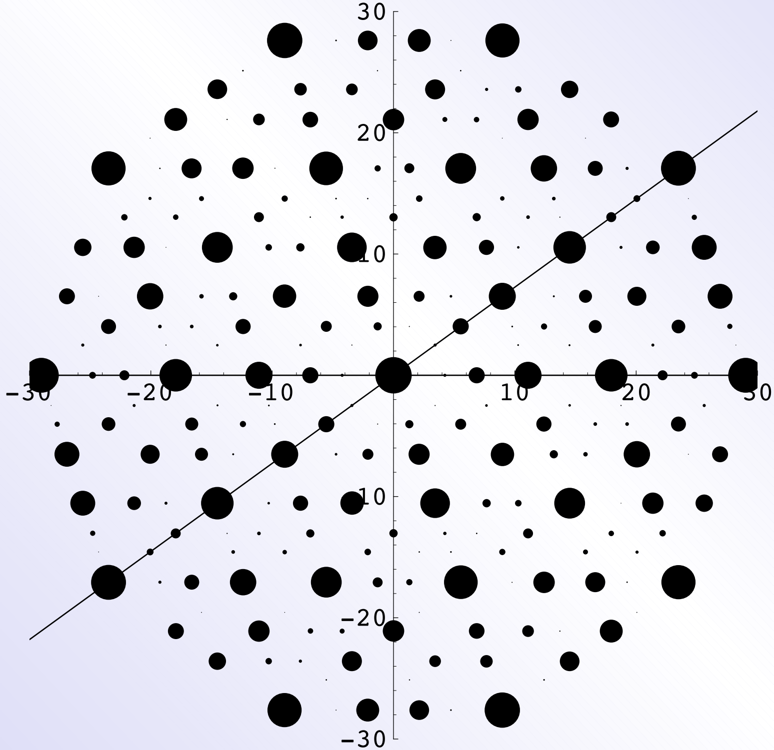
$$\Pi = \bigcup_{i,j=-\infty}^{\infty} R_{i,j},$$

where

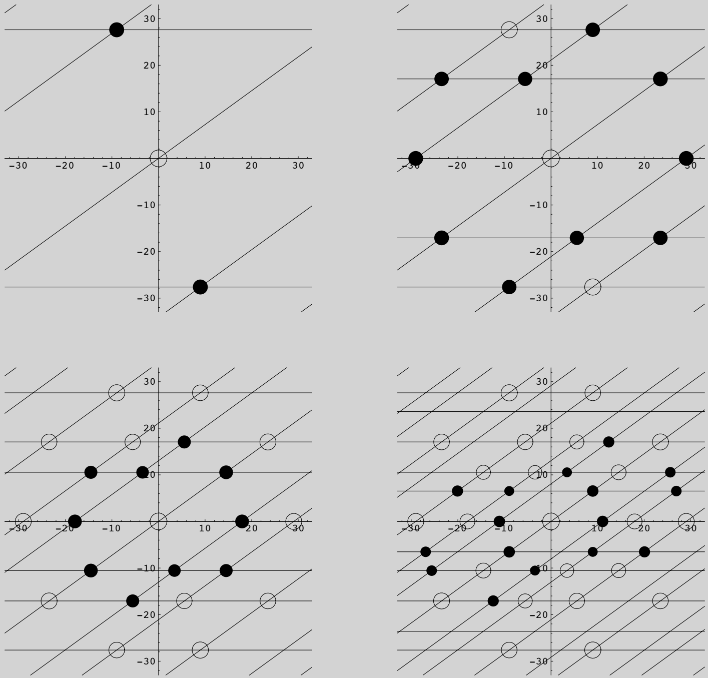
$$\begin{aligned} R_{i,j} &= D_i^P \cap D_j^G \\ &= \big\{ p = (\mathbf{x}(p), I_{\mathbf{x}}(p)) \in \Pi \;\mid \mathbf{x}(p) \in \widetilde{\Gamma}_j \setminus \widetilde{\Gamma}_{j-1} \\ &\text{and } X_i \leq I_{\mathbf{x}}(p) < X_{i-1} \big\} \end{aligned}$$

The table of values $|R_{i,j}|$ is the fingerprint.

