COHERENT and DISSIPATIVE TRANSPORT

in

APERIODIC SOLIDS: B

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III - Aperiodic Solids

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in *From Number Theory to Physics*, pp. 538-630, Les Houches March 89, Springer,
J.M. Luck, P. Moussa & M. Waldschmidt Eds., (1993).

J. BELLISSARD, D. HERRMANN, M. ZARROUATI, *Hull of Aperiodic Solids and Gap Labelling Theorems*,
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Aperiodic Materials:

- Perfect Crystals
- Crystal with disorder (metals)
- Impurities in Semiconductors
- Quasicrystals
- Glasses

III.1)- The Hull

Equilibrium positions of atomic nuclei make up a point set $\mathcal{L} \subset \mathbb{R}^d$ *the set of lattice sites*. $\mathcal{L}$ may be:

1. *Discrete*.
2. *Uniformly discrete*: $\exists r > 0$ s.t. each ball of radius r contains at most one point of $\mathcal{L}$. Then $\mathcal{L}$ is r-discrete.
3. A *Delone* set: $\mathcal{L}$ is r-uniformly discrete and *relatively dense* : $\exists R > 0$ s.t. each ball of radius R contains at least two points of $\mathcal{L}$. Then $\mathcal{L}$ is (r, R)-Delone.
4. A *Meyer* set: $\mathcal{L}$ and $\mathcal{L} - \mathcal{L}$ are Delone sets. Correspondingly $\mathcal{L}$ is $(r, R; r', R')$-Meyer.

Examples:

1. A random Poissonian set in $\mathbb{R}^d$ is almost surely discrete but not uniformly discrete nor relatively dense.
2. Due to Coulomb repulsion and Quantum Mechanics, **lattices of atoms are always uniformly discrete**.
3. Impurities in semiconductors are not relatively dense.
4. In amorphous media $\mathcal{L}$ is Delone.
5. In a quasicrystal $\mathcal{L}$ is Meyer.

Point Measures

$\mathfrak{M}(\mathbb{R}^d)$ is the set of Radon measures on $\mathbb{R}^d$ namely the dual space to $\mathcal{C}_c(\mathbb{R}^d)$ (continuous functions with compact support), endowed with the weak* topology.

For $\mathcal{L}$ a *uniformly discrete* point set in $\mathbb{R}^d$:

$$\nu := \nu^{\mathcal{L}} = \sum_{y \in \mathcal{L}} \delta(x-y) \qquad \in \mathfrak{M}(\mathbb{R}^d) \ .$$

The *Hull* is the closure in $\mathfrak{M}(\mathbb{R}^d)$

$$\Omega = \overline{\left\{ \mathrm{T}^a \nu^{\mathcal{L}} ; a \in \mathbb{R}^d \right\}} \ ,$$

where $\mathrm{T}^a \nu$ is the translated of ν by a.

Facts:

1. Ω is compact and $\mathbb{R}^d$ acts by homeomorphisms.
2. If $\omega \in \Omega$, there is a uniformly discrete point set $\mathcal{L}_\omega$ in $\mathbb{R}^d$ such that ω coincides with $\nu_\omega = \nu^{\mathcal{L}_\omega}$.
3. If $\mathcal{L}$ is *Delone* (resp. *Meyer*) so are the $\mathcal{L}_\omega$'s.

Properties

(a) Minimality

$\mathcal{L}$ is *repetitive* if for any finite patch p there is $R > 0$ such that each ball of radius R contains an ϵ-approximant of a translated of p.

Proposition 1 *$\mathbb{R}^d$ acts minimaly on Ω if and only if $\mathcal{L}$ is repetitive.*

(b) Transversal

The closed subset $X = \{\omega \in \Omega \; ; \; \nu_\omega(\{0\}) = 1\}$ is called the *canonical transversal*. Let G be the subgroupoid of $\Omega \rtimes \mathbb{R}^d$ induced by X.

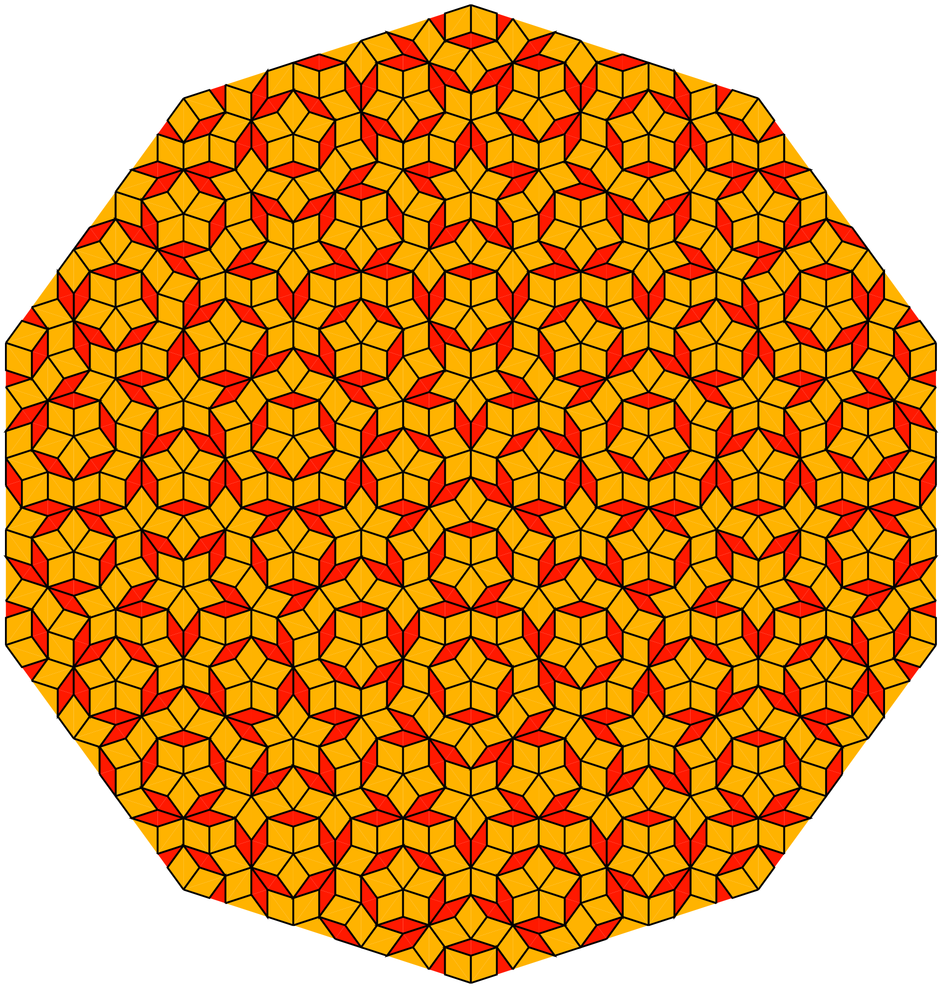
A Delone set $\mathcal{L}$ has *finite type* if $\mathcal{L} - \mathcal{L}$ is closed and discrete.

