The
NONCOMMUTATIVE GEOMETRY
of
APERIODIC SOLIDS

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Main References


Important References

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Content

1. Quasicrystals
2. The Hull as a Dynamical System
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4. The Noncommutative Brillouin Zone
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I - Quasicrystals
I.1)- Aperiodic Solids

1. *Perfect crystals* in $d$-dimensions: translation and crystal symmetries. Translation group $\mathcal{T} \simeq \mathbb{Z}^d$.

2. *Quasicrystals*: no translation symmetry, but icosahedral symmetry. Ex.:
   (a) $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$;
   (b) $\text{Al}_{70}\text{Pd}_{22}\text{Mn}_8$;
   (c) $\text{Al}_{70}\text{Pd}_{22}\text{Re}_8$;

3. *Amorphous media*: short range order
   (a) Glasses;
   (b) Silicium in amorphous phase;

4. *Disordered media*: random atomic positions
   (a) Normal metals (with defects or impurities);
   (b) Doped semiconductors ($\text{Si, AsGa, ...}$);
I.2) Quasicrystalline Alloys

1. Metastable QC’s: \( \text{AlMn} \)


\( \text{AlMnSi} \)

\( \text{AlMgT} \) \((T = \text{Ag, Cu, Zn})\)

2. Defective stable QC’s: \( \text{AlLiCu} \)

(Sainfort-Dubost, (1986))

\( \text{GaMgZn} \)

(Holzen et al., (1989))

3. High quality QC’s: \( \text{AlCuT} \) \((T = \text{Fe, Ru, Os})\)

(Hiraga, Zhang, Hirakoyashi, Inoue, (1988))

(Gurnan et al., Inoue et al., (1989))

(Y. Calvayrac et al., (1990))

4. “Perfect” QC’s: \( \text{AlPdMn} \)

\( \text{AlPdRe} \)
1.3) Quasiperiodicity

1. A periodic crystal admits $\mathbb{Z}^3$ as symmetry group. A rotation symmetry must be represented by a $3 \times 3$ matrix $R$ with integer coefficients. Thus, if $\theta$ is the rotation angle

$$\text{Tr}(R) = 2 \cos \theta \in \mathbb{Z}$$

implying

$$\theta = 0, \pm \frac{\pi}{3}, \pm \frac{\pi}{2}, \pm \frac{2\pi}{3}, \pi.$$ 

2. Unusual symmetries such as 5-fold symmetries: *incompatible with periodicity*

Pointlike diffraction $\Rightarrow$ quasiperiodicity
- The icosahedral quasicrystal $AlPdMn$ -
- The icosahedral quasicrystal $HoMgZn$-
Typical TEM diffraction pattern
- with 5-fold symmetry -
I.4) - Transport Properties

Typical values of the resistivity

1. $Al$, $Fe$, $Cu$, $Pd$ are very good metals: why is conductivity so low?

2. Why does it decreases with temperature (opposite to metals)?

3. At high temperature

$$\sigma \propto T^\gamma \quad 1 < \gamma < 1.5$$

**Such behavior was never seen before.**

4. At low temperature for $Al_{70.5}Pd_{22}Mn_{7.5}$,

$$\sigma \approx \sigma(0) > 0$$

5. At low temperature for $Al_{70.5}Pd_{21}Re_{8.5}$,

$$\sigma \propto e^{-(T_0/T)^{1/4}}$$

*C. R. Wang et al. (1997); C. Berger et al. (1998)*
Comparison of conductivities for two QC’s
II - The Hull as a Dynamical System

J. Bellissard, D. Herrmann, M. Zarrouati,
Hull of Aperiodic Solids and Gap Labelling Theorems,
In Directions in Mathematical Quasicrystals, CRM Monograph Series,
II.1)- Point Sets

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 $\mathcal{L}$.

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:* $\mathcal{L} - \mathcal{L}$ is discrete.

6. *Meyer* set: $\mathcal{L}$ and $\mathcal{L} - \mathcal{L}$ are Delone.

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.
II.2)- Point Measures and Tilings

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

Conversely, given a Delone set, a tiling is built through the \textit{Voronoi cells}

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

1. \( V(x) \) is an \textit{open convex polyhedron} containing \( B(x; r) \) and contained into \( B(x; R) \).

