

DISORDERED SOLIDS AND THE DYNAMICS OF
BOUNDED GEOMETRY

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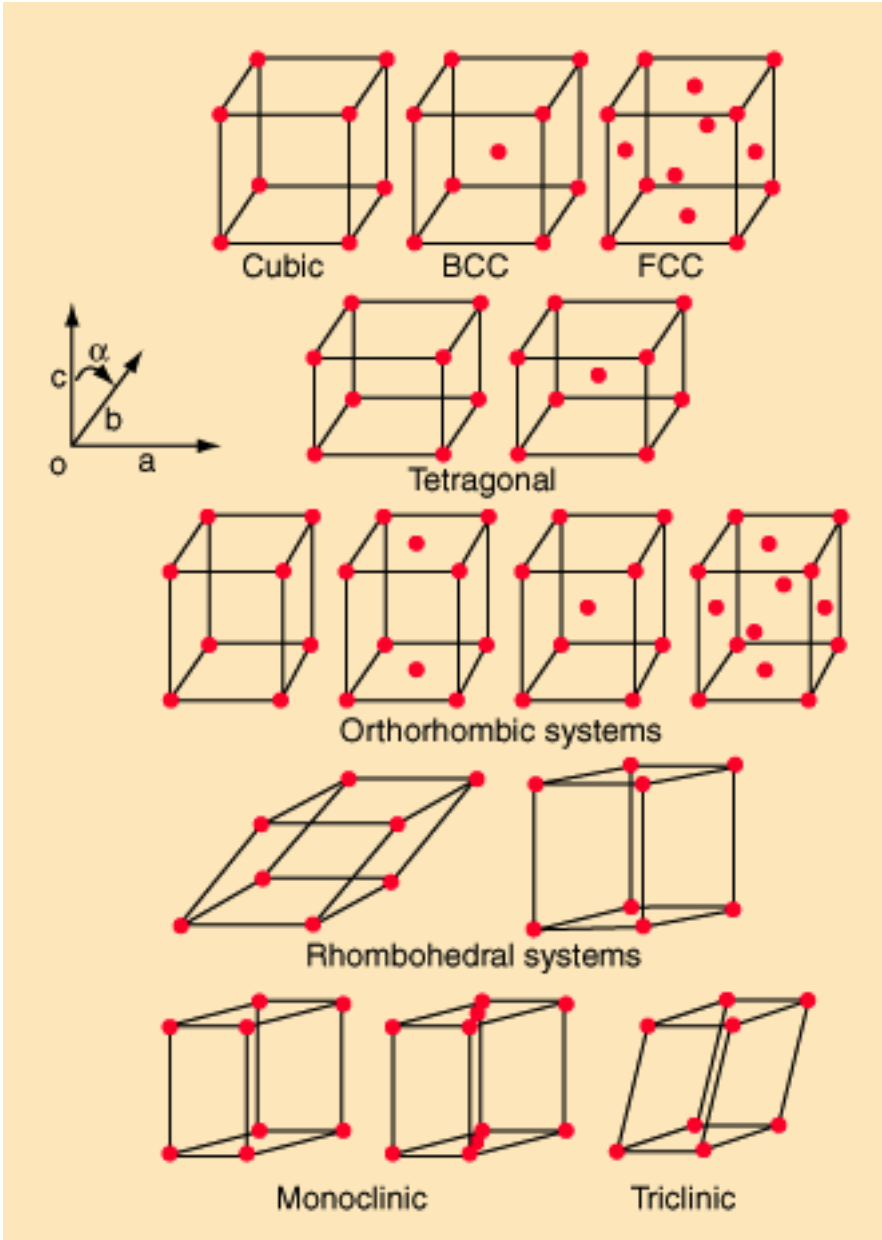
Some Ordered Solids



The facets that are visible must reflect the facets that are present on the molecular level.

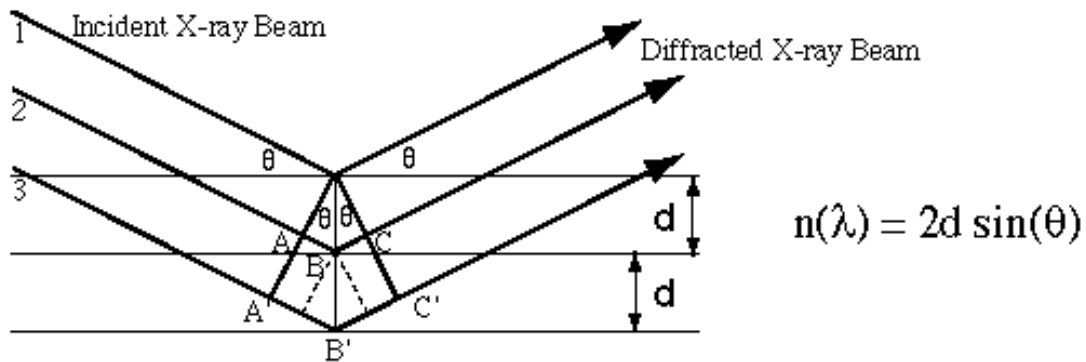
Crystals are modeled via their groups of symmetries, the crystallographic groups, together with extra data, about where the atoms are located.

(Of course, most important, is the translational symmetry that is always present and finite index. However, there are effects that do depend on the group and the extra structure.)



This is probed via diffraction.

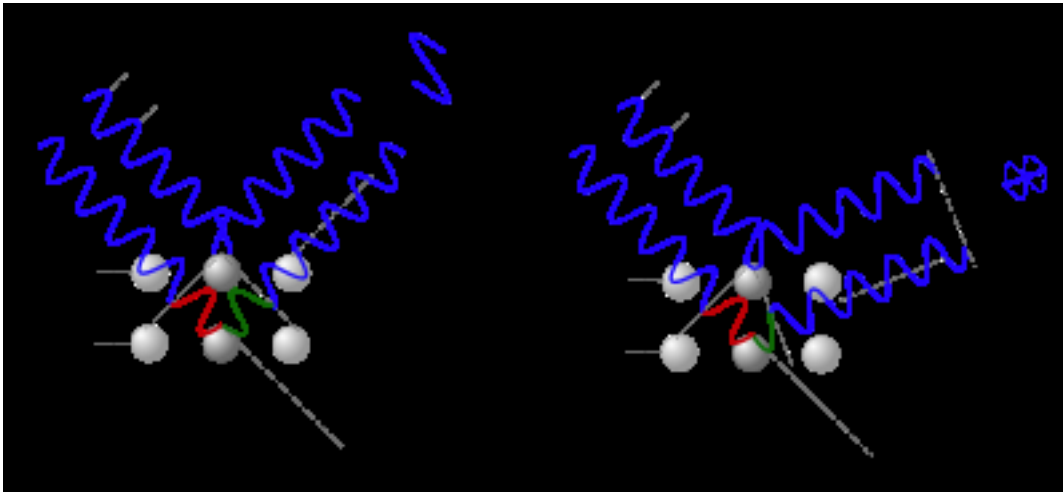
Bragg's Law.



$$AB = d \sin(\theta) = BC \quad \therefore \quad ABC = 2d \sin(\theta)$$

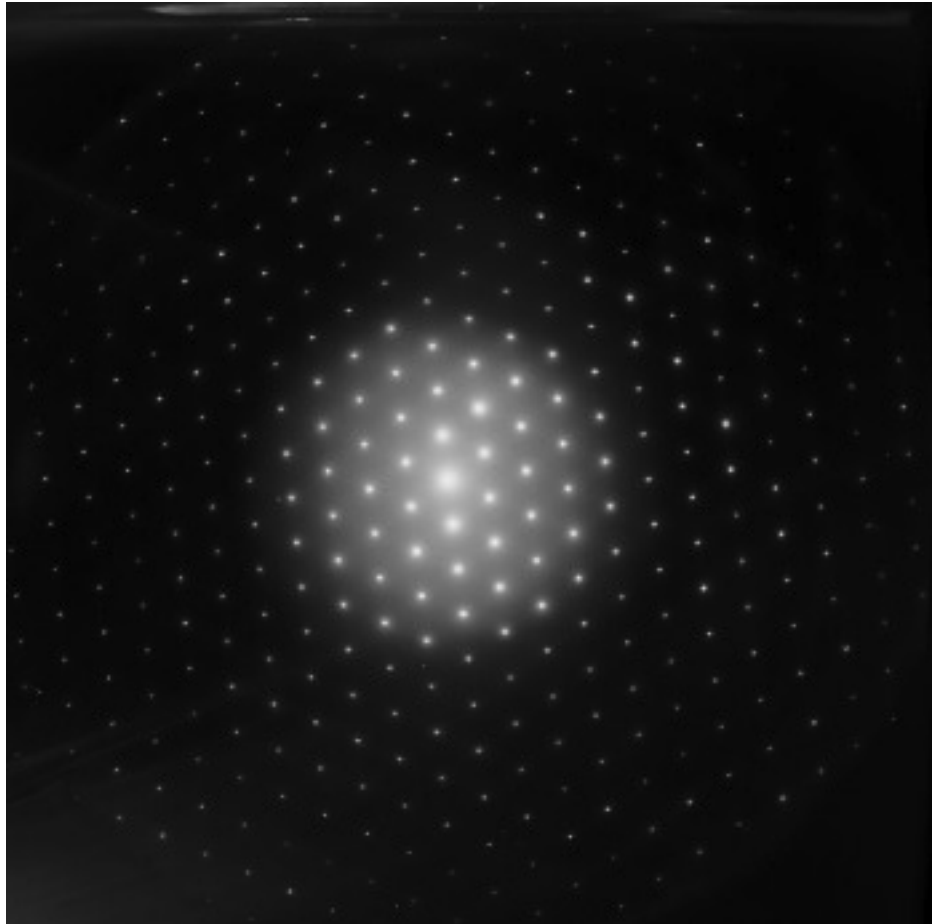
$$A'B' = 2d \sin(\theta) = B'C' \quad \therefore \quad A'B'C' = 2ABC = 4d \sin(\theta)$$

If this doesn't hold then there will be (destructive) interference and the waves cancel out.



Note that associated to a lattice, one sees the dual lattice via diffraction. (AKA the reciprocal lattice).