(c) Cantorian Transversal

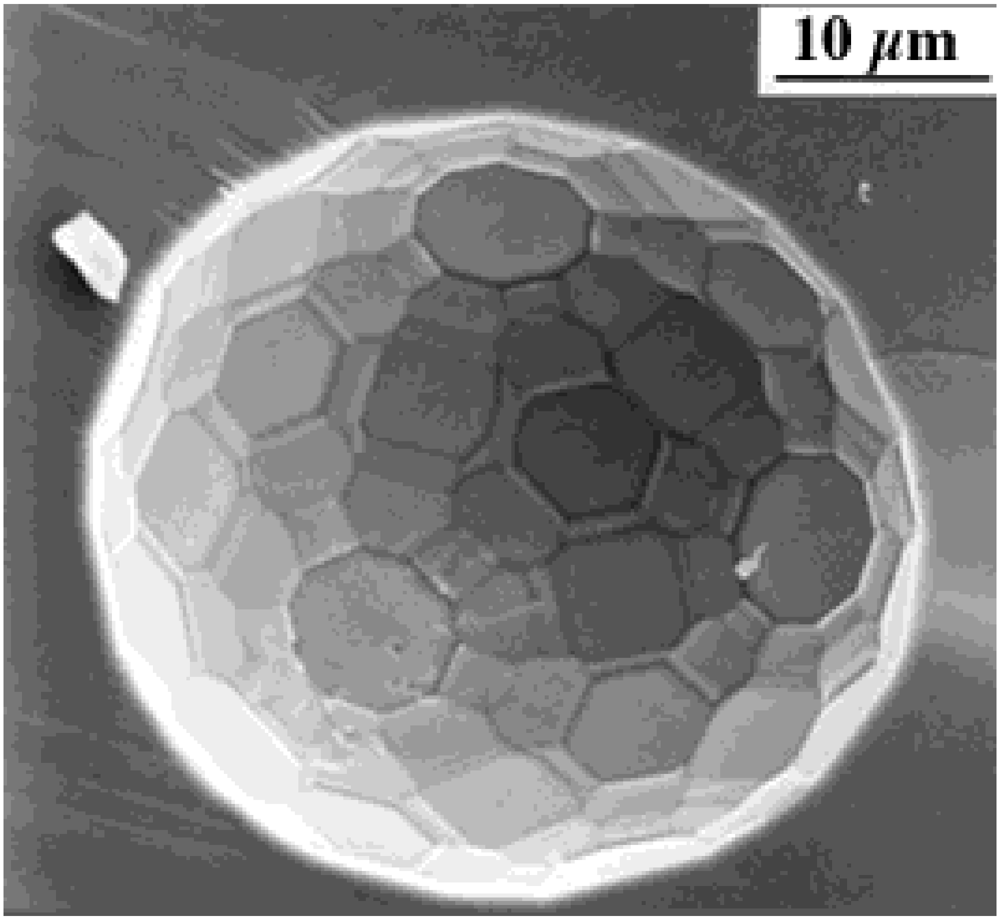
Proposition 2 *If $\mathcal{L}$ has finite type, then the transversal is completely discontinuous (Cantor).*

III.2)- Examples of Hulls

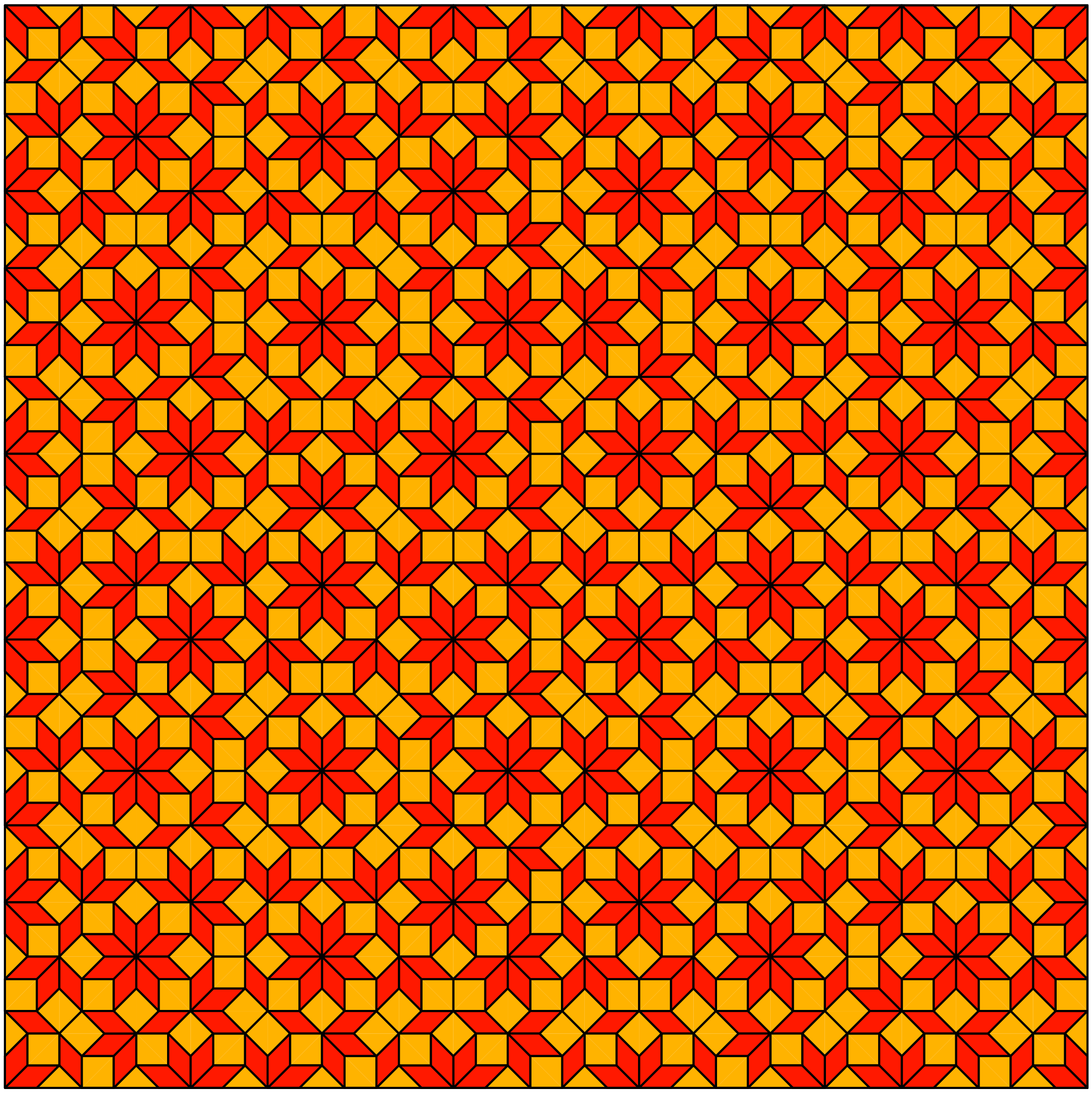
- For a perfect crystal $\mathcal{L}$ in $\mathbb{R}^d$ with period group Γ, the Hull is the torus $\Omega = \mathbb{R}^d/\Gamma$.
  The transversal is $\Sigma = \mathcal{L}/\Gamma$. It is finite.
- The Hull of a quasicrystal can be built by the *cut-and-project* method.
  Its transversal is Cantorian.
- Impurities in a Si-crystal:
  1. the lattice $\mathcal{L}$ of Si has diamond type it is $\mathbb{Z}^3$-invariant;
  2. if $x \in \mathcal{L}$, $\sigma_x \in \mathfrak{A}$ denotes the impurity at x;
  3. $\mathfrak{A} = \{0 = Si, P, I, \cdots\}$ is the *alphabet* labelling impurities;
  4. $\underline{\sigma} = (\sigma_x)_{x\in\mathcal{L}}$, $\quad a \in \mathbb{Z}^3 \Rightarrow a \cdot \underline{\sigma} = (\sigma_{x-a})_{x\in\mathcal{L}}$;
  5. *the transversal is* $\Sigma = \mathfrak{A}^{\mathcal{L}}$
     it is Cantorian and $\mathbb{Z}^3$-invariant;
  6. *the Hull is the suspension* $\Omega = \Sigma \times \mathbb{R}^3/\mathbb{Z}^3$, with action $a : (\underline{\sigma}, y) \mapsto (a\underline{\sigma}, y + a)$.