(Academic) example : Fingerprint of Tau-Lattice Diffraction Pattern - I

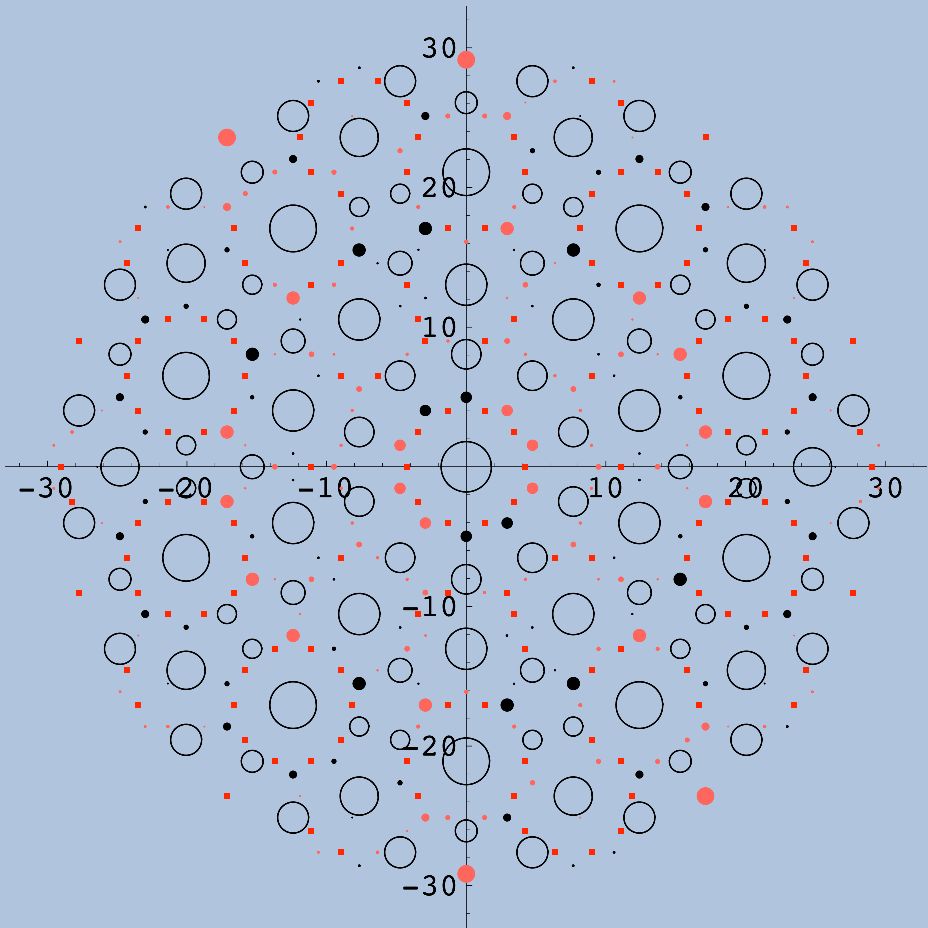


(Academic) example : Fingerprint of Tau-Lattice Diffraction Pattern - II

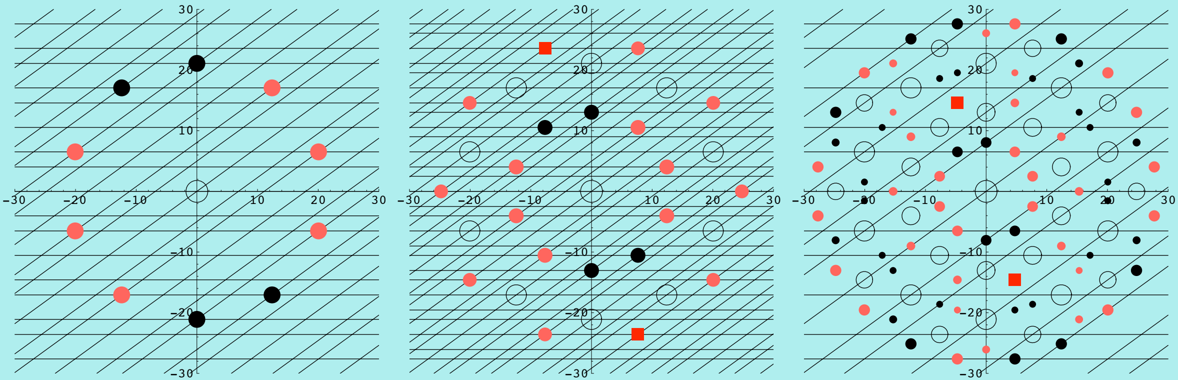


$(\lvert R_{ij}\rvert)\ j\backslash i$	0	1	2	3	4	5	6	7
$X_0 = 1$	1							
$X_1 = 0.970673$		2						
$X_2 = 0.924877$			10					
$X_3 = 0.814151$				10				
$X_4 = 0.642199$					16			
$X_5 = 0.300888$					18	46		
$X_6 = 0.046841$						32	62	
$X_7 = 0.02$						2	32	12

