ELECTRONS in APERIODIC MEDIA

Jean BELLISSARD

Georgia Institute of Technology, Atlanta School of Mathematics & School of Physics e-mail: jeanbel@math.gatech.edu





This material is based upon work supported by the National Science Foundation Grant No. DMS-1160962



Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

Contributors

H. SCHULZ-BALDES, Dep. of Math., Friedrich-Alexander Universität, Erlangen-Nürnberg, Germany.

Main References

J. Bellissard, *K-Theory of C*-algebras in Solid State Physics,* Lecture Notes in Physics, **257**, Springer (1986), pp. 99-156.

J. Bellissard, *Gap labeling theorems for Schrödinger operators*, *From number theory to physics (Les Houches, 1989)*, pp. 538-630, Springer, Berlin, 1992.

H. Schulz-Baldes, J. Bellissard, Rev. Math. Phys., 10, (1998), 1-46.

H. Schulz-Baldes, J. Bellissard, J. Stat. Phys., 91, (1998), 991-1026.

J. BELLISSARD, *Coherent and dissipative transport in aperiodic solids*, Lecture Notes in Physics, **597**, Springer (2003), pp. 413-486.

Content

- 1. Aperiodic Materials
- 2. Harper's Model
- 3. C*-algebras: an apology
- 4. Hull
- 5. The Noncommutative Brillouin Zone

I - Aperiodic Materials

A List of Materials

- 1. Aperiodicity for Electrons
 - Crystals in a Uniform Magnetic Field
 - Semiconductors at very low temperature
- 2. Atomic Aperiodicity
 - Quasicrystals
 - Glasses
 - Bulk Metallic Glasses

Quasicrystals

- 1. Stable Ternary Alloys (*icosahedral symmetry*)
 - High Quality: AlCuFe ($Al_{62.5}Cu_{25}Fe_{12.5}$)
 - Stable Perfect: AlPdMn (Al_{70} , $Pd_{22}Mn_{7.5}$) AlPdRe (Al_{70} , $Pd_{21}Re_{8.5}$)

- 2. Stable Binary Alloys
 - Periodic Approximants: **YbCd**₆, **YbCd**_{5.8}
 - Icosahedral Phase **YbCd**_{5.7}

Quasicrystals

A hole in a sample of AlPdMn





A sample of HoMgZn compared with a US one cent coin

Bulk Metallic Glasses

1. Examples (Ma, Stoica, Wang, Nat. Mat. '08)

- $\mathbf{Zr}_{\mathcal{X}}\mathbf{Cu}_{1-\mathcal{X}}$ $\mathbf{Zr}_{\mathcal{X}}\mathbf{Fe}_{1-\mathcal{X}}$ $\mathbf{Zr}_{\mathcal{X}}\mathbf{Ni}_{1-\mathcal{X}}$
- $Cu_{46}Zr_{47-x}Al_7Y_x$ $Mg_{60}Cu_{30}Y_{10}$
- 2. Properties (Hufnagel web page, John Hopkins)
 - High *Glass Forming Ability* (GFA)
 - High *Strength*, comparable or larger than steel
 - Superior *Elastic limit*
 - High *Wear* and *Corrosion* resistance
 - *Brittleness* and *Fatigue* failure

Bulk Metallic Glasses

Applications (Liquidemetal Technology www.liquidmetal.com)

- Orthopedic implants and medical Instruments
- Material for *military components*
- Sport items, golf clubs, tennis rackets, ski, snowboard, ...



Pieces of Titanium-Based Structural Metallic-Glass Composites

(Johnson's group, Caltech, 2008)

II - Harper's Model

P. G. HARPER, Proc. Phys. Soc. A, 68, 874-878, (1955)

D. R. Hofstadter, Phys. Rev. B, 14, 2239-2249, (1976)

- Perfect *square lattice*, nearest neighbor hoping terms, *uniform magnetic field B* perpendicular to the plane of the lattice
- Translation operators U_1, U_2



- a = lattice spacing
- ϕ = flux through unit cell

• Commutation rules (*Rotation Algebra*)

$$U_1 U_2 = e^{2i\pi\alpha} U_2 U_1$$
 $\alpha = \frac{\phi}{\phi_0}$ $\phi = Ba^2 \quad \phi_0 = \frac{h}{e}$