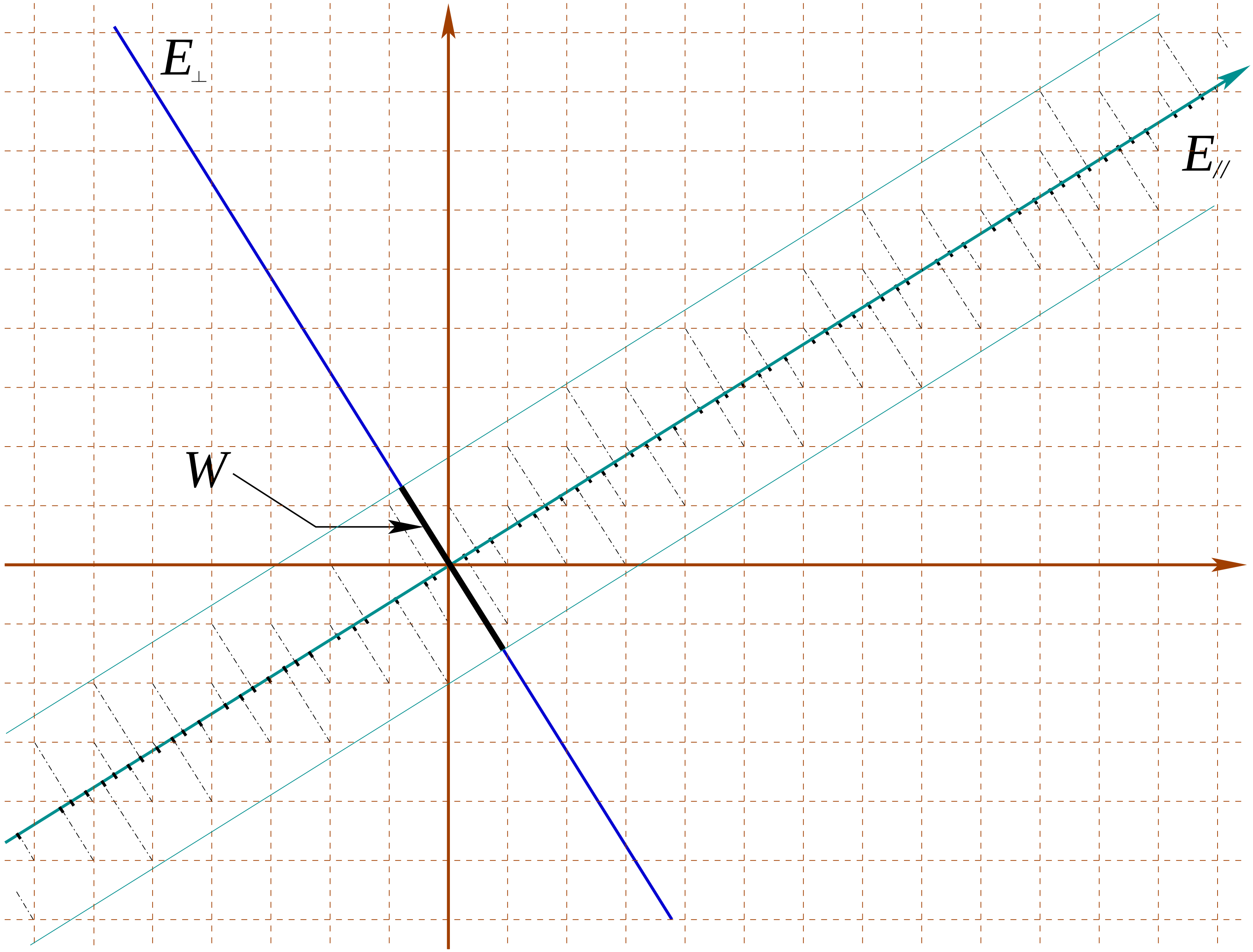
- The Penrose Tiling -



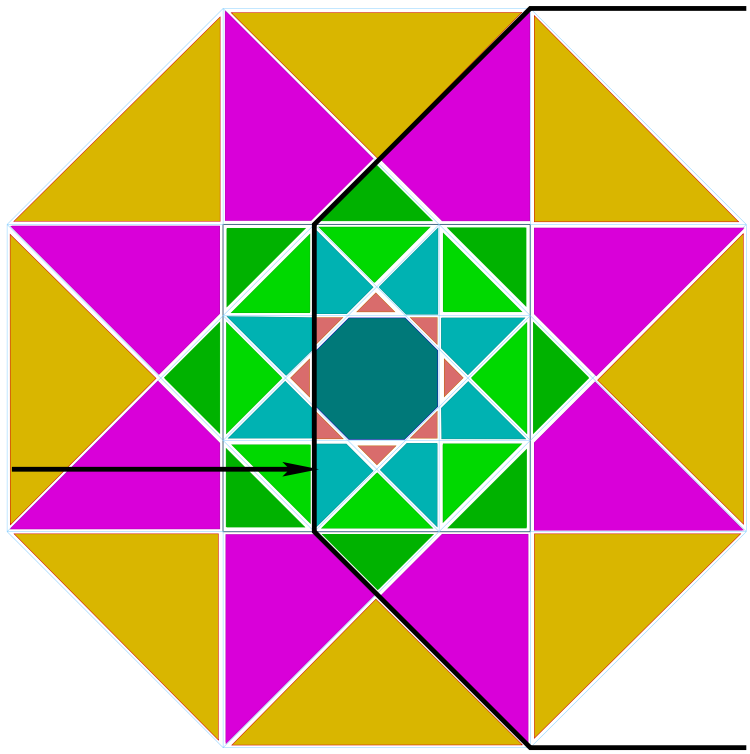
- A hole in icosahedral $AlPdMn$ -

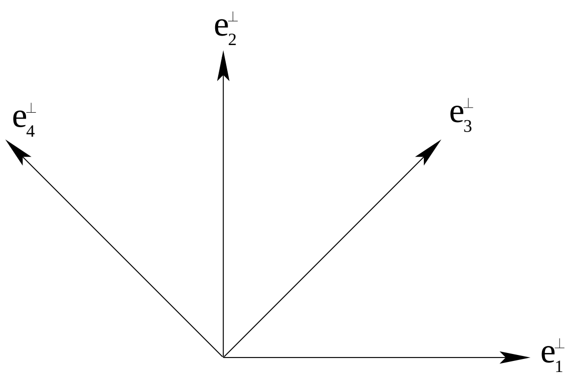


- The Octagonal Tiling -



− The cut−and−project construction −

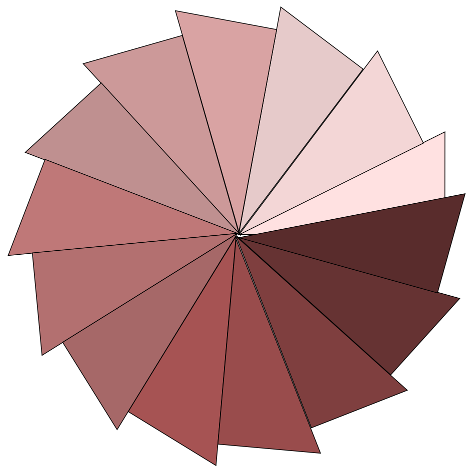


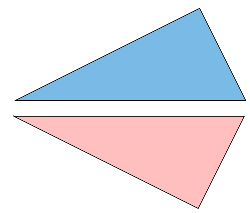


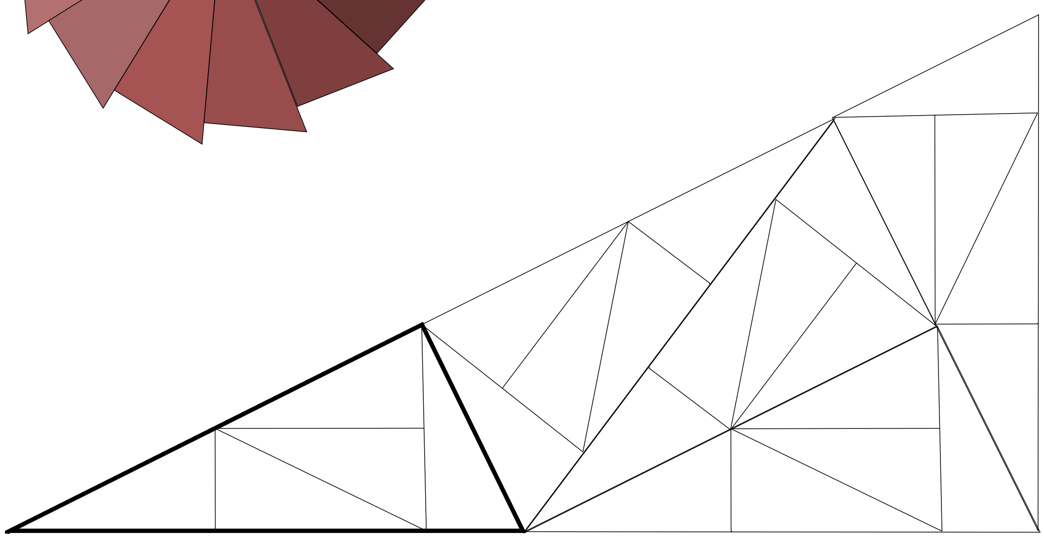
- The Window of the Octagonal Tiling -

The intersections $W \cap (W - a_1) \cap \cdots \cap (W - a_n)$ are clopen sets for any family $a_1, \cdots a_n$ in the $\mathbb{Z}$-module generated by $e_1^\perp, \cdots, e_4^\perp$.

$\Rightarrow$ *W is a Cantor set*.







- *The pinwheel tiling is NOT FPC !* -

Its Hull is invariant by $U(1)$.

III.3)- $T = 0$ Gibbs States