Laue Method.



Use white light and get a pattern from all wavelengths of how the various scattered lights from different atoms interfere.

i.e. produces a Fourier transform of the crystal.
As a result, a key role is played by the **Brillouin zone**, the torus **dual** to \mathbf{R}^n/L .

Basic Theorem.

In dimension ≤ 3 there is no 5-fold symmetry.

Proof:

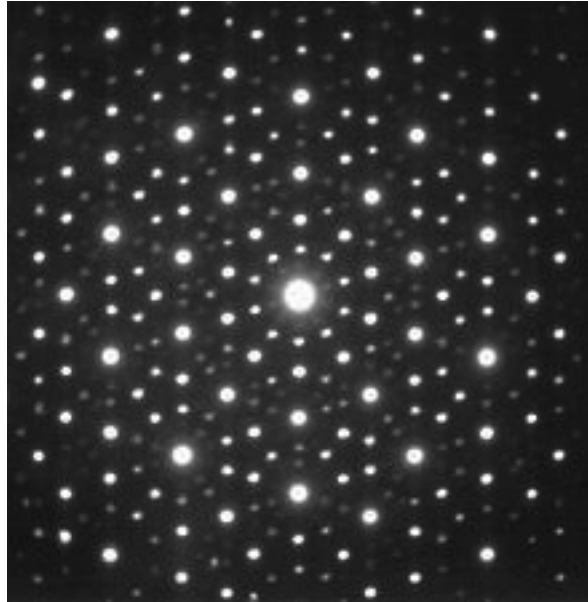
In $E(n)$ (the Euclidean group) we are just concerned with the rotational part image in $SO(n)$. Our element will be an element of $SL_n(\mathbf{Z})$. Note that it has a quadratic integral characteristic polynomial. (For $n=3$, use that 1 is automatically an eigenvalue of an orthogonal matrix.)

Hence the trace of the eigenvalue, i.e. its real part, must be $\frac{1}{2}$ * an integer.

So the only possible roots of unity are 1st, 2nd, 3rd, 4th, and 6th.

(This was used as evidence that atoms are real, not just computational conveniences.)

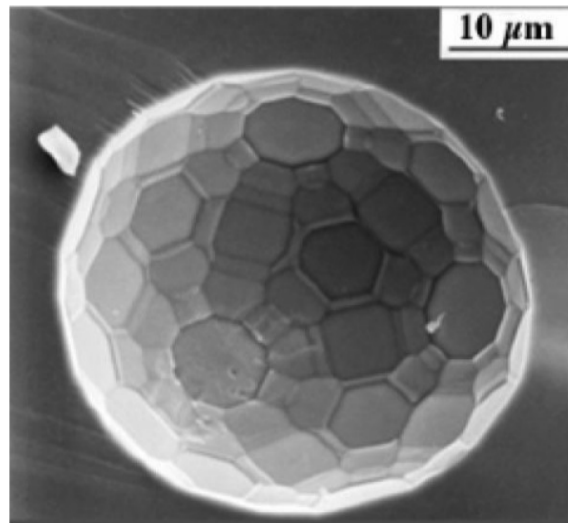
Quasicrystals



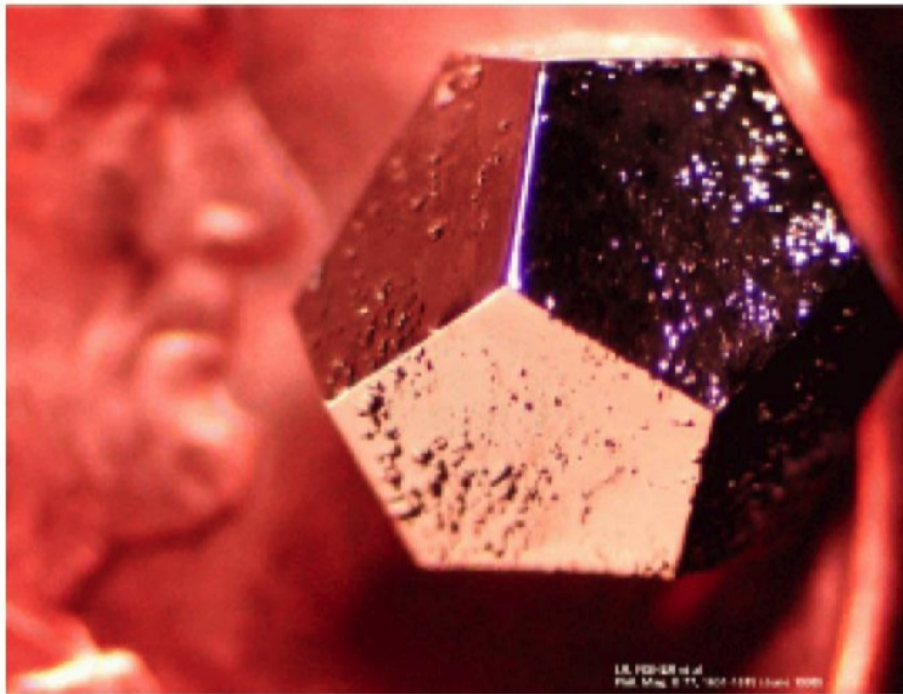
Electron diffraction pattern of an icosahedral Zn-Mg-Ho quasicrystal (Zinc-Magnesium-Holmium)

D. Shechtman, I. Blech, D. Gratias and J.W. Cahn, "Metallic phase with long-range orientational order and no translational symmetry," *Phys. Rev. Lett.* 53 (1984), 1951-1953.

Shechtman won the Nobel prize this December for this work.



- The icosahedral quasicrystal $AlPdMn$ -



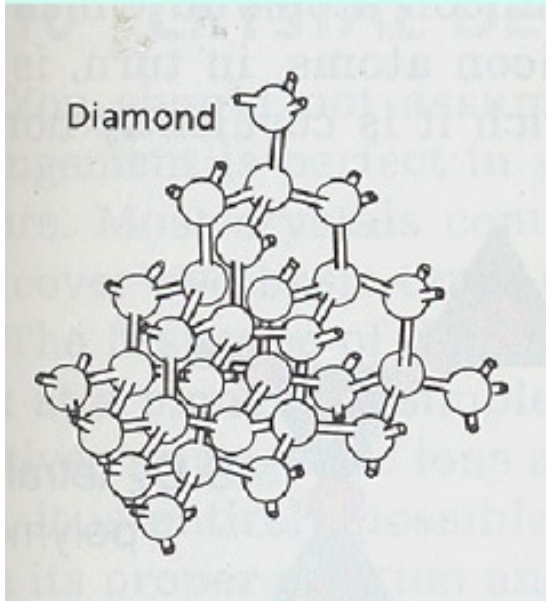
- The icosahedral quasicrystal $HoMgZn$ -

These cannot be modeled as crystals.

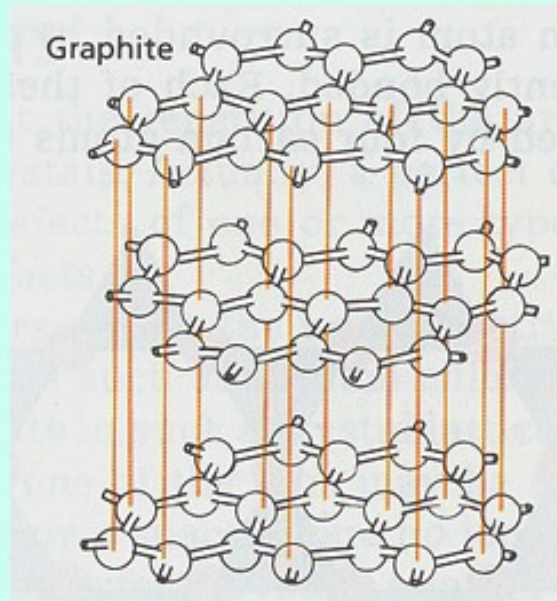
Some other examples of rather different material structure:

Diamond & Graphite

Allotropes of Carbon



**Three dimensional
network solid**

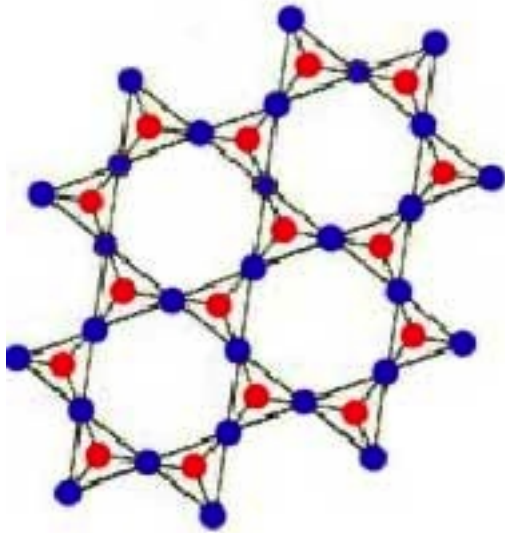


**Two dimensional
network solid**

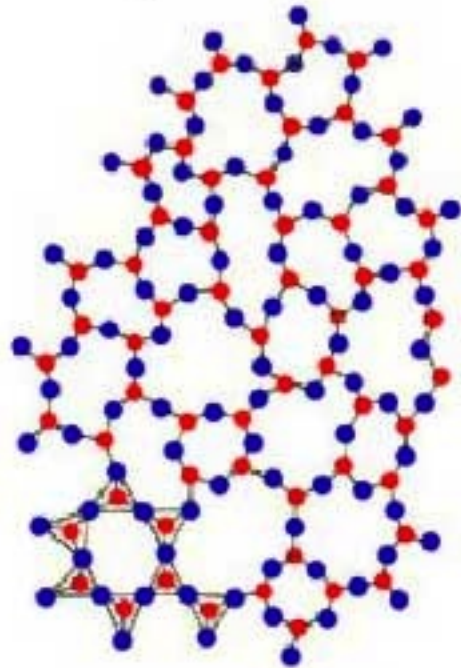
Diamond has a crystalline structure with face centered cubic lattice.

Graphite is a lubricant because there is essentially no connection between the 2-dimensional crystal sheets.