• Kinetic Energy (*Hamiltonian*)

$$H = t \left(U_1 + U_2 + U_1^{-1} + U_2^{-1} \right)$$

• Landau gauge $\psi(m, n) = e^{2i\pi mk}\varphi(n)$. Hence $H\psi = E\psi$ means

$$\varphi(n+1) + \varphi(n-1) + 2\cos 2\pi(n\alpha - k)\varphi(n) = \frac{E}{t}\varphi(n)$$



For $\alpha = p/q$, the following properties hold

• The spectrum has q nonoverlapping bands, *touching only at* E = 0

(Bellissard-Simon '82,..., Avila-Jitomirskaya '09)

• The spectral gaps are bounded below by e^{-Cq} for some C > 0(*Helffer-Sjöstrand '86-89, Choi-Elliot-Yui. 90*)

For $\alpha \notin \mathbb{Q}$,

• The spectrum is a Cantor set

(Bellissard-Simon '82,..., Avila-Jitomirskaya '09)

• The spectrum has zero Lebesgue measure

(Avron-van Mouche-Simon, '90, ..., Avila-Jitomirskaya '09)

• The gap edges are Lipshitz continuous as long as they do not close, otherwise they are Hölder with exponent 1/2

(Bellissard '94, Avron-van Mouche-Simon, '90, Haagerup et al.)

• The derivative of gap edges *w.r.t.* α is discontinuous at each rational

(Wilkinson '84, Rammal '86, Bellissard-Rammal '90)

Rotation Algebra

- The *C**-algebra \mathcal{A}_{α} generated by two unitaries U_1, U_2 such that $U_1 U_2 = e^{2i\pi\alpha} U_2 U_1$ is called the *rotation algebra* (*Rieffel '81*)
- \mathcal{A}_{α} has a *trace* defined by

 $\mathcal{T}(U_1^m \, U_2^n) = \delta_{m,0} \, \delta_{n,0}$

• \mathcal{A}_{α} admits two *-*derivations* ∂_1, ∂_2 defined by (Connes '82)

 $\partial_i U_j = 2\imath \pi \, \delta_{i,j} U_j$

Rotation Algebra

• Rieffel's projection $P_{R} = -f(U_{2})U_{1} + g(U_{2}) - U_{1}^{-1}f(U_{2})$



• If $P \in \mathcal{A}_{\alpha}$ is a *projection*, then

$$\mathcal{T}(P_{R}) = \alpha$$

$$\frac{1}{2i\pi} \mathcal{T}(P_{R}[\partial_{1}P_{R}, \partial_{2}P_{R}]) = 1$$

(Rieffel '81, Pimsner-Voiculescu '80, Connes '82)

$$\mathcal{T}(P) = n\alpha - [n\alpha] \qquad n = \operatorname{Ch}(P) = \frac{1}{2i\pi} \mathcal{T}(P[\partial_1 P, \partial_2 P]) \in \mathbb{Z}$$

Gap Labels

• If $H = U_1 + U_1^{-1} + U_2 + U_2^{-1}$, and if *E* belongs to a gap of the spectrum of *H*, set



• Then $P_E \in \mathcal{A}_{\alpha} !!$ Hence $\mathcal{T}(P_E) = n\alpha - [n\alpha]$ for some $n \in \mathbb{Z} !!$ (Bellissard '81, '86)

Gap Labels

- The spectral projection of the Harper model between any two gaps can be labelled by an integer, using the previous results, *(Claro-Wannier '78)*
- This integer corresponds to the quantization of the Hall conductivity in such systems (Thouless-Kohmoto-den Nijs-Nightingale '82)



Each color corresponds to the integer gap label, for the eigenprojection between the l.h.s and the gap. (Avron-Osadchy-Seiler '03) III - C*-algebras: an apology

Fourier Transform

JOSEPH FOURIER, Mémoire sur la propagation de la chaleur dans les corps solides, Nouveau Bull. Sci. Soc. Philomatique Paris, I (6), (1808), 112-116.