- Let $\mathfrak{M}$ be the space of Radon measure on $\mathbb{R}^d$ endowed with the weak$*$-topology with respect to $\mathcal{C}_c(\mathbb{R}^d)$.
- $UD_r(\mathbb{R}^d)$ is the set of Radon measures $\nu_{\mathcal{L}}$ with $\mathcal{L}$ being r-discrete. Set
  $UD(\mathbb{R}^d) = \bigcup_{r>0} UD_r(\mathbb{R}^d)$.
- $Del_{(r,R)}(\mathbb{R}^d)$ is the set of Radon measures $\nu_{\mathcal{L}}$ with $\mathcal{L}$ being (r, R)-Delone. Set
  $Del(\mathbb{R}^d) = \bigcup_{0<r\leq R} Del_{(r,R)}(\mathbb{R}^d)$.
- $Mey_{(r,R;r',R')}(\mathbb{R}^d)$ is the set of Radon measures $\nu_{\mathcal{L}}$ with $\mathcal{L}$ being $(r, R; r', R')$-Meyer. Set
  $Mey(\mathbb{R}^d) = \bigcup_{0<r\leq R, 0<r'\leq R'} Mey_{(r,R;r',R')}(\mathbb{R}^d)$.
- $QD(\mathbb{R}^d)$ is the closure of $UD(\mathbb{R}^d)$. An element of QD is called a *quasidiscrete set*.