(Academic) example : Fingerprint of Penrose Diffraction Pattern - I

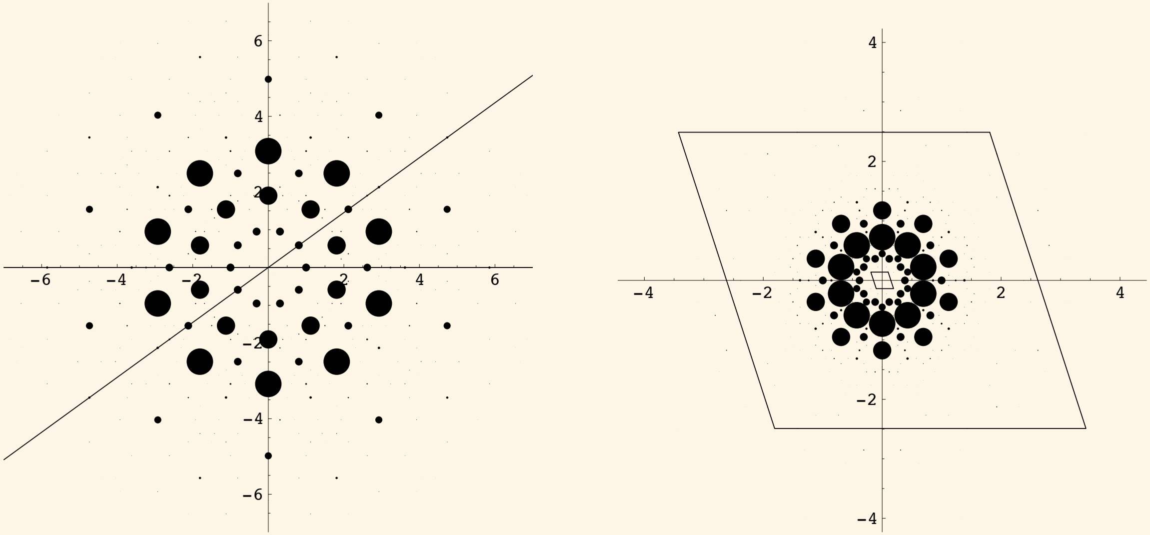


(Academic) example : Fingerprint of Penrose Diffraction Pattern - II



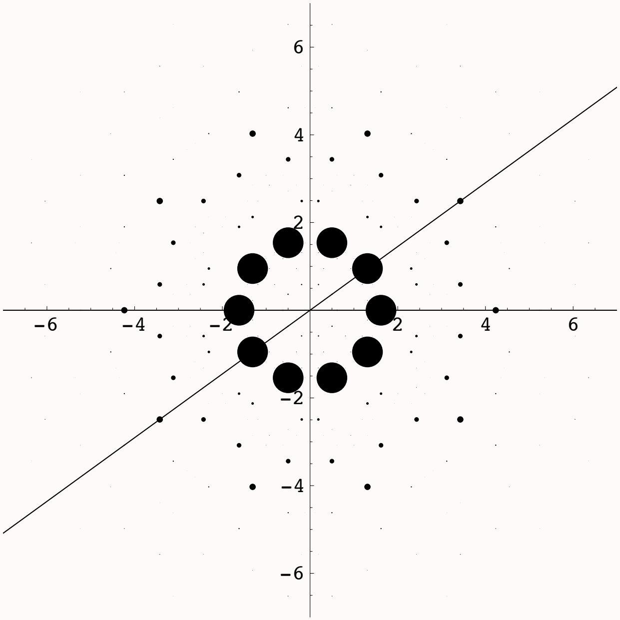
$(\|R_{ij}\|)\ j\backslash i$	0	1	2	3	4	5	6	7	8	9
$X_0 = 1$	1									
$X_5 = 0.92691$					6	4				
$X_6 = 0.757223$					2	14	4			
$X_7 = 0.378328$						5	34	34		
$X_8 = 0.038948$		2	8	2	12	34	86	136	90	
$X_9 = 0.02$							10	34	40	16