**Crystalline SiO₂
(Quartz)**



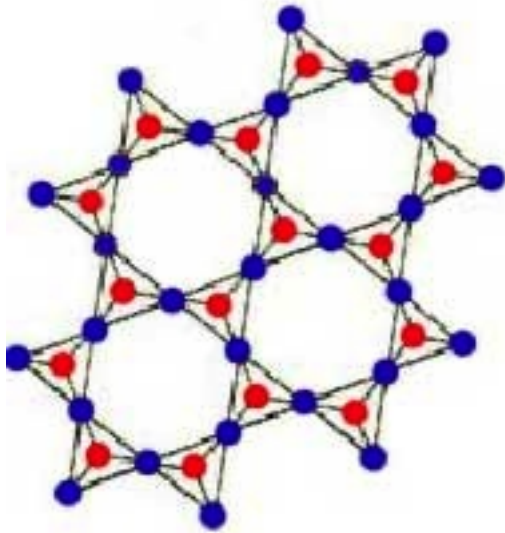
**Amorphous SiO₂
(Glass)**



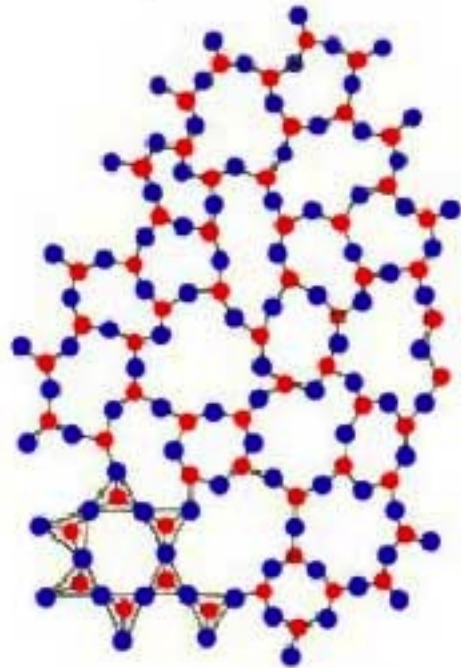
● Si ● O

(Quartz crystal can withstand much higher temperatures and pressures than glass. Quartz generates very precise acoustic modes when excited by an electric potential, which can be used in the design of watches; glass cannot be used in this way.)

**Crystalline SiO₂
(Quartz)**



**Amorphous SiO₂
(Glass)**



● Si ● O

(Quartz crystal can withstand much higher temperatures and pressures than glass. Quartz is an electrical conductor and Glass is an insulator.)

Normal metals (with defects or impurities) and alloys.

Also....semiconductors. At low temperatures, electrical properties can be modeled as essentially random, Poisson distributed, impurities. Shades of TDA..

Plan for the rest of the talk.

(1) A quick view of one method in the mathematical theory of quasicrystals.

The “Noncommutative Brillouin Zone”

(2) Generalizations of some of the basic constructions.

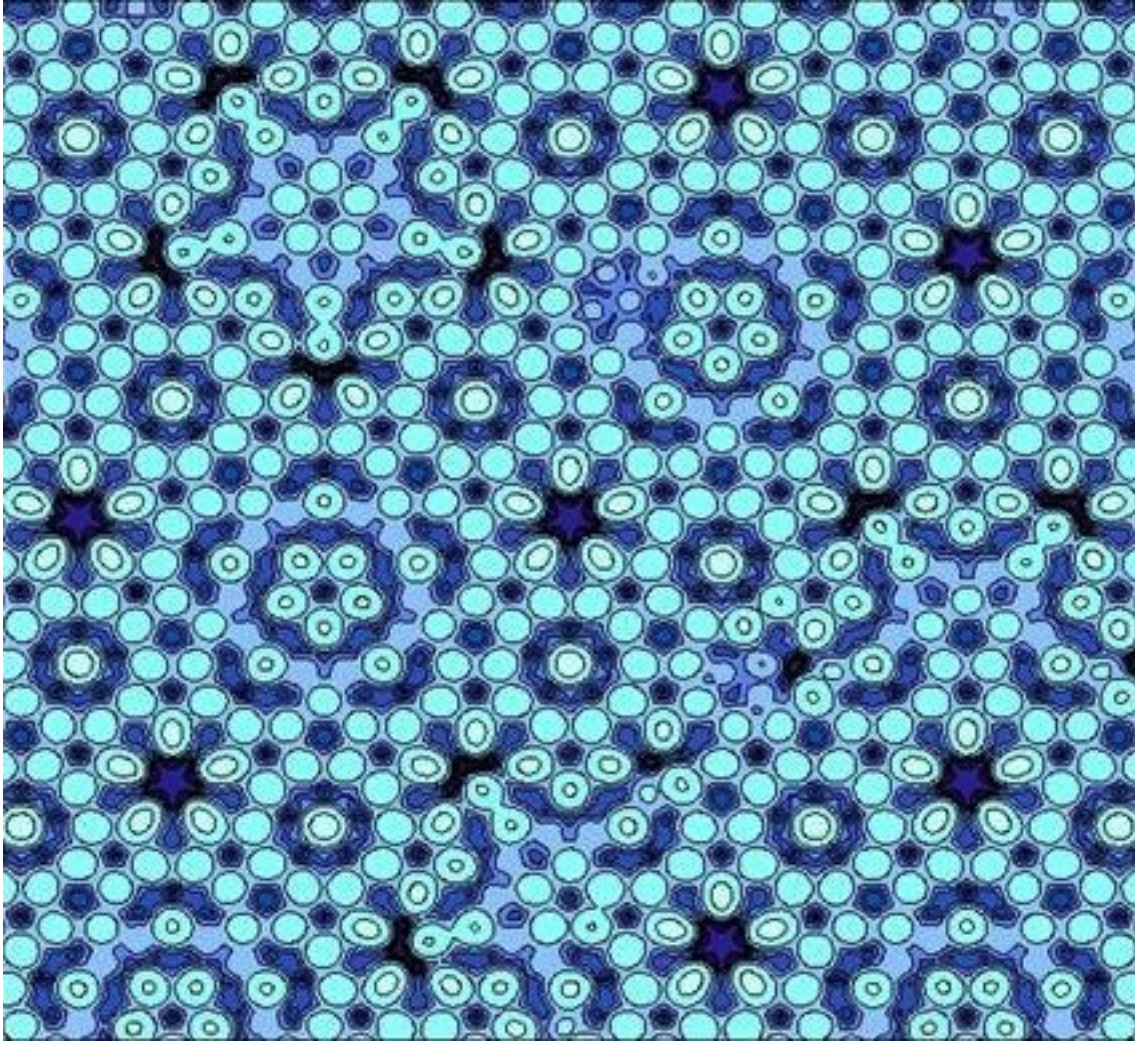
Hulls for manifolds with bounded geometry. K-theory of an associated convolution algebra

(3) Some other applications of this idea to completely different problems within pure math (mainly topology and geometry).

Positive Scalar Curvature The principle of descent (for the Novikov conjecture) Random perturbations of periodic operators.

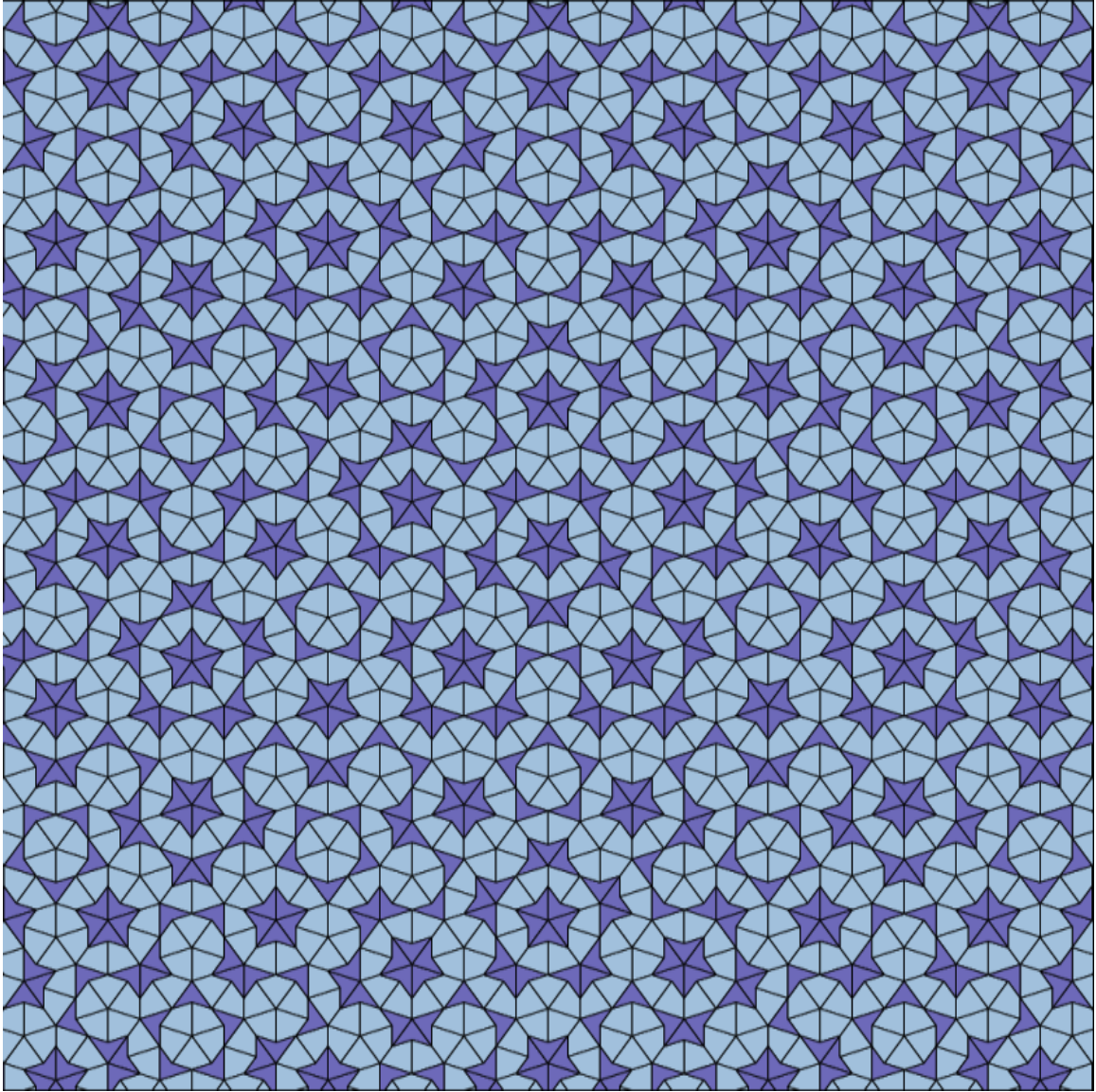
(4) Future directions and summary.