• *"All"* complex valued functions defined on the interval [0,1] can be written as a Fourier series

$$f(x) = \sum_{n \in \mathbb{Z}} \hat{f}_n \ e^{2i\pi \ n \ x} \qquad \qquad \hat{f}_n \in \mathbb{C}$$

• "All" complex valued functions defined on \mathbb{R} can be written as a Fourier integral

$$f(x) = \int_{\mathbb{R}} \hat{f}(p) \ e^{\iota p x} \ dp$$

Fourier Transform

• The expansion extends to a parallelepiped $P = \prod_{i=1}^{d} [a_i, b_i]$ or to \mathbb{R}^d

$$f(x) = \sum_{n \in \mathbb{Z}^d} \hat{f}_n \ e^{2i\pi \sum_{i=1}^d n_i (x_i - a_i)/(b_i - a_i)} \qquad \qquad f(x) = \int_{\mathbb{R}^d} \hat{f}(p) \ e^{i p \cdot x} \ d^d p$$

• It was used by Fourier to *"solve"* the *heat equation* in a parallelepipedic box and to compute the heat transfer

$$\frac{\partial f}{\partial t} = \Delta f \qquad \Leftrightarrow \qquad \frac{\partial \hat{f}_n}{\partial t} = -\left(\sum_i \frac{4\pi^2 n_i^2}{(b_i - a_i)^2}\right) \hat{f}_n$$

An amazingly efficient tool

• The entry *Fourier transform* on Google produces

8,100,000 results !!

- Used to analyze *partial differential equations*
- Used to solve PDE's by numerical computations through (*fast Fourier transform*), in
 - Celestial Mechanics (satellites),
 - weather forecast
 - Optic, gratings,
 - Quantum Physics: nuclei, atoms, molecules, band calculations,...

Reconstruction Formula & Hilbert Spaces

(Second half of 19th century, PARSEVAL, orthonormal polynomials, HILBERT)

• The Fourier coefficients \hat{f}_n can be computed from f

$$\hat{f_n} = \int_0^1 e^{-2inx} f(x) \, dx$$

• The sequence $(\hat{f_n})_{n \in \mathbb{Z}}$ as an analog of the *coordinates of a vector* in the complex analog of Euclidean spaces, a *Hilbert space*

$$\sum_{n \in \mathbb{Z}} |\hat{f}_n|^2 = \int_0^1 |f(x)|^2 \, dx = ||f||^2 \qquad \text{(Parseval)}$$

Pontryagin Duality

L.S. PONTRYAGIN, The theory of topological commutative groups, Ann. of Math., **35**, (1934), 361-388

- If *G* is an *abelian group*, a *character* is a group homomorphism $\chi: G \to \mathbb{S}^1$
- The set G^* of character is an abelian group for the *pointwise* multiplication $\chi \eta : g \in G \mapsto \chi(g)\eta(g) \in \mathbb{S}^1$ and $G \subset G^{**}$
- If **G** is a *topological group* the weak*-topology make **G*** topolog-ical
- If **G** is locally compact
 - so is G^*
 - $-G = G^{**}$
 - *G* and *G*^{*} have a *Haar measure* dg, $d\chi$

Pontryagin Duality

If $F : G \to \mathbb{C}$ is *continuous*, there is a suitable normalization of the dual Haar measure $d\chi$ such that, its *Fourier transform* satisfies

$$\widehat{F}(\chi) = \int_{G} \chi(g) F(g) dg \quad \Leftrightarrow \quad F(g) = \int_{G^*} \overline{\chi(g)} \widehat{F}(\chi) d\chi$$
$$\int_{G} |F(g)|^2 dg = \int_{G^*} |\widehat{F}(\chi)|^2 d\chi \quad \text{(Parseval)}$$
Fourier transform : $L^2(G) \to L^2(G^*)$ is unitary.

Fourier transform is (abelian) group theory !

Convolution & Product

• Dual aspect of the group law: *convolution* If $F, F' : G \rightarrow \mathbb{C}$ are continuous with comact support

$$F * F'(g) = \int_G F(h) F'(h^{-1}g) dh$$

• The Fourier transform it into the *pointwise product*

$$\widehat{F \ast F'}(\chi) = \widehat{F}(\chi) \ \widehat{F'}(\chi)$$

Fourier transform is (abelian) algebra !

C*-Algebras

A very long story: from Gelfand *et al.* 1940, to the mid sixties G. K. PEDERSEN, *C**-algebras and their automorphism groups, Academic Press, 1979.

A *C**-*algebra* \mathcal{A} is a Banach space with a bilinear associative product $(a, b) \mapsto ab$ and an antilinear involution $a \mapsto a^*$ such that

 $||ab|| \le ||a|| ||b|| \qquad ||a^*a|| = ||a||^2$

The *r.h.s* implies that the norm is of purely algebraic origin because

- 1. The norm of $||a^*a||$ coincides with the *spectral radius* of a^*a (namely the minimum of |z| for $z \in \mathbb{C}$ such that $(z a^*a)$ is invertible in \mathcal{A})
- 2. If $\rho : \mathcal{A} \to \mathcal{B}$ is an injective *-homomorphism between C*-algebras, then it is *isometric*.