Theorem 1 *(i) $UD_r \supset Del_{(r,R)} \supset Mey_{(r,R;r',R')}$ are compact subsets of $\mathfrak{M}$ for all $0 < r \leq R$ and $0 < r' \leq R'$.*

(ii) $\bigcup_{0<r'\leq R'} Mey_{(r,R;r',R')}$ is dense in $Del_{(r,R)}$;

(iii) $\bigcup_{0<R} Del_{(r,R)}$ is dense in UD_r;

(iv) A Radon measure μ belongs to QD iff there is a discrete point set $\mathcal{L}$ such that

$$\mu = \sum_{x\in\mathcal{L}} n_x \, \delta(\cdot - x)$$

where $n_x \in \mathbb{N}_*$ for all $x \in \mathcal{L}$.

Thus a *quasidiscrete set* can be seen as a discrete subset of $\mathbb{R}^d$ with finitely many atoms on top of each other at each site. If $\mu \in \mathfrak{M}$, $a \in \mathbb{R}^d$, $\tau^a\mu$ denote the a-translated of μ.

Theorem 2 *QD, UD_r, $Del_{(r,R)}$ and $Mey_{(r,R;r',R')}$ $\mathbb{R}^d$-invariant subsets of $\mathfrak{M}$.*

Gibbs measures are basic tools in Thermodynamics and describe the equilibrium states of the atomic array. They have the following properties:

1. A *Gibbs state* describing the atomic equilibrium is given by a probability measure $\mathbb{P}$ on $QD(\mathbb{R}^d)$.
   (*Note that* $QD(\mathbb{R}^d)$ *is a polish space*).

2. Whenever unique, $\mathbb{P}$ is $\mathbb{R}^d$-invariant and ergodic.
   (*Non-uniqueness means coexistence of phases*).

3. To describe a solid, *at* $T = 0$, $\mathbb{P}$ is expected to give probability one to UD, Del or Mey.
   $\mathbb{P}$ is called *uniformly discrete, Delone or even Meyer* if it gives probability one to UD, Del, Mey respectively.

Theorem 3 *If $\mathbb{P}$ is a $\mathbb{R}^d$-invariant ergodic uniformly discrete probability measure on $QD(\mathbb{R}^d)$, then:*
(i) There is $r > 0$ unique such that $\mathbb{P}\{UD_r\} = 1$ and for every $r' > r$, $\mathbb{P}\{UD_{r'}\} = 0$.
(ii) for $\mathbb{P}$-almost all $\nu \in QD(\mathbb{R}^d)$, the Hull of ν is compact and given by the topological support of $\mathbb{P}$.

Thus a *uniformly discrete Gibbs measure* $\mathbb{P}$ determines the Hull $\Omega_{\mathbb{P}}$ with probability one.

Proposition 3 *(i) If $\mathbb{P}$ is an $\mathbb{R}^d$-invariant ergodic Delone probability measure on $QD(\mathbb{R}^d)$, there is $0 < r \leq R$ unique such that $\mathbb{P}\{Del_{(r,R)}\} = 1$ and, for every $(r', R') \neq (r, R)$ with $r' \geq r, R' \leq R$, $\mathbb{P}\{Del_{(r',R')}\} = 0$.*
(i) If $\mathbb{P}$ is a $\mathbb{R}^d$-invariant ergodic Meyer probability measure, there are $0 < r \leq R$, $0 < r' \leq R'$ unique such that $\mathbb{P}\{Mey_{(r,R;r',R')}\} = 1$ and, for every $(r_1, R_1; r'_1, R'_1) \neq (r, R; r', R')$ with $r_1 \geq r$, $r'_1 \geq r'$, $R_1 \leq R$, $R'_1 \leq R'$, $\mathbb{P}\{Mey_{(r_1,R_1;r'_1,R'_1)}\} = 0$.

III.4)- Diffraction Measure

For Λ a ball in $\mathbb{R}^d$, the *diffraction measure* associated with $\nu_{\mathcal{L}} \in UD$ is given by the density

$$\rho_\Lambda^{(\mathcal{L})}(k) \;=\; \frac{1}{|\Lambda|}\left|\sum_{x\in\mathcal{L}\cap\Lambda} e^{\imath k\cdot x}\right|^2$$

Theorem 4 *If $\mathbb{P}$ is a $\mathbb{R}^d$-invariant ergodic uniformly discrete probability measure on $QD(\mathbb{R}^d)$, then for $\mathbb{P}$-almost every $\nu \in QD$ the family $\left(\rho_\Lambda^{(\mathcal{L})}\right)_{\Lambda\subset\mathbb{R}^d}$ converges as $\Lambda \uparrow \mathbb{R}^d$ to a measure $\rho_{\mathbb{P}} \in \mathfrak{M}(\mathbb{R}^{d*})$ such that:*
(i) $\rho_{\mathbb{P}}$ is positive,
(ii) its Fourier transform is positive and supported by the closure of $\mathcal{L} - \mathcal{L}$.

Thus the diffraction picture seen by an experimentalist depends only upon the Gibbs measure describing the atomic equilibrium.

III.4)- Bloch Theory

- If $\mathcal{L}$ is periodic with period group $\mathbb{G}$, the Voronoi cell, called *the Bravais zone*, can be identified with

$$\mathbb{V} = \mathbb{R}^d/\mathbb{G}$$

- The group $\mathbb{G}^\perp$ orthogonal to $\mathbb{G}$ in the dual space $\mathbb{R}^{d\,*}$ is *the reciprocal lattice*. By Pontryagin duality

$$\mathbb{G}^\perp \simeq \mathbb{V}^*$$

- The corresponding Voronoi cells are called *Brillouin zones*. They can also be identified with the quotient

$$\mathbb{B} = \mathbb{R}^{d\,*}/\mathbb{G}^\perp \simeq \mathbb{G}^*$$

  $\mathbb{B}$ is topologically a torus $\mathbb{T}^d$.
  It represents the *momentum space* of the crystal.

- Let now $\mathcal{H} = L^2(\mathbb{R}^d)$. Translation $a \in \mathbb{R} \mapsto T(a)$ on $\mathcal{H}$: $T(a)\psi(x) = \psi(x-a)$.
- textcolorequa$H = H^*$: selfadjoint operator on $\mathcal{H}$ with $\mathbb{G}$-invariant dense domain. H is *$\mathbb{G}$-periodic* if

$$T(a)HT(a)^{-1} = H\,, \qquad a \in \mathbb{G}$$

- **Example:** the Schrödinger operator

$$H = -\Delta + V \qquad V(x+a) = V(x) \ \forall a \in \mathbb{G}$$

with $\Delta = d$-Laplacian, $V \in L^1 + L^p$ with $p > d/2$.