2. Two Voronoi cells touch face-to-face.

3. If \( \mathcal{L} \) is \textit{FLC}, then the Voronoi tiling has finitely many tiles modulo translations.
- Building a Voronoi cell-
- A Delone set and its Voronoi Tiling-
II.3)- Point Measures

\( \mathcal{M}(\mathbb{R}^d) \) 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 \( \mathbb{R}^d \):

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

The \textit{Hull} is the closure in \( \mathcal{M}(\mathbb{R}^d) \)

\[
\Omega = \{ T^a \nu^\mathcal{L}; a \in \mathbb{R}^d \},
\]

where \( T^a \nu \) is the translated of \( \nu \) by \( a \).

\textbf{Results:}

1. \( \Omega \) 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 \( \omega \) coincides with \( \nu_\omega = \nu^\mathcal{L}_\omega \).
3. If \( \mathcal{L} \) is \textit{Delone} (resp. \textit{Meyer}) so are the \( \mathcal{L}_\omega \)'s.
II.4)- Properties

(a) Minimality

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

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

(b) Transversal

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

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

(c) Cantorian Transversal

\textbf{Proposition 2} If $\mathcal{L}$ has finite type, then the transversal is completely discontinuous (Cantor).
III - Building Hulls

J. Bellissard, R. Benedetti, J.-M. Gambaudo,
Spaces of Tilings, Finite Telescopic Approximations and Gap-Labelling,
III.1)- Examples

1. **Crystals**: \( \Omega = \mathbb{R}^d / \mathcal{T} \cong \mathbb{T}^d \) with the quotient action of \( \mathbb{R}^d \) on itself. (Here \( \mathcal{T} \) is the translation group leaving the lattice invariant. \( \mathcal{T} \) is isomorphic to \( \mathbb{Z}^D \).)

2. **Quasicrystals**: \( \Omega \simeq \mathbb{T}^n, \ n > d \) with an irrational action of \( \mathbb{R}^d \) and a completely discontinuous topology in the transverse direction to the \( \mathbb{R}^d \)-orbits.

3. **Impurities in Si**: let \( \mathcal{L} \) be the lattices sites for Si atoms (it is a Bravais lattice). Let \( \mathcal{A} \) be a finite set (alphabet) indexing the types of impurities. One sets \( \tilde{\Omega} = \mathcal{A}^\mathbb{Z}^d \) with \( \mathbb{Z}^d \)-action given by shifts. Then \( \Omega \) is the mapping torus of \( \tilde{\Omega} \).
- The Hull of a Periodic Lattice -
– The cut–and–project construction –
- The Penrose tiling -
Trieste, May 26, 2008

- Kites and Darts -

\[ \phi = \frac{1 + \sqrt{5}}{2} \]
\[ \phi^2 = \phi + 1 \]
\[ \phi = 1 + 1/\phi \]
- Rhombi in Penrose's tiling -
- The Penrose tiling -
- The octagonal tiling -
- Octagonal tiling: inflation rules -
- The transversal of the Octagonal Tiling -

- is completely disconnected -
III.2)- Finite Type Tilings

Let $\mathcal{L}$ be a finite type Delone set, and let $\mathcal{T}$ be its Voronoi tiling. Then

**Theorem 1** The dynamical system

$$(\Omega, \mathbb{R}^d, \mathcal{T}) = \lim_{\leftarrow} (B_n, f_n)$$

obtained as inverse limit of branched oriented flat manifolds, is conjugate to the Hull of the Delone set of the tiling $\mathcal{T}$ by an homemorphism.

1. A **Branched Oriented Flat manifold** (BOF) is a family of colored tiles glued on their edges.

2. As $n \to \infty$ the tiles of $B_n$ cover more and more of $\mathcal{T}$.

3. **BOF-submersion** $f_n : B_{n+1} \rightarrow B_n$ such that $Df_n = 1$. Each tile in $B_{n+1}$ is tiled by tiles of $B_n$: $f_n$ identifies them.