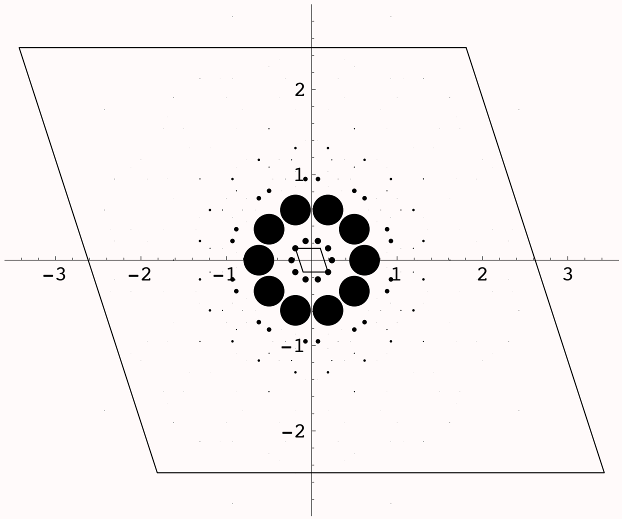
Steurer Kao model



Diffraction pattern of the Steurer and Kuo model for the plane $l = 0$*. On the left-hand side : in the physical space together with the grid* Γ_0 *; on the right-hand side : in the internal space together with the envelope* $\tau^8 R_\tau$*.*