- Then

$$\mathcal{H} \simeq \int_{\mathbb{B}}^{\oplus} \frac{d^d k}{|\mathbb{B}|}\, \mathcal{H}_k \qquad H \simeq \int_{\mathbb{B}}^{\oplus} \frac{d^d k}{|\mathbb{B}|}\, H_k$$

$$\mathcal{H}_k = L^2(\mathbb{V})\,, \quad H_k = \left(\frac{\hbar}{\imath}\vec{\nabla} + k\right)^2 + V(.)\,.$$

- The spectrum of H_k is *discrete*. Eigenvalues $E_n(k)$ are continuous (analytic) on $\mathbb{B}$

$$\sigma(H) = \cup_n B_n\,, \quad B_n = \{E_n(k); k \in \mathbb{B}\}$$

B_n is called a *band*.

III.5)- Noncommutative Brillouin Zone

- Here $\mathcal{L}$ is a uniformly discrete set with Hull Ω and $\mathbb{R}^d$-action τ. $(\Omega, \mathbb{R}^d, \tau)$ is a topological dynamical system with at least one dense orbit.
- The crossed product

$$\mathcal{A} = \mathcal{C}(\Omega) \rtimes_\tau \mathbb{R}^d$$

is (almost) the smallest C^*-algebra containing both the space of continuous functions on Ω and the action of $\mathbb{R}^d$ submitted to the commutation rules (for $f \in \mathcal{C}(\Omega)$)

$$T(a) f T(a)^{-1} = f \circ \tau^{-a}, \qquad a \in \mathbb{R}^d$$

- For a crystal $\Omega = \mathbb{V}$, $\mathbb{R}^d$ acts by quotient action

$$\mathcal{C}(\mathbb{V}) \rtimes_\tau \mathbb{R}^d \simeq \mathcal{C}(\mathbb{B}) \otimes \mathcal{K},$$

where $\mathcal{K}$ is the algebra of compact operators.

- *$\mathcal{A}$ is the Noncommutative version of the space of $\mathcal{K}$-valued function over the Brillouin zone*.

Construction of $\mathcal{A}$:

Endow $\mathcal{A}_0 = \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ with (here $A, B \in \mathcal{A}_0$):

1. Product
$$A \cdot B(\omega, x) = \int_{y \in \mathbb{R}^d} d^d y \, A(\omega, y) \, B(\tau^{-y}\omega, x - y)$$

2. Involution
$$A^*(\omega, x) = \overline{A(\tau^{-x}\omega, -x)}$$

3. A faithfull family of representations in $\mathcal{H} = L^2(\mathbb{R}^d)$
$$\pi_\omega(A) \, \psi(x) = \int_{\mathbb{R}^d} d^d y \; A(\tau^{-x}\omega, y - x) \cdot \psi(y)$$
if $A \in \mathcal{A}_0$, $\psi \in \mathcal{H}$.

4. C^*-norm
$$\|A\| = \sup_{\omega \in \Omega} \|\pi_\omega(A)\| \; .$$

Definition 1 *The C^*-algebra $\mathcal{A}$ is the completion of $\mathcal{A}_0$ under this norm.*

Calculus on $\mathcal{A}$:

Integration: Let $\mathbb{P}$ be an $\mathbb{R}^d$-invariant ergodic probability measure on Ω. Then set (for $A \in \mathcal{A}_0$)):

$$\mathcal{T}_{\mathbb{P}}(A) = \int_{\Omega} d\mathbb{P}\ A(\omega, 0) = \overline{< 0|\pi_\omega(A)0 >}^{dis.}$$

Then $\mathcal{T}_{\mathbb{P}}$ extends as a *positive trace* on $\mathcal{A}$.

Trace per unit volume:
thanks to Birkhoff's theorem:

$$\mathcal{T}_{\mathbb{P}}(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \mathrm{Tr}(\pi_\omega(A) \restriction_\Lambda) \quad \text{a.e. } \omega$$

Differential calculus:
A commuting set of $*$-derivations is given by

$$\partial_i A(\omega, x) = \imath x_i\ A(\omega, x)$$

on $\mathcal{A}_0$. Then $\pi_\omega(\partial_i A) = -\imath[X_i, \pi_\omega(A)]$ where $X = (X_1, \cdots, X_d)$ is the *position operator*.

III.6)- Electronic Hamiltonian

- The Schrödinger Hamiltonian for an electron in $\mathcal{L}$ is typically

$$H_\omega = -\Delta + \sum_{y \in \mathcal{L}_\omega} v(X - y)\,, \qquad \omega \in \Omega\,.$$

acting on $\mathcal{H} = L^2(\mathbb{R}^d)$.
$v \in L^p(\mathbb{R}^d) \cap \mathcal{C}(\mathbb{R}^d)$ is the *atomic potential*.

Theorem 5 *For any $z \in \mathbb{C} \setminus \mathbb{R}$ there is $R(z) \in \mathcal{A}$ such that*

$$\pi_\omega(R(z)) \;=\; \frac{1}{z \;-\; H_\omega}$$

The *algebraic spectrum* of H is defined by

$$\Sigma \;=\; \bigcup_{\omega \in \Omega} \sigma(H_\omega) \;\;\Leftrightarrow\;\; \sigma(R(z)) \;=\; \frac{1}{z - \Sigma}$$

Density of States:

- The Density of States (DOS) is the positive measure $\mathcal{N}_{\mathbb{P}}$ on $\mathbb{R}$ defined by

$$\int_{\mathbb{R}} \frac{d\mathcal{N}_{\mathbb{P}}(E)}{z - E} = \mathcal{T}_{\mathbb{P}}(R(z))$$