4. call $\Omega$ the **projective limit** of the sequence

$$\cdots \rightarrow f_{n+1} B_{n+1} f_n B_n f_{n-1} \cdots$$

5. **parallel transport** of constant vector fields on $B_n$, generates the infinitesimal $\mathbb{R}^d$-action on $\Omega$. 
- Vertex branching for the octagonal tiling -
IV - NC Brillouin Zone

IV.1)- Algebra

Set $\mathcal{A} = \mathcal{C}(\Omega) \rtimes \mathbb{R}^d$. For any $\omega \in \Omega$, let $\pi_\omega$ be the left regular representation on $\mathcal{H} = L^2(\mathbb{R}^d)$:

$$
\pi_\omega(A)\psi(x) = \int_{\mathbb{R}^d} d^dy \ A(T^{-x}\omega, y - x) \psi(y),
$$

and $\psi \in \mathcal{H}$. If $\mathbb{P}$ is an $\mathbb{R}^d$-invariant ergodic probability measure on $\Omega$, let $\mathcal{T}_\mathbb{P}$ be the trace on $\mathcal{A}$ defined by (for $A \in \mathcal{C}_c(\Omega \times \mathbb{R}^d)$ )

$$
\mathcal{T}_\mathbb{P}(A) = \int_{\Omega} \mathbb{P}(d\omega) A(\omega, 0),
$$

In much the same way, $\mathcal{C}^*(\Gamma_{tr})$ is the $\mathcal{C}^*$-algebra of the transversal, endowed with the induced trace $\mathcal{T}_{\mathbb{P}}^{tr}$.

**Theorem 2** If $\mathcal{L}$ is $\mathcal{G}$-periodic in $\mathbb{R}^d$, with Brillouin zone $\mathbb{B} = \mathbb{R}^d^*/\mathcal{G}^\perp = \mathcal{G}^*$ then :

1. $\mathcal{A}$ is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$,
2. $\mathcal{C}^*(\Gamma_{tr})$ is isomorphic to $\mathcal{C}(\mathbb{B}) \otimes M_n$ if $n = |\mathcal{L}/\mathcal{G}|$. 

IV.2)- Electrons

Schrödinger’s equation (ignoring interactions) on \( \mathbb{R}^d \)

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

acting on \( \mathcal{H} = L^2(\mathbb{R}^d) \). Here \( v \in L^1(\mathbb{R}^d) \) is real valued, decays fast enough, is the atomic potential.

Lattice case (tight binding representation)

\[
\tilde{H}_\omega \psi(x) = \sum_{y \in \mathcal{L}_\omega} h(t^{-x} \omega, y - x) \psi(y),
\]

**Proposition 3**

1. There is \( R(z) \in \mathcal{A} \), such that, for every \( \omega \in \Omega \) and \( z \in \mathbb{C} \setminus \mathbb{R} \)

\[
(z - H_\omega)^{-1} = \pi_\omega(R(z)).
\]

2. There is \( \tilde{H} \in C^*(\Gamma_{tr}) \) such that \( \tilde{H}_\omega = \pi_\omega(\tilde{H}) \).

3. If \( \Sigma_H = \bigcup_{\omega \in \Omega} \text{Sp}(H_\omega) \), then \( R(z) \) is holomorphic in \( z \in \mathbb{C} \setminus \Sigma_H \). The bounded components of \( \mathbb{R} \setminus \Sigma_H \) are called spectral gaps (same with \( \tilde{H} \)).
IV.3)- Density of States

• Let $\mathcal{P}$ be an invariant ergodic probability on $\Omega$. Let

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

It is called the $\textit{Integrated Density of states}$ or $\textit{IDS}$.

• The limit above exists $\mathcal{P}$-almost surely and

$$\mathcal{N}(E) = T_\mathcal{P}(\chi(H \leq E)) \quad (\text{Shubin, '76})$$

$\chi(H \leq E)$ is the eigenprojector of $H$ in $\mathcal{L}_\infty(\mathcal{A})$.

• $\mathcal{N}$ is non decreasing, non negative and constant on gaps. $\mathcal{N}(E) = 0$ for $E < \inf \Sigma_H$. For $E \to \infty$, $\mathcal{N}(E) \sim \mathcal{N}_0(E)$ where $\mathcal{N}_0$ is the IDS of the free case (namely $\nu = 0$).

• $\textit{Gaps can be labelled by the value the IDS takes on them}$
- An example of IDS -
1. Phonons are *acoustic waves* produced by small displacements of the 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*. 
1. For identical atoms with *harmonic motion*, the classical equations of motion are:

\[ M \frac{d^2 \vec{u}(\omega, x)}{dt^2} = \sum_{x \neq y \in \mathcal{L}_\omega} K_\omega(x, y) (\vec{u}(\omega, y) - \vec{u}(\omega, x)) \]

where \( M \) is the atomic mass, \( \vec{u}(\omega, x) \) is its classical displacement vector and \( K_\omega(x, y) \) is the matrix of *spring constants*.