Aperiodic Tilings



Atomic model of an Ag-Al quasicrystal

(This picture was on the NY Times web page in December – taken from Wikipedia.)



The Penrose Tiling.

Towards the Hull of a tiling.

The moduli space of tilings with a given set of prototiles is locally a space modeled on Euclidean space \times a Cantor set.

Towards the Hull of a tiling.

Theorem: If a set of tiles tiles the 1st quadrant, then it tiles the whole plane.

Proof: Make a tree from partial tilings and apply Konig's lemma.

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Proof: Follow some direction that still has unbounded length.

Note: Konig's lemma is a form of compactness. (Also false without the local finiteness.)

Proposition: If X_k, f_k is an inverse system of finite sets, then the inverse limit is nonempty.

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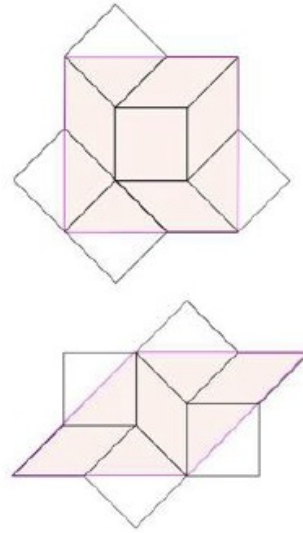
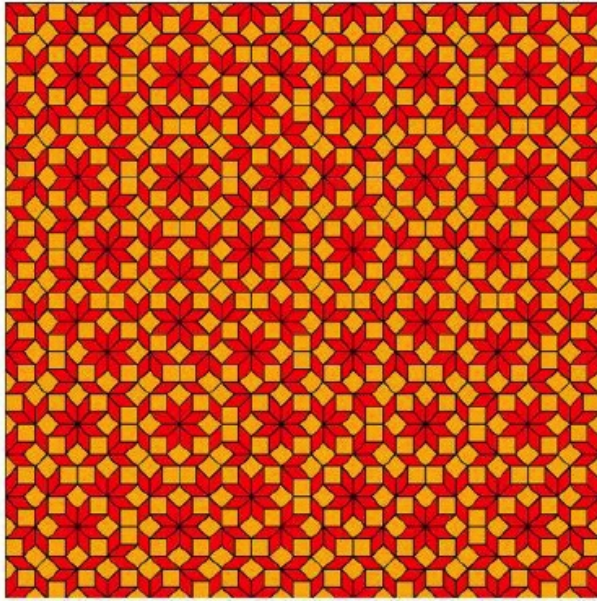
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Proposition: If X_k, f_k is an inverse system of finite sets, then the inverse limit is nonempty.

This proof has several implications:

- We can build tilings using larger and larger pieces.
- There is a compact space of tilings.
- There is a substantial and interesting literature on analyzing this space.

It has an essentially "Cantor structure".



An Octagonal Tiling via substitution.

Later we will use this method for “pinwheel tilings”.

It is possible to go back and forth between the language of tiles in Euclidean space and of Delone sets.

Modelling the positions of the atoms.

Point Sets

A subset $\mathcal{L} \subset \mathbb{R}^d$ 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} .
3. *Relatively dense*: $\exists R > 0$ s.t. each ball of radius R contains at least one points of \mathcal{L} .
4. A *Delone* set: \mathcal{L} is uniformly discrete and relatively dense.
5. *Finite Local Complexity (FLC)*: $\mathcal{L} - \mathcal{L}$ is discrete and closed.
6. *Meyer* set: \mathcal{L} and $\mathcal{L} - \mathcal{L}$ are Delone.

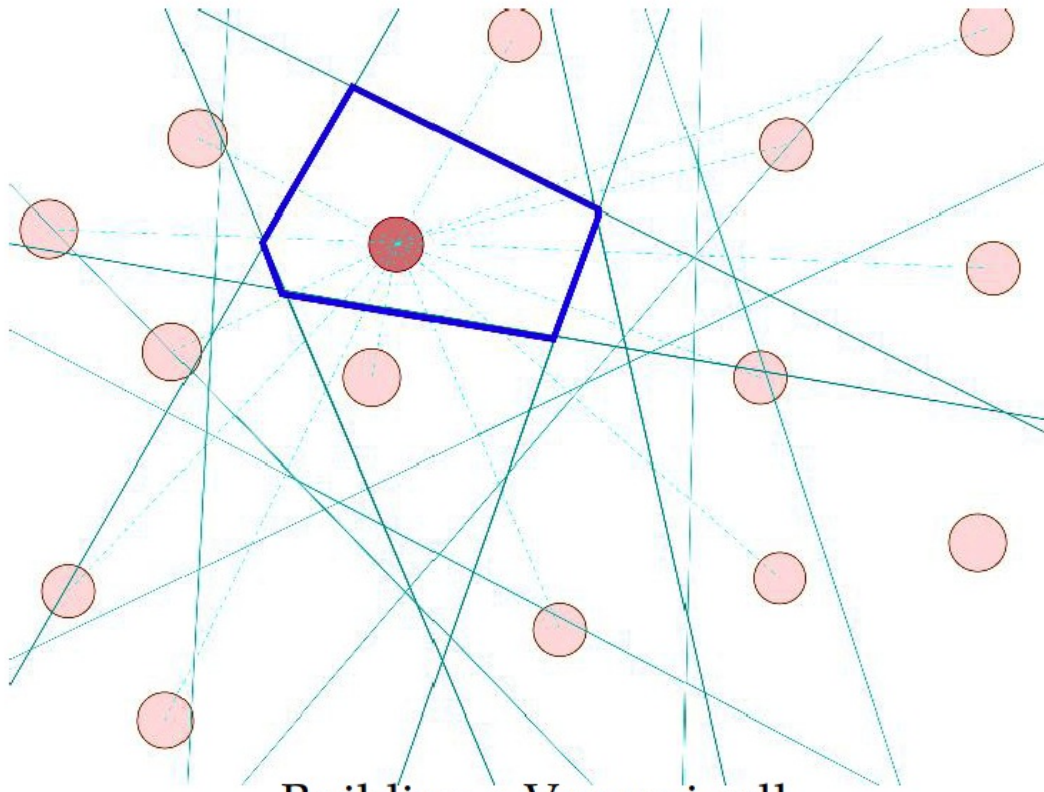
Point Sets and Tilings

Given a tiling with finitely many tiles (*modulo translations*), a Delone set is obtained by defining a point in the interior of each (*translation equivalence class of*) tile.

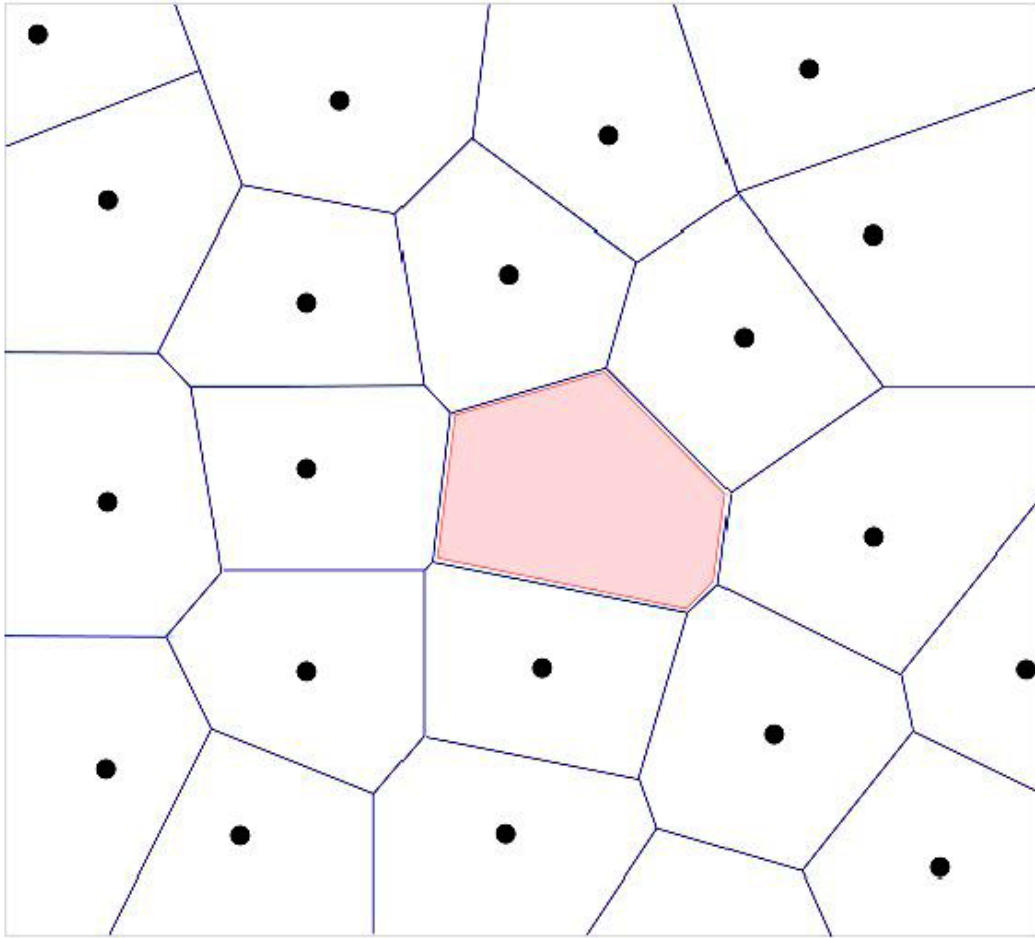
Conversely, given a Delone set, a tiling is built through the *Voronoi cells*

$$V(x) = \{a \in \mathbb{R}^d; |a - x| < |a - y|, \forall y \in \mathcal{L} \setminus \{x\}\}$$

1. $V(x)$ is an *open convex polyhedron* containing $B(x; r)$ and contained into $\overline{B(x; R)}$.
2. Two Voronoi cells touch face-to-face.
3. If \mathcal{L} is *FLC*, then the Voronoi tiling has finitely many tiles modulo translations.