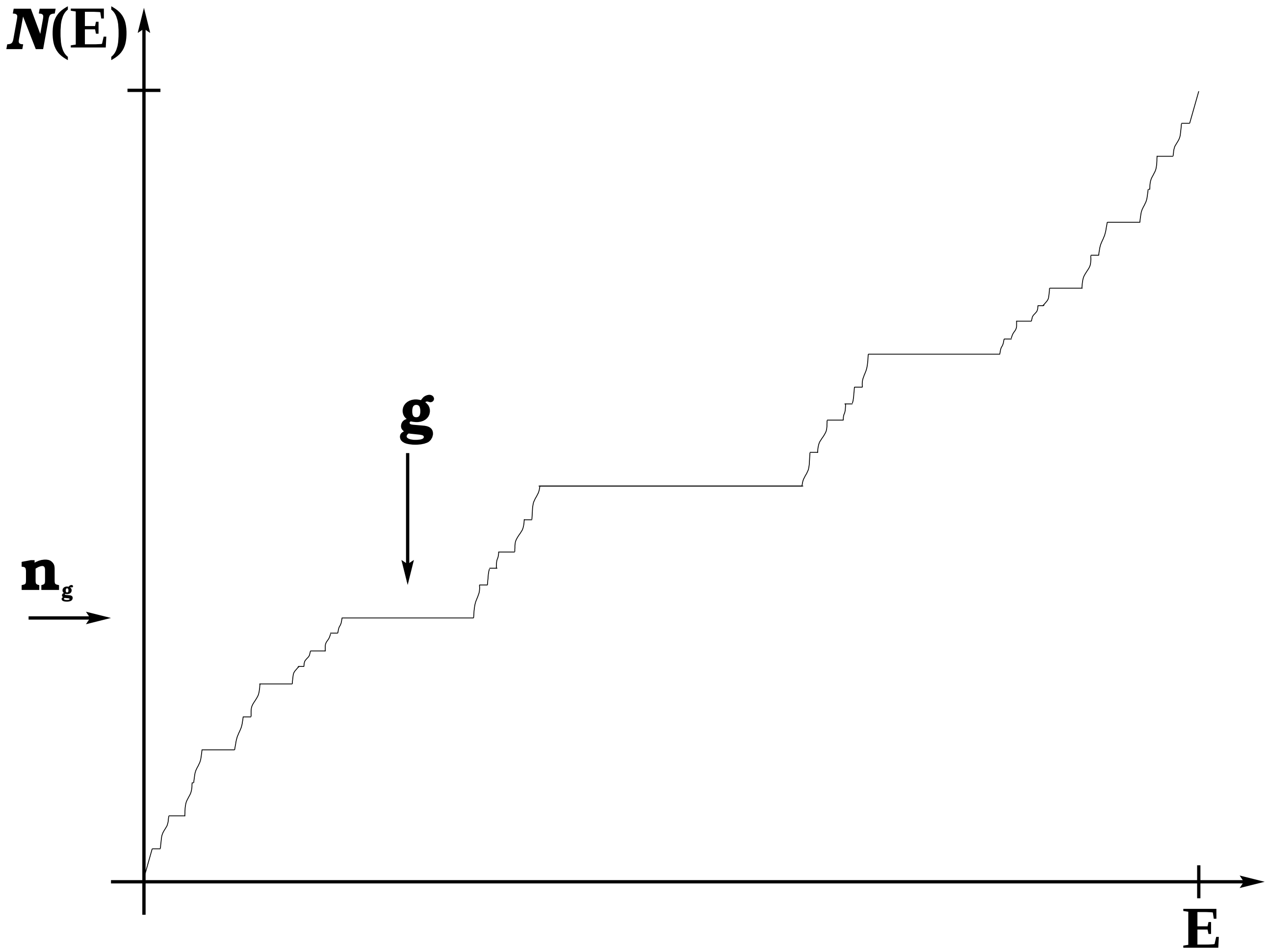
- Set $\mathcal{N}_{\mathbb{P}}(E) = \int_{-\infty}^{E} d\mathcal{N}_{\mathbb{P}}$. If E is a continuity point of $\mathcal{N}_{\mathbb{P}}$, *Shubin's formula* holds $\mathbb{P}$-almost all ω's:

$$\mathcal{N}_{\mathbb{P}}(E) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \# \{\text{eigenvalues of } H_\omega \restriction_\Lambda \leq E\}$$

- The *support* of $\mathcal{N}_{\mathbb{P}}$ is contained in Σ.
  If $\mathfrak{g} = (E_-, E_+)$ is a spectral gap, let $P_{\mathfrak{g}}$ be the spectral projection of H on $(-\infty, E_-]$, so that

$$n_{\mathfrak{g}} = \mathcal{N}_{\mathbb{P}}(E_- + 0) = \mathcal{N}_{\mathbb{P}}(E_+ - 0) = \mathcal{T}_{\mathbb{P}}(P_{\mathfrak{g}})$$

- **Fact:** $P_{\mathfrak{g}}$ is a projection belonging to $\mathcal{A}$!!



- An example of DOS -

III.7)- Tight Binding Representation

- Let Σ be the transversal of $\mathcal{L}$. Then

$$\Gamma = \{\gamma = (\omega, a) \in \Sigma \times \mathbb{R}^d ; \tau^{-a}\omega \in \Sigma\}$$

  is a *locally compact groupoid*:

  1. range, source: $r(\omega, a) = \omega, \; s(\omega, a) = \tau^{-a}\omega$
     $r, \; s : \Gamma \mapsto \Sigma$.
  2. product: $\gamma, \gamma')$ are *composable* if $s(\gamma) = r(\gamma')$. Then

$$(\omega, a) \circ (\tau^{-a}\omega, a') = (\omega, a + a')$$

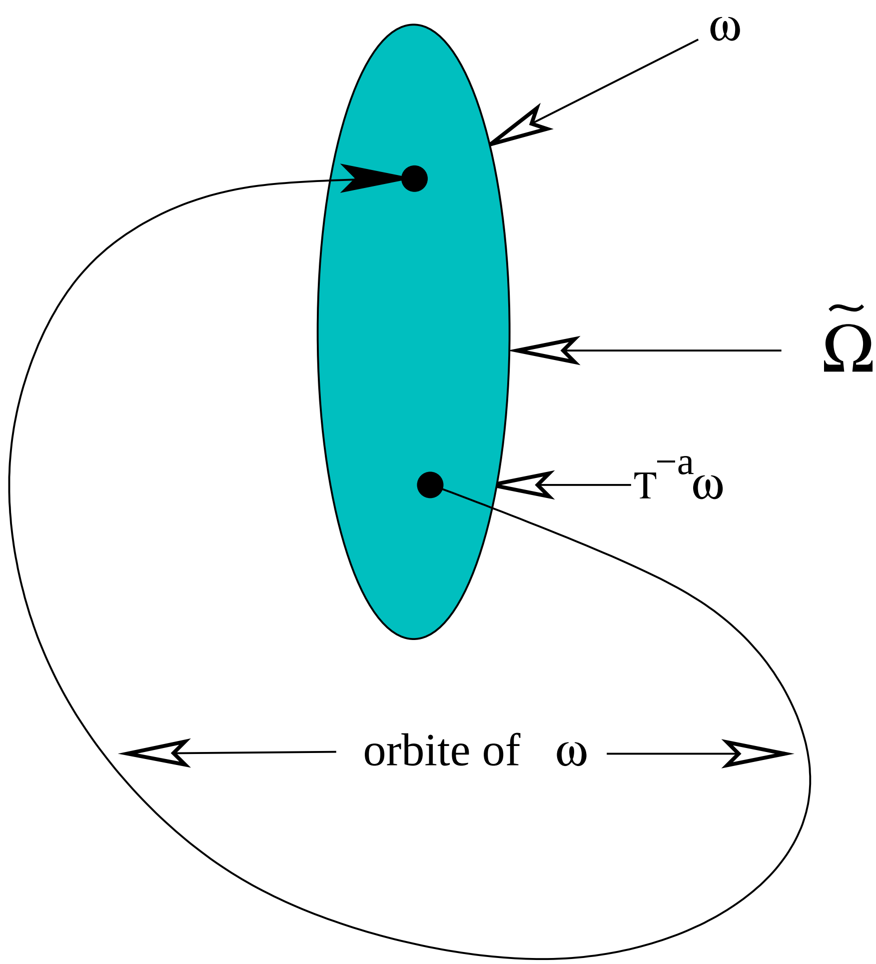
  3. Units: $e_\omega = (\omega, 0)$ are units