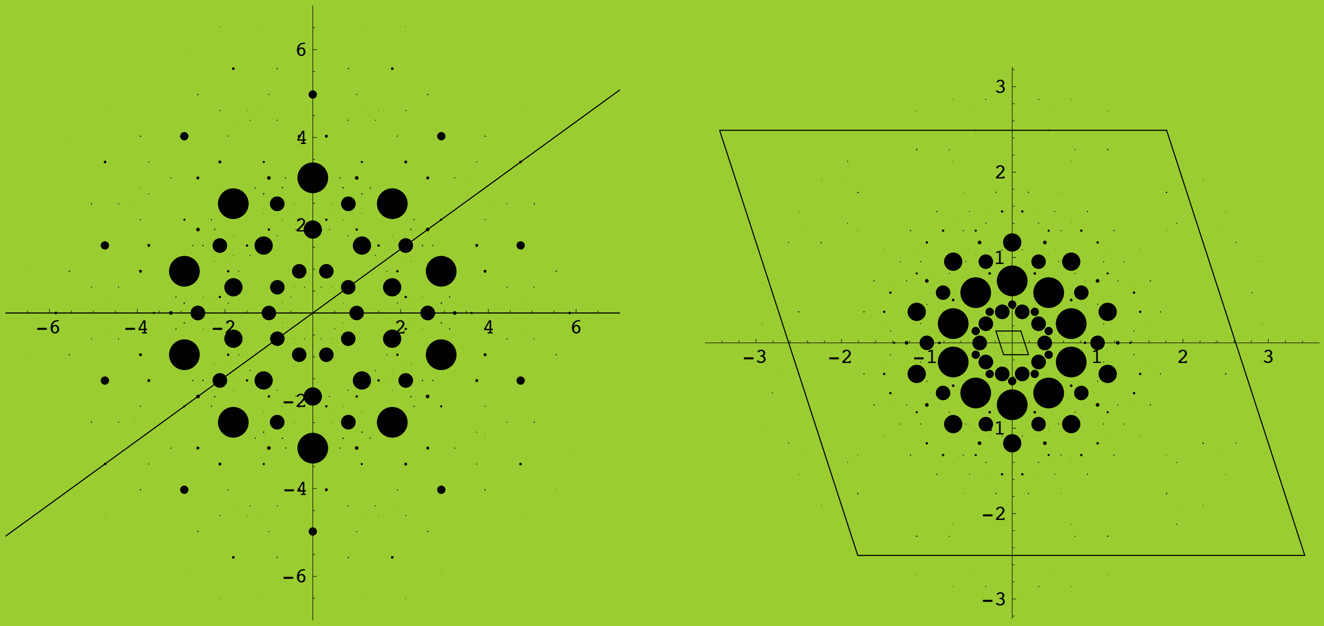
Steurer Kao model





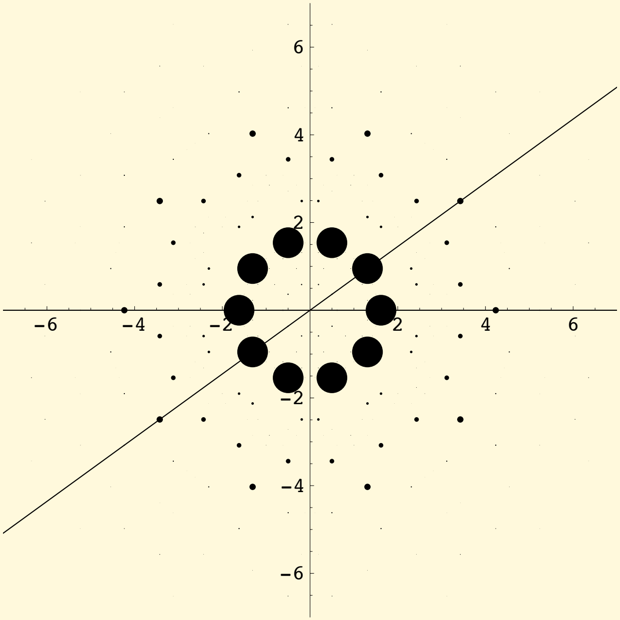
plane $l = 1$

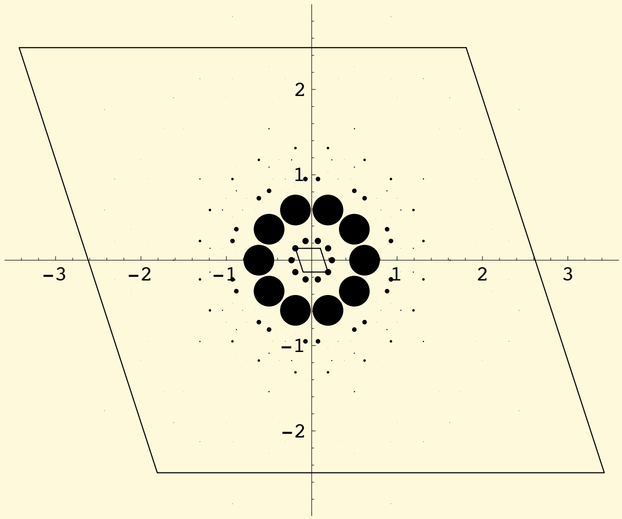
Steurer Kao model



plane $l = 2$.

Steurer Kao model





plane $l = 3$

0.1. plane $l = 0$

$X_i \diagdown j$	0	1	2	3	4	5	6	7	8	9
$X_6 = 51.65$						6	4			
$X_7 = 10.59$				2	16	28	36	28		
$X_9 = 3.8$		2	10	8	6	32	80	110	66	16

0.2. plane $l = 1$

$X_i \diagdown j$	0	1	2	3	4	5	6	7	8	9
$X_5 = 30.19$			2	8	2	8				
$X_6 = 25.75$						4	16			
$X_7 = 9.72$					12	16	38	24		
$X_8 = 9.47$								4	16	
$X_9 = 5.56$						12	34	96	40	

0.3. plane $l = 2$

$X_i \diagdown j$	0	1	2	3	4	5	6	7	8	9
$X_6 = 38.38$						6	4			
$X_7 = 10.71$				2	16	28	36	28		
$X_8 = 6.98$					4	20	32	28	16	
$X_9 = 2.85$		2	8			4	54	142	122	28

0.4. plane $l = 3$

$X_i \diagdown j$	0	1	2	3	4	5	6	7	8	9
$X_5 = 23.05$			2	8	2	8				
$X_6 = 19.19$						4	16			
$X_7 = 6.23$				2	20	16	52	40		
$X_8 = 6.11$								4	16	
$X_9 = 3.37$					4	28	24	92	72	

Practical use of this approach

- *Equipped with these nested sequences of inflated/deflated versions of beta-integers and beta-lattices, we become able to build "catalogues" of diffraction patterns due to standard or manageable well-identified site occupation distributions, and then implement our multiresolution analysis of each of them.*
- *The issue will be a catalogue of diffraction patterns. Having this catalogue at our disposal, one can then examine experimental diffraction patterns, those ones displayed by real quasicrystals or other more or less exotic structures.*
- *The next step will be a (patient !) labor of (statistical) comparison, classification, and identification.*