C*-Algebras

A *character* is a *-homomorphism $\chi : \mathcal{A} \to \mathbb{C}$. Then the *kernel* of a character is a *closed* *-*ideal*.

If \mathcal{A} is simple, there are no characters other than 0, 1.

The set $X = X(\mathcal{A})$ of characters is equipped with the *weak*^{*}-*topology*: then X is *locally compact* (*compact* if \mathcal{A} has a unit).

Gelfand Theorem *A* C^* -algebra \mathcal{A} is an abelian if and only if there is a *-isomorphism $\mathcal{G} : \mathcal{A} \to C_0(X)$

C*-Algebras

Let *G* be a *locally compact abelian group*. The convolution and the adjoint $(F, F' \in C_c(G))$ are continuous with compact support)

$$F * F'(g) = \int_G F(h)F'(h^{-1}g) dh$$
 $F^*(g) = \overline{F(g^{-1})}$

 $C_c(G)$ becomes a **-algebra*. It has a unique C^* -*norm* with completion $C^*(G)$.

Theorem If G is a locally compact abelian group $C^*(G)$ is commutative and its space of character is homeomorphic to G^* . The Gelfand transform G coincides with the Fourier transform

Fourier transform is (abelian) C*-algebras !

C*-Algebras as Noncommutative Spaces

- A C*-algebra can be seen as the space of continuous functions (*vanishing at infinity*) on an hypothetical locally compact "*non-commutative*" space X.
- Hence expressing algebraically operations like integrals, derivatives, vector fields, connections, *etc.*, leads to *"noncommutative geometry"*.
- Similarly a C*-algebra can be seen as a *Fourier transform without symmetries* !

VI - The Hull

Fundamental Properties

- **Pointlike Nuclei:** The *atomic nuclei* in a solid are located on a discrete subset of \mathbb{R}^3 . These nuclei can be considered as pointlike.
- Exclusion Principle: Due to the electron-electron repulsion, produced by the Pauli's *exclusion principle*, there is a *minimum distance* between nuclei. Hence the nuclei positions make up a uniformly discrete subset of \mathbb{R}^3 .
- **Condensed Media:** Both in liquid and solids, big holes are unstable, hence unlikely.
- **Homogeneity:** All solids considered are *homogeneous*, namely their large scale physical properties are invariant by translation

Uniformly Discrete Sets

- A discrete subset $\mathcal{L} \subset \mathbb{R}^d$ is called *uniformly discrete* whenever there is r > 0 such that $\#\{B(x;r) \cap \mathcal{L}\} = 0, 1$ for any $x \in \mathbb{R}^d$
- Associated with *L* is the *Radon measure*

$$v^{\mathcal{L}} = \sum_{y \in \mathcal{L}} \delta_y$$

- $\nu^{\mathcal{L}}$ is characterized by two properties
 - If *B* is any bounded *Borel* subset of \mathbb{R}^d then $\nu^{\mathcal{L}}(B) \in \mathbb{N}$
 - For all $x \in \mathbb{R}^d$ then $\nu^{\mathcal{L}}(B(x; r)) \in \{0, 1\}$
- Let UD_r be the set of such measures on \mathbb{R}^d .

UD-sets

• The space $\mathfrak{M}(\mathbb{R}^d)$ of *Radon measures* on \mathbb{R}^d is the dual to the space $C_c(\mathbb{R}^d)$ of continuous functions with compact support. It will be endowed with the *weak*-topology*. \mathbb{R}^d acts on it and this action is weak*-continuous. Then **T** will denote this action.

• Theorem:

- A Radon measure μ belongs to UD_r if and only if it has the form $v^{\mathcal{L}}$ with \mathcal{L} being r-uniformly discrete
- UD_r is invariant by the translation group \mathbb{R}^d
- **Theorem:** For any r > 0, the space UD_r is compact

• **Hull of** μ : if $\mu \in UD_r$ its Hull is the closure of its translation orbit.