$$e_\omega(\omega, a) = (\omega, a) , \qquad (\tau^a\omega, a)e_\omega = (\tau^a\omega, a)$$

  4. inverse: $(\omega, a)^{-1} = (\tau^{-a}\omega, -a)$.

- The *fiber* $\Gamma^\omega = \{\gamma \in \Gamma ; r(\gamma) = \omega\}$ coincides with

$$\Gamma^\omega = \{\omega\} \times \mathcal{L}_\omega$$



- Transversal and Groupoid Arrows -

- The C^*-algebra $C^*(\Gamma)$ is built from $\mathcal{C}_c(\Gamma)$ in a similar way to $\mathcal{A}_0$. Just replace the integral over a by the discrete sum.

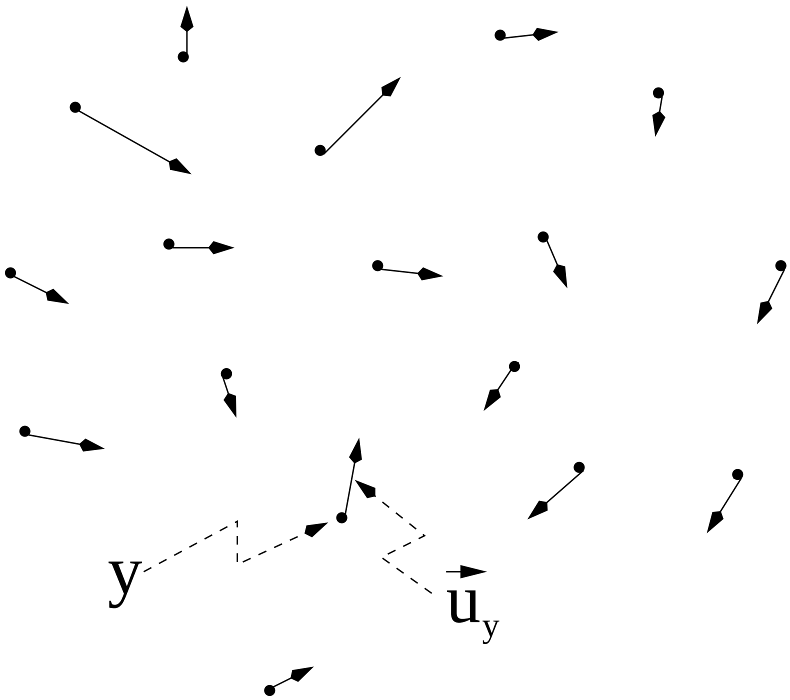
- the representation π_ω acts on $\ell^2(\mathcal{L}_\omega)$ through the same formula.

- The translation maps $\ell^2(\mathcal{L}_\omega)$ onto $\ell^2(\mathcal{L}_{T^a\omega})$ unitarily

- The rules for calculus are similar: $\mathbb{P}$ is replaced by the transversal measure $\mathbb{P}_{tr}$ induced by $\mathbb{P}$ on Σ.

- For periodic crystals, $C^*(\Gamma) \simeq \mathcal{C}(\mathbb{B})$

III.8)- Phonons



1. Phonons are *acoustic waves* produced by small displacements of atomic nuclei.
2. These waves are polarized with d-directions of polarization: $d-1$ are *transverse* one is *longitudinal*.
3. The nuclei motion is approximatively harmonic and quantized according to the *Bose-Einstein* statistics.
4. The charged nuclei interact with electrons, leading to an *electron-phonon interaction*.

The Harmonic Approximation:

1. If the nuclei motion is harmonic, the equations of motion are
$$M_{(\omega,x)} \frac{d^2 \vec{u}_{(\omega,x)}}{dt^2} = \sum_{x \neq y \in \mathcal{L}_\omega} K_\omega(x,y) \left(\vec{u}_{(\omega,y)} - \vec{u}_{(\omega,x)}\right)$$
where $M_{(\omega,x)}$ is the *mass* of the nucleus located at x, $\vec{u}_{(\omega,x)}$ is its *classical displacement* and $K_\omega(x,y)$ is the matrix of *spring constants*.

2. $K_\omega(x,y)$ decays fast in $x - y$, uniformly in ω..

3. Covariance gives
$$M_{(\omega,x)} = m(\tau^{-x}\omega) \qquad K_\omega(x,y) = k(\tau^{-x}\omega, y - x)$$
thus $m \in \mathcal{C}(X) \subset C^*(\Gamma)$, $k \in C^*(\Gamma) \otimes M_d(\mathbb{C})$.

4. Let $\hat{\Omega} \in C^*(\Gamma)$ be defined by (for $\vec{s}_x \in \mathbb{C}^d$).
$$\sum_{x,y} \frac{\vec{s}_x^{\,*}}{\sqrt{M_{\omega,x}}} \left(\hat{\Omega}^2_\omega\right)_{x,y} \frac{\vec{s}_y}{\sqrt{M_{\omega,x}}} = \sum_{x \neq y} (\vec{s}_x - \vec{s}_y)^* K_\omega(x,y)(\vec{s}_x - \vec{s}_y)$$
Then $\hat{\Omega}^\alpha(\omega,x)_{\rho,\rho'} \geq 0$ if $\alpha < 2$.

5. The spectrum of $\hat{\Omega}$ gives the *phonon modes*.
The *density of phonon modes* is defined like the DOS with $\hat{\Omega}$ replacing the Hamiltonian.