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

3. Covariance gives

\[ K_\omega(x, y) = k(\tau^{-x} \omega, y - x) \]

thus

\[ k \in C^*(\Gamma_{tr}) \otimes M_d(\mathbb{C}) \]

4. Then the spectrum of \( k/M \) gives the *eigenmodes* propagating in the solid. Its density (DPM) is given by Shubin’s formula again.
IV.5) K-group labels

- If $E$ belongs to a gap $g$, the characteristic function $E' \in \mathbb{R} \mapsto \chi(E' \leq E)$ is continuous on the spectrum of $H$. Thus:
  $$P_g = \chi(H \leq E) \text{ is a projection in } \mathcal{A}!$$
- $\mathcal{N}(E) = \mathcal{T}_P(P_g) \in \mathcal{T}_P^*(K_0(\mathcal{A}))!$

**Theorem 3 (Abstract gap labelling theorem)**

- $S \subset \Sigma_H$ clopen, $n_S = [\chi_S(H)] \in K_0(\mathcal{A})$. If $S_1 \cap S_2 = \emptyset$ then $n_{S_1 \cup S_2} = n_{S_1} + n_{S_2}$ (additivity).
- Gap labels are invariant under norm continuous variation of $H$ (homotopy invariance).
- For $\lambda \in [0, 1] \mapsto H(\lambda) \in \mathcal{A}$ continuous, if $S(\lambda) \subset \Sigma_H$ clopen, continuous in $\lambda$ with $S(0) = S_1 \cup S_2$, $S(1) = S'_1 \cup S'_2$ and $S_1 \cap S_2 = \emptyset = S'_1 \cap S'_2$ then $n_{S_1} + n_{S_2} = n_{S'_1} + n_{S'_2}$ (conservation of gap labels under band crossings).
Theorem 4 If $\mathcal{L}$ is an finite type Delone set in $\mathbb{R}^d$ with Hull $(\Omega, \mathbb{R}^d, \tau)$, then, for any $\mathbb{R}^d$-invariant probability measure $\mathbb{P}$ on $\Omega$
\[ T_{\mathbb{P}}^*(K_0(A)) = \int_X d\mathbb{P}_{tr} \ C(X, Z) . \]
if $A = C(\Omega) \rtimes \mathbb{R}^d$, $X$ is the canonical transversal and $\mathbb{P}_{tr}$ the transverse measure induced by $\mathbb{P}$.

Main ingredient, for the proof

*Connes measured Index Theorem for foliations*

IV.6) - History

- For $d = 1$ this result follows from the Pimsner & Voiculescu exact sequence (*Bellissard, '92*).

- For $d = 2$, a double use of the Pimsner & Voiculescu exact sequence provides the result (*van Elst, '95*).

- For $d \geq 3$ whenever $(\Omega, \mathbb{R}^d, \mathbf{T})$ is Morita equivalent to a $\mathbb{Z}^d$-action, using spectral sequences (*Hunton, Forrest*) this theorem was proved for $d = 3$ (*Bellissard, Kellendonk, Legrand, '00*).

- The theorem has also been proved for all $d$’s recently and independently by (*Benameur, Oyono, 2001*) (*Kaminker, Putnam, 2001*) and (*Bellissard, Benedetti, Gambaudo, 2001*).
V - NC Fermi Surface

V.1) Quasilocal Algebra

Here $\mathcal{L}$ is a Delone set, electrons are described in the tight binding representation. $X$ denotes its transversal. Then $\mathcal{A} = C^*(\Gamma_{tr})$.

1. For $\omega \in X$, with each site $x \in \mathcal{L}_\omega$ are associated *creation-annihilation* operators for electrons (*fermions*) and phonons (*bosons*).

2. These operators generate a *quasilocal algebra* $\mathfrak{A}_\omega$. The translation $\gamma = (\omega, a)$ in $\Gamma_{tr}$ allows to generate a *-isomorphism $\alpha_\gamma : \mathfrak{A}_{T-a\omega} \mapsto \mathfrak{A}_\omega$.

3. The second quantized Hamiltonian with electron-phonon interactions, generates a dynamics (*Bratteli, Robinson, ’72*) $\eta_\omega(t) \in \text{Aut}(\mathfrak{A}_\omega)$ that is covariant. Adding the various Lagrange multipliers (chemical potential,...) gives a *KMS-dynamics* $\phi$ in much the same way.