- Building a Voronoi cell-



- A Delone set and its Voronoi Tiling-

The Hull

A point measure is $\mu \in \mathfrak{M}(\mathbb{R}^d)$ such that $\mu(B) \in \mathbb{N}$ for any ball $B \subset \mathbb{R}^d$. Its support is

1. *Discrete*.
2. *r-Uniformly discrete*: iff $\forall B$ ball of radius r , $\mu(B) \leq 1$.
3. *R-Relatively dense*: iff for each ball B of radius R , $\mu(B) \geq 1$.

\mathbb{R}^d acts on $\mathfrak{M}(\mathbb{R}^d)$ by translation.

The Hull Λ is the closure of the orbit of a given tiling.

Abstractly the hull is a space modeled by $\mathbf{R}^d \times \text{Cantor set}$.

For many concrete tilings e.g. associated to “cut and project method”, or substitution tilings, etc. these can be calculated explicitly, see e.g. work of Anderson-Putnam, Bellissard and collaborators, Priebe-Franck-Sadun, Kallendock, Savinien, Moustafa and others.

The Hull Λ is the closure of the orbit of a given tiling.

The **Noncommutative Brillouin zone** is the cross product C^* -algebra $C^*(\Lambda) \rtimes \mathbb{R}^d$.

The Hull Λ is the closure of the orbit of a given tiling in the space of measures.

The **Noncommutative Brillouin zone** is the cross product C^* -algebra $C^*(\Lambda) \rtimes \mathbb{R}^d$.

(Gross Oversimplification)

The cohomology of the Hull is related to “Pattern Equivariant Cohomology” (cocycles can only take values that take into account some size neighborhood of the point).

This regulates the deformations of the tiling in ways that don't affect the diffraction data. (Sadun & Clarke)

The spectrum of the group action on Λ .

What is the x-ray diffraction pattern of the crystal?
i.e. the Fourier transform of the autocorrelation function.
And well definedness of densities of patterns.
(Like the relation of the golden mean to the Penrose tiling)

The K-theory of this algebra.

What are the possible energy levels of electrons?
What is the spectrum of Schroedinger operators with potentials associated to the given locations of the atoms?
What is the density of states associated to gaps in the spectrum?

Schrödinger's Operator

Ignoring electrons-electrons interactions, the one-electron Hamiltonian is given by

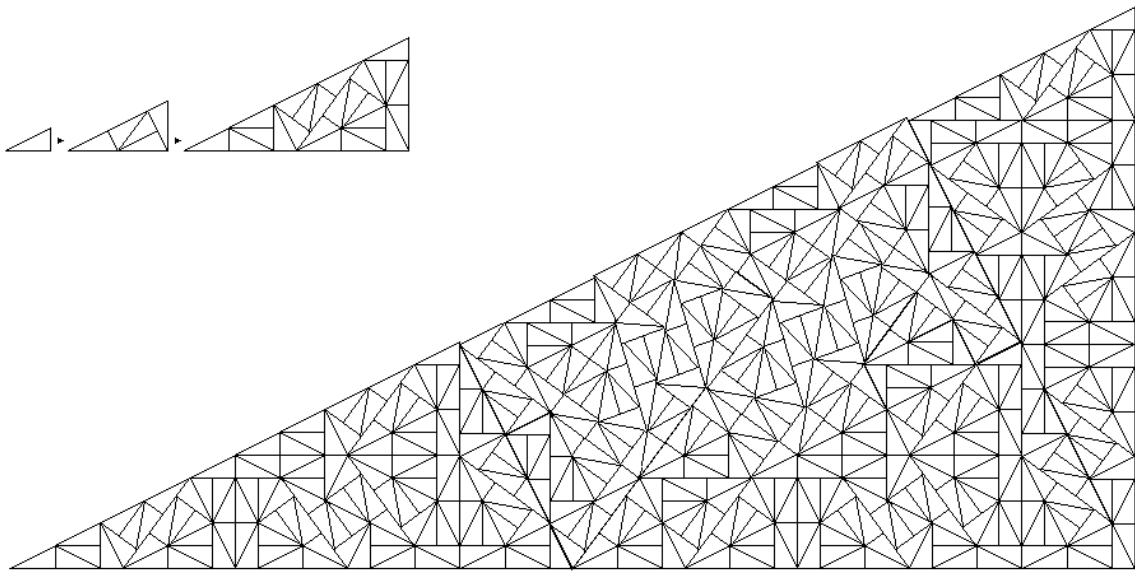
$$H_\omega = -\frac{\hbar^2}{2m} \Delta + \sum_{y \in \mathcal{L}_\omega} v(\cdot - y)$$

Its *integrated density of states (IDS)* is defined by

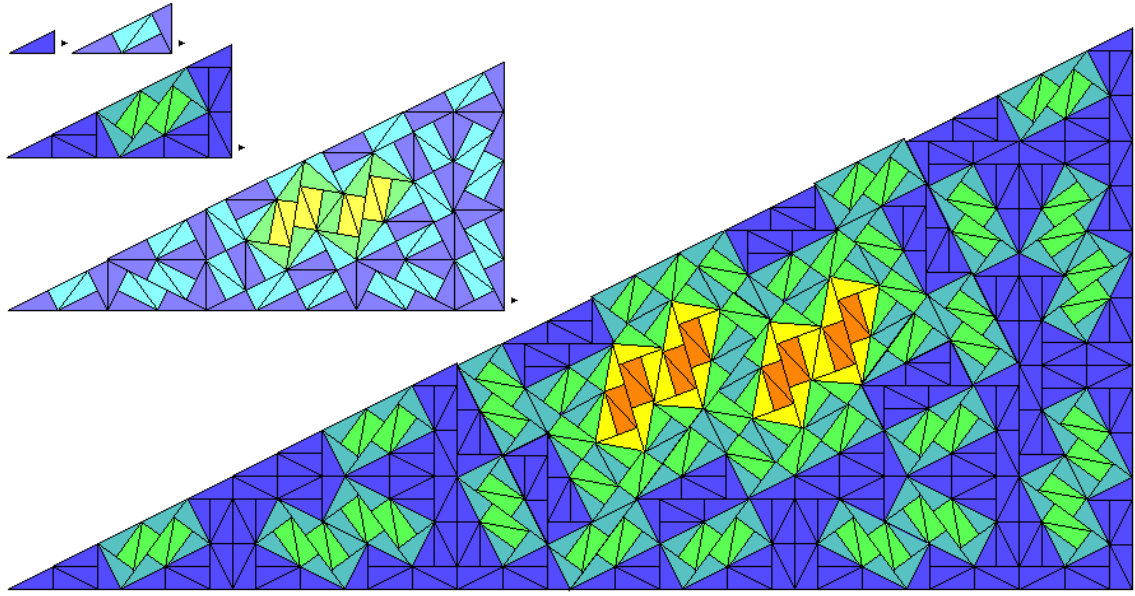
$$\mathcal{N}(E) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \#\{\text{eigenvalues of } H_\omega \upharpoonright_\Lambda \leq E\}$$

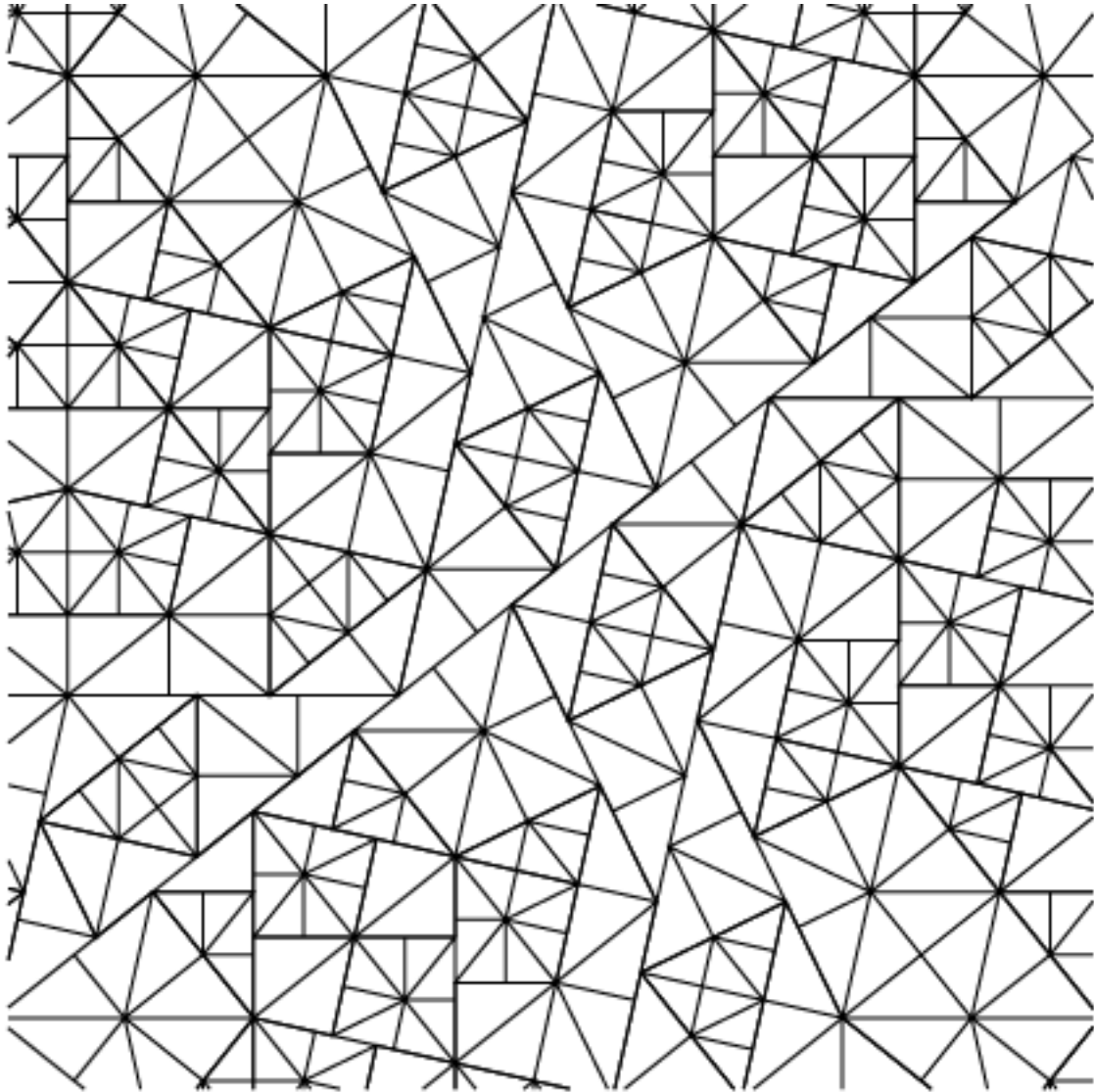
For any \mathbb{R}^d -invariant probability measure \mathbb{P} on Ω the limit exists a.e. and is independent of ω . It defines a nondecreasing function of E constant on the spectral gaps of H_ω . It is asymptotic at large E 's to the IDS of the free Hamiltonian.