 $\operatorname{Hull}(\mu) = \{ \mathrm{T}^a \mu \, ; \, a \in \mathbb{R}^d \}$

• It follows immediately that the *Hull* is *compact* and that \mathbb{R}^d acts on it by *homeomorphisms*. Hence

(Hull(μ), \mathbb{R}^d , τ) is a topological dynamical system

• The support of μ is denoted by \mathcal{L}_{μ}

The Canonical Transversal

- If $\mu \in UD_r$ its *canonical transversal* is the subset $Trans(\mu)$ defined by those elements $\xi \in Hull(\mu)$ with $\xi(\{0\}) = 1$
- If $\xi \in \text{Trans}(\mu)$ and if $a \in \mathbb{R}^d$ is small enough and nonzero 0 < |a| < r then $\tau^a \xi \notin \text{Trans}(\mu)$
- $Trans(\mu)$ is also compact.
- $\xi \in \text{Trans}(\mu)$ then its *fiber* is the set of points $\mathcal{L}_{\xi} \subset \mathbb{R}^d$ such that $a \in \mathcal{L}_{\xi} \Rightarrow \tau^{-a} \xi \in \text{Trans}(\mu)$. Hence \mathcal{L}_{ξ} is nothing but the *support* of ξ

Delone Sets

• A measure $\mu \in UD_r$ is *Delone* if there is $R \ge r$ so that $\mu(\overline{B}(x; R)) \ge 1 \qquad \forall x \in \mathbb{R}^d$

The space of *R*-Delone sets is closed, thus $\operatorname{Hull}(\mu) \subset \operatorname{Del}_{r,R}$

- A Delone set \mathcal{L} has *finite local complexity* (*FLC*), if the set $\mathcal{L} \mathcal{L}$ is discrete and closed (Lagarias '99) where $\mathcal{L} \mathcal{L} = \{y z; y, z \in \mathcal{L}\}$ Then its transversal is *completely disconnected*.
- *L* is a *Meyer set* whenever both *L* and *L L* are Delone. *Quasicrystal* are described by Meyer sets.

V - The Noncommutative Brillouin Zone

Set Up

- Ω is a *compact metrizable* space equipped with an *action* of the translation group \mathbb{R}^d by homeomorphism (for example $\Omega = \text{Hull}(\mu)$)
- $\Xi \subset \Omega$ is a *closed* subspace (for example $\Xi = \Omega$, Trans(μ))
- $\Gamma^{\xi} = \{x \in \mathbb{R}^d : \tau^{-x} \xi \in \Xi\}$. Let *dy* denotes either the Lebesgue or the counting measure on Γ^{ξ} .
- **Magnetic field:** $(x, y) \in \mathbb{R}^d \mapsto \mathcal{B}(x, y) \in \mathbb{R}$ is bilinear, antisymmetric.

The lack of periodicity makes *homogeneity* (translation invariance at large scale) more complicate to express.

Instead of a *group* action, it is rather a *groupoid* action.

A groupoid can be seen as a *category*, with objects and morphisms being *sets*.



A groupoid can be seen as a group with *several units* (objects) and a *partially defined product*. It can be endowed with a topology, a probability on the set of units, ...

 $\Gamma \subset \Xi \times \mathbb{R}^d$ is the *groupoid* induced Ξ :

- Elements of Γ are pairs $\gamma = (\xi, x) \in \Xi \times \mathbb{R}^d$ such that $\tau^{-x} \xi \in \Xi$
- $\Gamma \subset \Xi \times \mathbb{R}^d$ is closed.
- Source, Range: $r(\gamma) = \xi$, $s(\gamma) = \tau^{-x}\xi$ are continuous maps $s, r: \Gamma \to \Xi$
- **Product:** if $r(\gamma') = s(\gamma)$ and $\gamma = (\xi, x), \gamma' = (\xi', x') = (\tau^{-x}\xi, x')$

$$\gamma \circ \gamma' = (\xi, x + x')$$

• Inverse: $\gamma^{-1} = (\tau^{-\chi}\xi, -\chi)$

- In the *periodic case* $\mathcal{L} = \mathbb{Z}^d$ then $\Omega = \mathbb{R}^d / \mathbb{Z}^d = \mathbb{T}^d$
- If $\Xi = \{0\} \subset \mathbb{T}^d$ then $\Gamma \simeq \mathbb{Z}^d$ is the *period group*.

 Γ is the remnant of the translation group !