4. The field $\mathfrak{A} = (\mathfrak{A}_\omega)_{\omega \in X}$ becomes continuous and covariant.

5. The crossed product $\mathfrak{B} = \mathfrak{A} \rtimes_\alpha \Gamma$ is well-defined (*Renault, ’86*). The dynamics induced by $\eta, \phi$ give corresponding automorphism groups of $\mathfrak{B}$.
V.2)- Bimodule over the NC Brillouin Zone

1. $\mathfrak{B}$ is generated by continuous funtions

$$\gamma \in \Gamma \mapsto A(\gamma) \in A_\omega$$

if $\omega = r(\gamma)$, with compact support.

2. The product is given by

$$(AB)(\gamma) = \sum_{\gamma' \in \Gamma^\omega} A(\gamma')\alpha(\gamma')B(\gamma'^{-1} \circ \gamma)$$

3. the adjoint by:

$$A^*(\gamma) = \alpha(\gamma)A(\gamma^{-1})^*$$

4. The (reduced) norm is obtained through covariant representations.

5. $\mathfrak{B}$ is also a $C^*(\Gamma)$-bimodule.
V.3) Covariant States & GNS Representation

1. A **covariant state** on $\mathfrak{A}$ is a continuous family $\Phi_\omega$ of states on $\mathfrak{A}_\omega$ such that

$$\Phi_\omega \circ \alpha(\gamma) = \Phi_{\omega'} \quad \text{if} \quad \gamma : \omega' \mapsto \omega$$

2. A Hilbert $C^*$-module structure over $C^*(\Gamma)$ is defined on $\mathfrak{B}$ by:

$$\langle A|B\rangle(\gamma) = \Phi_\omega (A^* B(\gamma))$$

After quotienting and completion we get a Hilbert $C^*$-module $\mathcal{F}$.

3. In particular

(a) $\langle A|B\rangle \in C^*(\Gamma)$,

(b) If $h \in C^*(\Gamma)$ then $\langle A|Bh\rangle = \langle A|B\rangle h$.

(c) $\langle A|B\rangle^* = \langle B|A\rangle$.

(d) $\langle A|CB\rangle = \langle C^* A|B\rangle$

4. So that the left multiplication by an element of $\mathfrak{B}$ defines an **endomorphisms** of $\mathcal{F}$, giving rise to the **GNS representation** of $\mathfrak{B}$ in $\mathcal{F}$. 

V.4)- Ground State

1. If $\Phi$ is $\eta$-invariant, $\eta^t$ is implemented by a one parameter group $U(t)$ of unitary endomorphisms of $\mathcal{F}$:

$$\langle A | U(t) B \rangle = \langle A | \eta^t(B) \rangle$$

2. If, in addition, $\Phi$ is a ground state for $\eta$, then the generator $H = -iU(t)^{-1}dU/dt$ is positive, namely

$$\langle A | HA \rangle \geq 0 \quad \forall A \in \mathcal{F}$$

3. This construction applies to the case of the electron-phonon dynamics in an aperiodic solid: a ground state is specified by the Fermi level $E_F$.

The Hilbert $C^*$-module $\mathcal{F}_F$ obtained in this way, plays the rôle of a fiber bundle over the Noncommutative Brillouin zone defined by $C^*(\Gamma)$, fixing the geometry of the Fermi surface. Hence :

**Definition 1** The Noncommutative Fermi surface associated with the dynamics defined by the total Hamiltonian $H$, and with the Fermi energy $E_F$ is the NC fiber bundle above the NC Brillouin zone associated with the Hilbert $C^*$-module $\mathcal{F}_F$ constructed above.
Conclusion

1. An aperiodic solid gives rise to a canonical dynamical system, its Hull, representing the configurations of lack of periodicity.

2. The $C^*$-algebra associated with the Hull can be interpreted as the Noncommutative Brillouin Zone.

3. Electrons and phonons are affiliated to this algebra.

4. The topology of the NCBZ can be computed via its $K$-theory. The Gap Labelling Theorem is a special example of application.

5. Interactions lead to a NC description of the Fermi surface, through a Hilbert $C^*$-bimodule over the NCBZ.

6. The NC Geometry can be described through the Cyclic Cohomology of the NCBZ. We conjecture that it plays a rôle in non dissipative transport (ex.: the Integer Quantum Hall Effect).