How do we go beyond the situation of tilings associated to these special aperiodic sets?



Stages in a pinwheel tiling





A Pinwheel Tiling (Following Conway, Radin, Sadun, etc.)

Note: The pinwheel tiling constructed above does not have a fault line. Such were constructed by Sadun, based on the work of N.Priebe-Franck.

Two aspects:

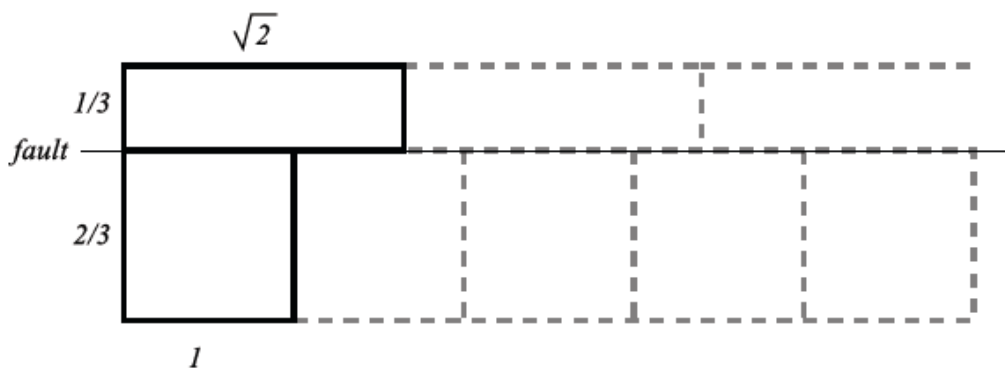
- (1) Infinite amount of rotational symmetry.
- (2) The existence of fault lines.

The first is easily dealt with by replacing the \mathbb{R}^2 group by the group $\text{Iso}(\mathbb{R}^2)$.

(which has other advantages in encoding symmetries even for periodic lattices).

The second leads to higher dimensional hulls because of the possibility of sliding along fault lines.

For example, there are aperiodic tilings of $S^2 \times \mathbb{R}$, but any such must have a fault line. (P.Nowak and SW)



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Our goal is to encompass these, also problems of imperfections, amorphous solids, other manifolds and tiled spaces, etc. all in one rubric.

Manifolds of bounded geometry

(in the sense of Roe, as opposed to Cheeger-Gromov)

M has **bounded geometry** if $\text{inj}(M) > c > 0$, and $|K| < C$.

If necessary, we will assume bounds on **higher covariant derivatives of the curvature tensor** if convenient.

Manifolds of bounded geometry

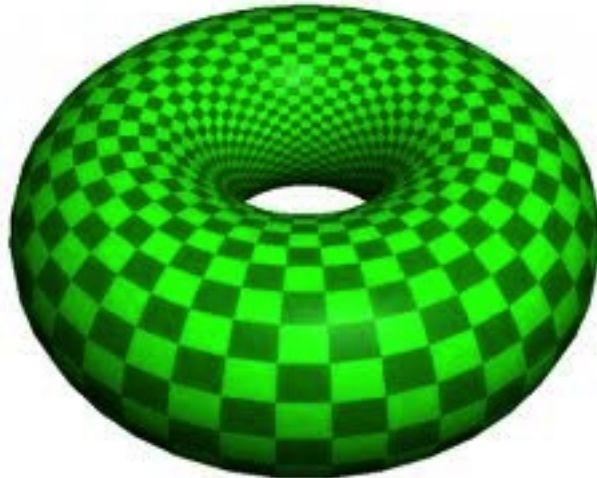
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+ Deformation using almost periodic or “totally bounded” functions.

- For example, $dx^2 + dy^2 + f(x,y) dx dy$

Where f is a suitable function.

Definition: A function f on E (=Euclidean space) is almost periodic if any sequence of translates of f has a uniformly convergent subsequence.

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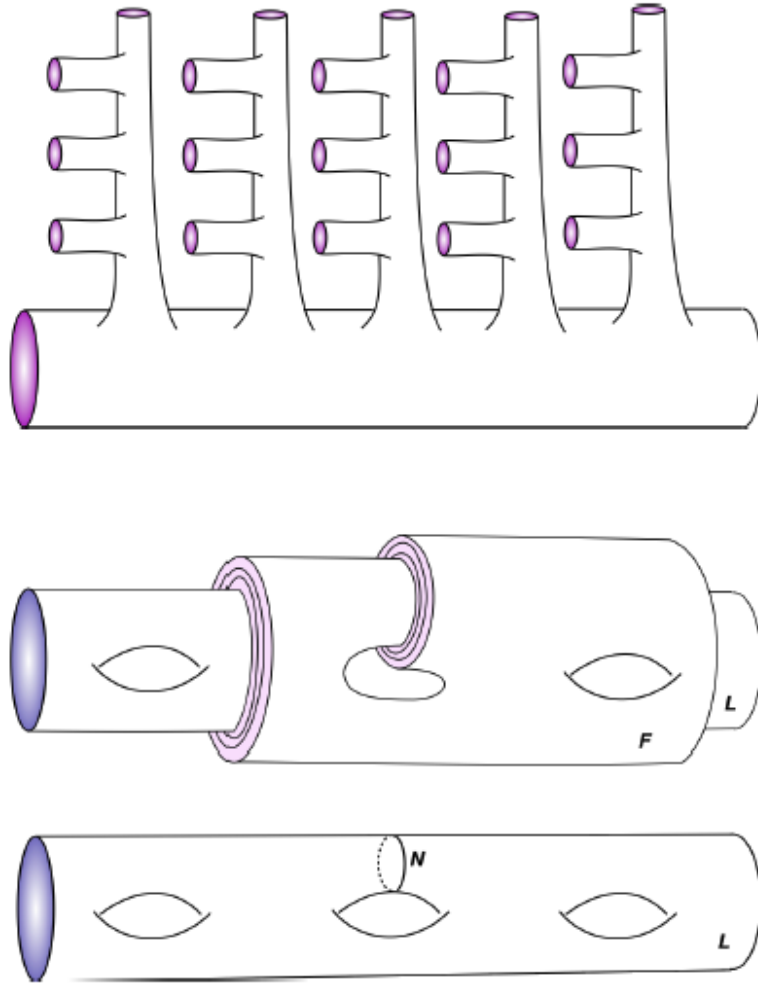
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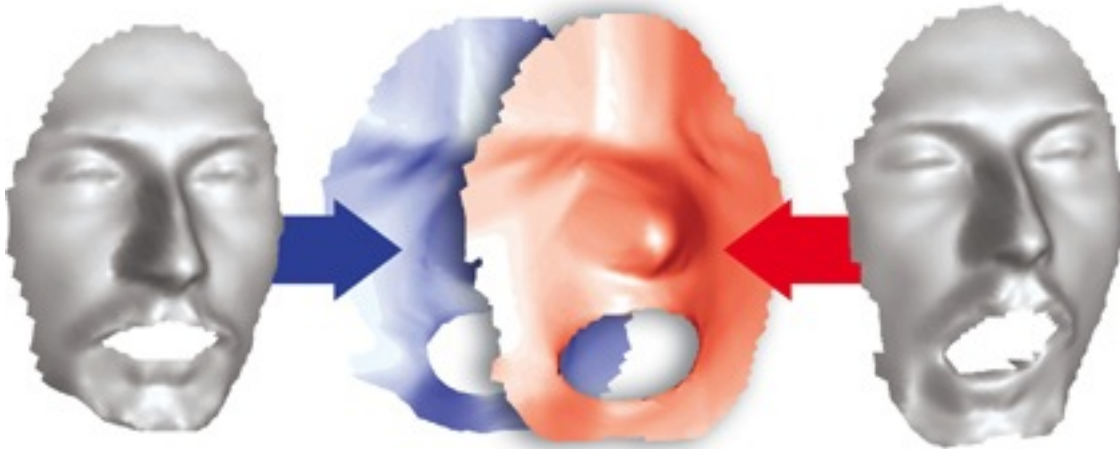
(Compare to the compact open version.)

✚ A Leaf of a smooth foliation of a smooth manifold.



A key feature of bounded geometry is the following compactness property, which requires the notion of Gromov-Hausdorff space to express.

Definition: (GH space) The distance between two metric spaces is the smallest separation possible between the metric spaces in any metric on the union.



Pointed Gromov Hausdorff space requires also aligning base points in these spaces.

We will denote by $\mathbf{GHB}(D)$ the Pointed Gromov Hausdorff space of Balls of radius $D/2$. Subsets with uniform covering functions are precompact.

Key Proposition. If M is a manifold of bounded geometry, then for every D , the map

$$\Psi_D: M \rightarrow \mathbf{GHB}(D)$$

given by $\Psi_D(m) = B_m(D/2)$ has precompact image.

Remarks:

(1) With our definitions, the converse does not hold. Finite volume hyperbolic manifolds are not bounded geometry in our sense, but for every D , the image **is** precompact.

(2) It is also useful to allow higher derivatives in the definition of GH distance (see Peterson's introduction to Differential geometry). And then we can define and exploit similar maps. Indeed, we will assume this done in what follows.

(3) This map is generically an embedding, but whenever there is some symmetry it fails to be. M is homogeneous iff the image is a point for all D .

The smallest D for which it fails to be trivial is related to the length of the shortest geodesic (in the compact case).

(4) If M has a flat region Ψ_D will shrink it.

Covering functions for $\Psi_D(M)$ as $D \rightarrow \infty$ give a useful measure of the **entropy** of the manifold.

Such invariants were used by Attie and Hurder to obstruct bounded geometry manifolds from being leaves of sufficiently smooth foliations of compact manifolds. We will see that they nevertheless are (often) leaves of compact **foliated spaces**.

Definition: Foliated spaces are spaces with foliations whose leaves are manifolds, but whose total spaces are not. Many tools of foliation geometry apply to these, e.g. Connes' foliated index theorem.

(See Moore-Schochet)

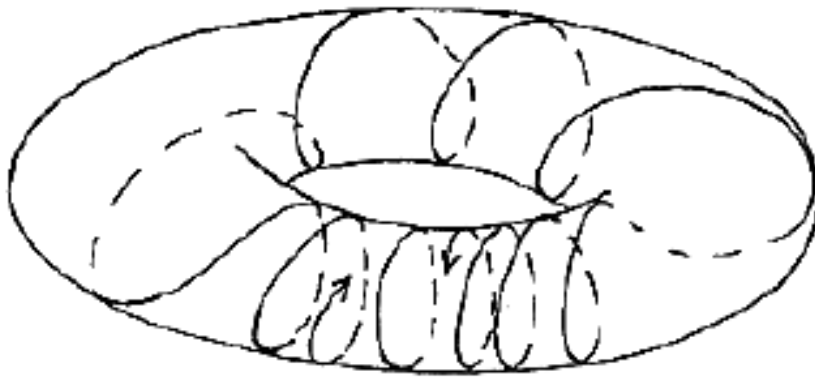
Definition. (The Hull of a Manifold with Bounded Geometry)

Let M have bounded geometry.

$$\Lambda(M) = \lim_{\leftarrow} \text{closure } (\Psi_D(M))$$

←

- + Note that the hull of a tiling, periodic or not is an example of this construction. Translation gives the foliation structure.
- + It also makes sense for tilings of other homogeneous spaces.



This leaf is the hull of a periodic tiling of the line with a single impurity.

1. The Hull of an **almost periodic** metric on a Euclidean space is a torus (usually of higher dimension).

$$dx^2 + [\sin(x)\sin(y) - \sin(\sqrt{2}(x-3y))]dxdy + dy^2$$

2. If f is a function with enough bounded derivatives with $|f| < 2$, then $dx^2 + f(x,y)dxdy + dy^2$ is a manifold with bounded geometry, whose hull is ...?
3. Foliation \rightarrow Leaf \rightarrow Foliation is not the identity even for minimal leaves. Here's a useful and interesting example. Let Γ be a finitely presented residually finite group with finite quotients Γ_k . Then Γ acts isometrically on the Cantor Set

$$CS = \lim(\Gamma_k)$$

with dense orbits. If X is the universal cover of a compact manifold with fundamental group Γ , then

$$(X \times CS)/\Gamma$$

is a compact foliated space. Using a partition of unity, one obtains a metric on X so that this space (rather than X/Γ) is the hull of the associated manifold with bounded geometry.

4. Now, if we choose a different Cantor set, we can get rather different behavior. As an example, consider $SL_n(\mathbb{Z}_p)/\mathbb{Z}_p$. This will have all leaves dense, but with different isotropy than each other. There are leaves isometric to X .

Definition: $H^*_{bg}(M)$ is the cohomology of the complex of differential forms so that the forms are continuous when plaques are placed close to each other using Gromov-Hausdorff correspondences.

Note that this is “Pattern Equivariant Cohomology” for aperiodic tilings with bounded local complexity.

This makes sense whether or not Ψ is an embedding; if Ψ is an embedding this corresponds to one of the usual “foliated cohomology theories” of the foliated hull (see below).

Remark: Using a fixed D , it is possible to define the bounded geometry at particular scales. This can be interesting even if the manifold is compact.

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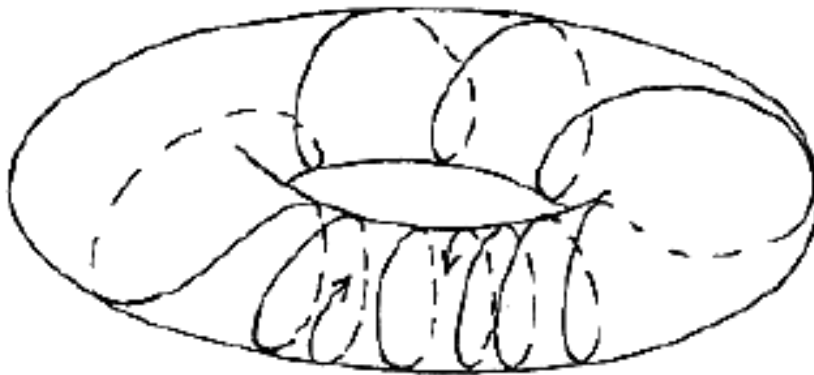
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Example: If B is a finite dimensional “generic” Banach space, then $H^{2k}_{bg}(B) = \Lambda^{2k}(B)$ (and the odd cohomology vanishes).

Example: If M is a symmetric space $K \backslash G$, then for all D , Ψ_D is trivial. However, even so the $H^*_{bg}(M)$ is the part of the cohomology of $H^*_{bg}(K \backslash G / \Gamma)$ that comes from the trivial representation in the Matsushima formula. So it’s the cohomology of CP^n in case $g = U(n,1)$, for instance.

Example: $H^*(K \backslash G / \Gamma)$ is $H^*_{bg}(K \backslash G)$ when $K \backslash G$ is tiled by a Γ equivariant tiling.

Example': Suppose that $K \backslash G$ is tiled by a Γ equivariant tiling with a single "impurity", then the hull is the union of $K \backslash G$ with $K \backslash G / \Gamma$ where they are glued together asymptotically using the covering map, as in the figure below.



The cohomology therefore is $\mathbf{R}[n] \oplus H^*(K \backslash G / \Gamma)$.

Example'': If there are an infinite number of impurities that are completely dispersed (i.e. $d(x, x') \rightarrow \infty$) then the cohomology is $\mathbf{R}^2[n] \oplus H^*(K \backslash G / \Gamma)$.

Example "": If one allows impurities to be Poisson distributed, then this is related to problems of TDA.

Definition: The prefoliated manifold structure on the limit.

If $\Lambda(M)$ is the hull of a manifold with bounded geometry, and we are given a point $p \in \Lambda(M)$, then to each D , there are balls $\pi_D(p) \in \text{GHB}(D)$, the pointed limit of which is a pointed manifold with bounded geometry, $M(p)$.

Note $\Psi: M(p) \rightarrow \Lambda(M)$ and $\Psi(p) = p$.

We call $\Psi(M(p))$ the leaf of the hull going through p .

Warning: If $M(p)$ is too homogeneous, the Ψ will not be an embedding, and this will not produce a foliated space.

Example: One Euclidean space with a single defect, the hull is a sphere. The prefoliated structure puts a whole copy of Euclidean space at the north pole, and topologizes this union in a non-Hausdorff fashion.

The prefoliated structure is Riemannian enough to enable the definition of an associated **topological groupoid** and **C*-algebra**.

This enables one to use methods of noncommutative geometry and index theory to exploit the recurrent structure of the manifolds to gain analytic and geometric information.

(I will not go into detail here.)

Some Applications of the Hull.

(1) Roe-Block-Weinberger theorem.

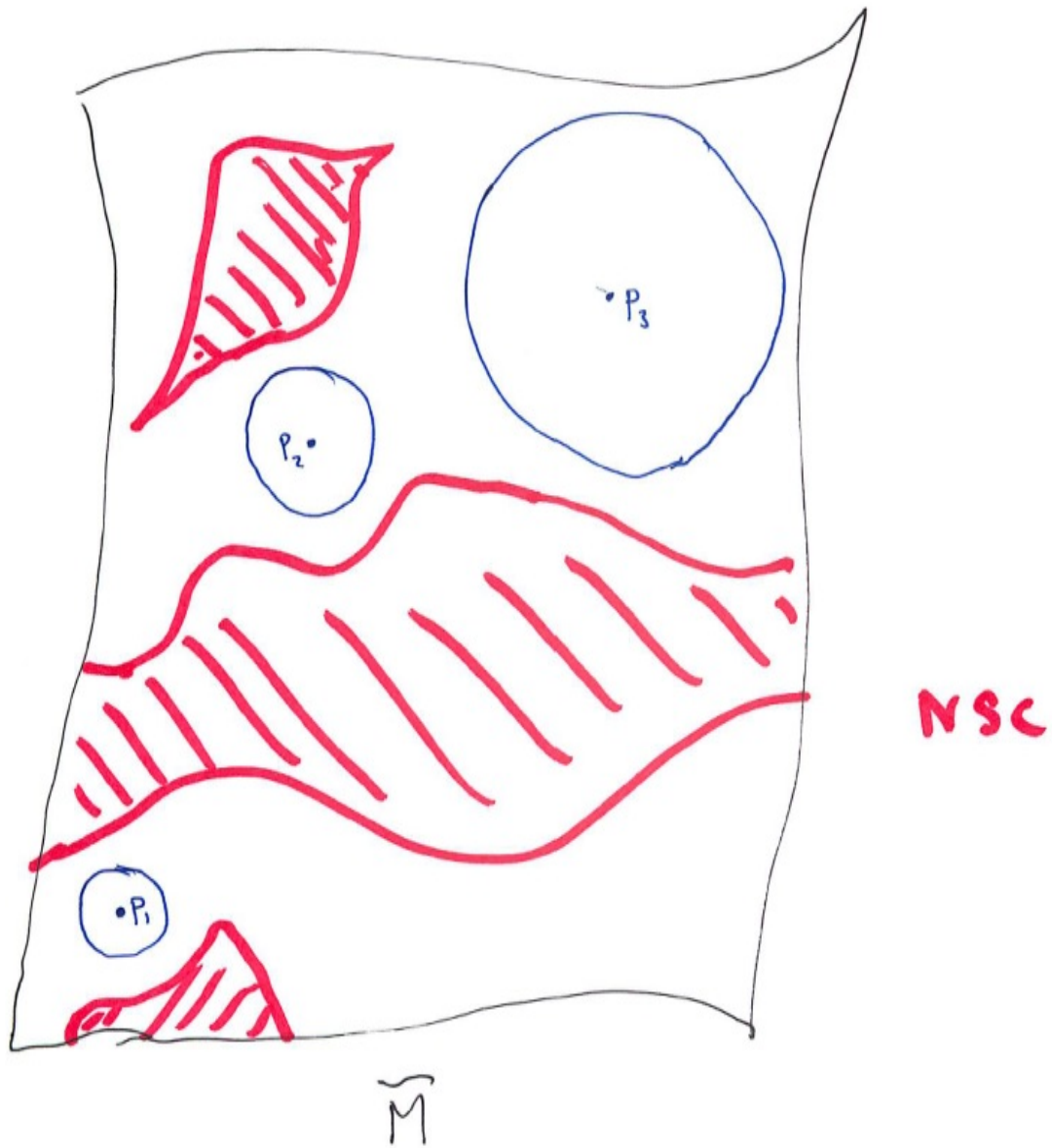
Theorem: (Atiyah-Lichnerowicz-Singer). If M is a closed spin manifold with positive scalar curvature, then

$$\langle A(M), [M] \rangle = 0.$$

Theorem: (Roe) If $\pi_1(M)$ is amenable and the universal cover has a bounded geometry metric with p.s.c. that is quasi-isometric to the universal cover, the same holds. Moreover, the same is true even if the n.s.c. set is merely assumed compact.

Theorem (Block-Weinberger). The same is true even if the n.s.c. is not C-dense.

Proof: Otherwise a suitable point on the hull contradicts Roe's original theorem.

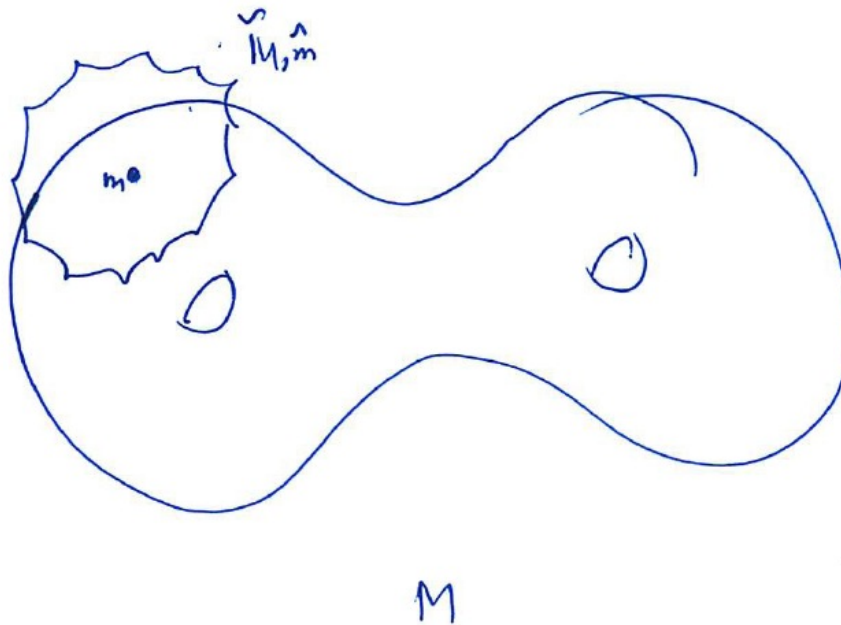


Remark: The original index theoretic approaches of Roe and Block-W probably still have application to very thinly doped matter.

(2) Principle of descent for the Novikov conjecture.

If M is a compact manifold of dimension > 1 , then for almost every metric on M , the hull of X = the universal cover of M is

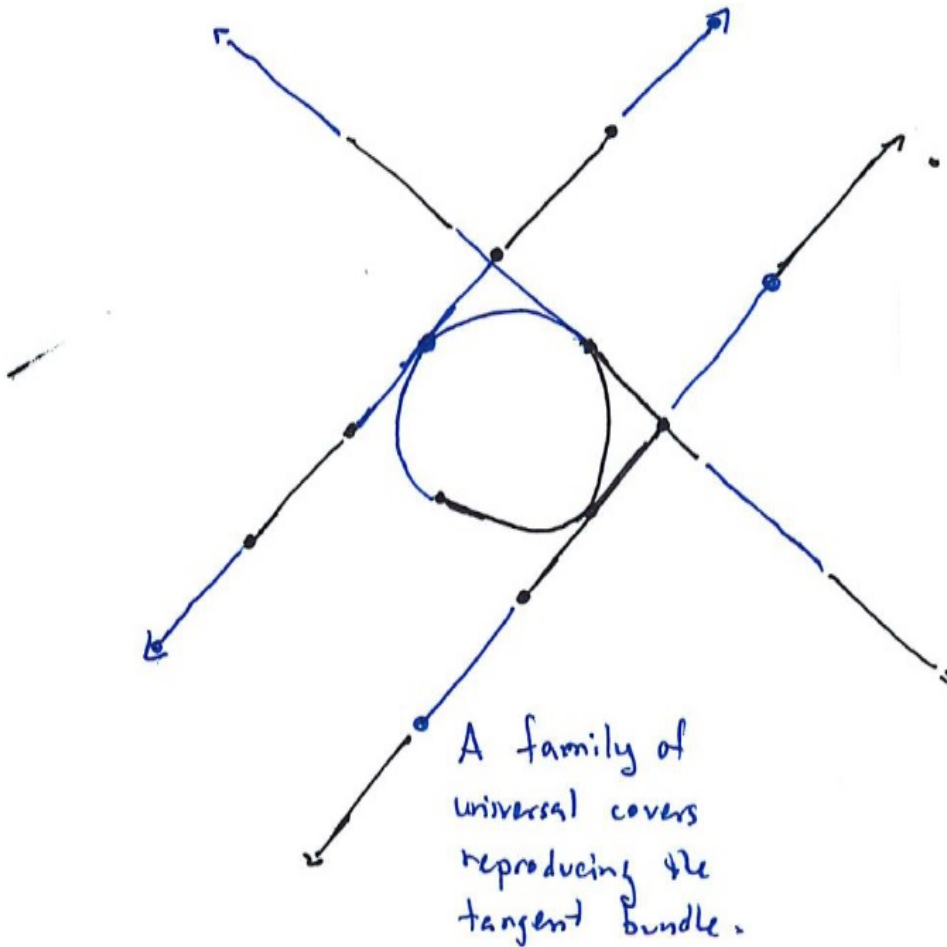
$$\Lambda(X) = M.$$



However, the prefoliated structure is in this case a fibration:

$$\begin{array}{c} X \times_{\pi_1 M} X \\ \downarrow \\ M \end{array}$$

It is precisely the study of this *family* of universal covers that allows one to prove the Novikov conjecture for e.g. linear groups, hyperbolic groups, etc. via the study of elliptic operators on the universal cover.



(A better picture of the foliated hull of a compact painted manifold.)

(3) Random unequivariant perturbations of an equivariant operator.

If Γ acts properly discontinuously on a manifold X , and D is an invariant operator, then it has an index, computed via the Atiyah L^2 index theorem.

For some purposes we might want to consider random perturbations of this.

Suppose in each fundamental domain we make a random choice of an element of a finite set F (e.g. a type of atom to put there). So our periodicity is now broken by a random element of F^Γ . Choosing a base point, each atom will add a bounded support potential $V_f(gm)$ to the operator.

This gives us an uncountable, but compact family of perturbations. All but $\#F$ of them are not actually periodic.

However since F^Γ has an invariant measure, we can take an average “ Γ -index” of these operators. The foliation index theorem says that this will equal the Atiyah index of the periodic leaf.

Ergodicity of the Γ action on F^Γ implies, for instance, that if the index is positive, then almost all of these random perturbations have nontrivial L^2 solutions of $Df = 0$.

Problems and future directions.

- (1) Develop a theory of “almost periodic manifolds” analogous to almost periodic functions.
- (2) Develop the index theory for elliptic operators on prefoliated spaces.
- (3) Develop tools for calculations of hulls in interesting cases (when infinite local complexity, for example or manifolds not associated to tilings). These can be both related to understanding better the hull as a space and technology related to the Baum-Connes conjecture (in its foliated version).
- (4) Of course, do some real Physics using these ideas, that were directly motivated by the work on gap labeling and the Quantum Hall effect for quasicrystals.

Summary.

- + There are analogies

Aperiodic tilings \longleftrightarrow Manifolds of bounded geometry

\longleftrightarrow Bounded u.c. functions
& Almost periodic functions

- + Such spaces have a dynamic aspect (similar in spirit to the ideas of additive combinatorics).
- + There is also an analogy to the Benjamini-Schramm limit in modern stochastic graph theory. Whether there is a benefit to this further unification is unclear.
- + The Brillouin zone of crystallography can be replaced by the study of the hull of such a space, and associated foliation dynamics (extending the noncommutative Brillouin zone from quasicrystals).
- + There are associated C^* -algebras whose K -theory should shed light on the elliptic theory of these spaces; and there are natural cohomology theories (with interesting mathematical interpretations) which should be the targets of Chern characters in these situations.
- + This construction unifies previous work on Quasicrystals with results on the theory of manifolds with bounded geometry and on the Novikov conjecture and random operators.

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