- Hilbert Space: $\mathcal{H}_{\xi} = L^2(\Gamma^{\xi})$
- **Γ-Action:** if $\gamma \in \Gamma : \eta = \tau^{-\chi} \xi \to \xi$ then

 $U(\gamma): \mathcal{H}_{\eta} \to \mathcal{H}_{\xi}$ $U(\gamma)\psi(y) = e^{-\imath \mathbb{B}(x,y)} \psi(y-x) \qquad \psi \in \mathcal{H}_{\eta} \ y \in \Gamma^{\xi}$

The Algebra $C^*(\Gamma)$

Endow $\mathcal{A}_0 = C_c(\Gamma)$ with (here $A, B \in \mathcal{A}_0$)

• **Product:** (convolution over the groupoid)

$$A \cdot B(\xi, x) = \int_{\Gamma^{\xi}} A(\xi, y) B(\tau^{-y}\xi, x - y) e^{i\mathcal{B}(x, y)} dy$$

• Adjoint: (Like
$$F^*(\gamma) = \overline{F(\gamma^{-1})}$$
)
$$A^*(\xi, x) = \overline{A(\tau^{-x}\xi, -x)}$$

• **Representation:** (*Left regular*) on $\mathcal{H}_{\xi} = L^2(\Gamma^{\xi})$

$$\pi_{\xi}(A)\,\psi(x) = \int_{\Gamma^{\xi}} A(\tau^{-x}\xi, y-x)\,e^{-\imath \mathcal{B}(x,y)}\,\psi(y)\,dy \qquad \psi \in \mathcal{H}_{\xi}$$

The Algebra $C^*(\Gamma)$

• **Covariance:** if $\gamma : \eta \to \xi$

$$U(\gamma)\pi_{\eta}(A)U(\gamma)^{-1} = \pi_{\xi}(A)$$

• C*-norm:

$$||A|| = \sup_{\xi \in \Xi} ||\pi_{\xi}(A)||$$

• $C^*(\Gamma, \mathcal{B})$ is the *completion* of \mathcal{A}_0 under this norm

The Algebra $C^*(\Gamma)$

• **Periodic Case:** \mathcal{L} is a discrete subgroup of \mathbb{R}^d , such that $\mathbb{B} = \mathbb{R}^d / \mathcal{L}$ is compact. \mathbb{B} is called the *Brillouin zone*.

$C^*(\Gamma) \simeq C(\mathbb{B}) \otimes \mathcal{K}$

• In particular any $A \in C^*(\Gamma)$ can be seen as a matrix valued function $A_{ij}(k), k \in \mathbb{B}$

Calculus

• Let \mathbb{P} be a Γ -invariant probability on Ξ and set

$$\mathcal{T}_{\mathbb{P}}(A) = \int_{\Xi} A(\xi, 0) \mathbb{P}(d\xi) \qquad A \in C_{\mathcal{C}}(\Gamma)$$

- $\mathcal{T}_{\mathbb{P}} : \mathcal{A}_0 \to \mathbb{C}$ is a trace:
 - $-\mathcal{T}_{\mathbb{P}}:\mathcal{A}_0\to\mathbb{C}$ is linear
 - It is positive $\mathcal{T}_{\mathbb{P}}(A^*A) \geq 0$
 - It is tracial $\mathcal{T}_{\mathbb{P}}(AB) = \mathcal{T}_{\mathbb{P}}(BA)$

Calculus

• $\mathcal{T}_{\mathbb{P}}$ is the *trace per unit volume*

$$\mathcal{T}_{\mathbb{P}}(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda \cap \Gamma^{\xi}|} \operatorname{Tr}\left(\pi_{\xi}(A)\chi_{\Lambda}\right) \qquad \forall \xi \mathbb{P} - a. \ s.$$

• In the periodic case

$$\mathcal{T}_{\mathbb{P}}(A) = \int_{\mathbb{B}} \operatorname{Tr}\left(\hat{A}(k)\right) \, dk$$

Trace per unit volume = integral over Brillouin's zone

Calculus

• Dual \mathbb{R}^d -action:

$$\eta_k(A)(\xi, x) = e^{\imath k \cdot x} A(\xi, x) \qquad \partial_i A = \frac{\partial}{\partial k_i} \eta_k(A) \upharpoonright_{k=0}$$

• Then if $X = (X_1, \dots, X_d)$ is the *position* operator defined by $(X_i\psi)(x) = x_i\psi(x)$ for $\psi \in \mathcal{H}_{\xi}$, then

 $\pi_{\xi}(\partial_i A) = -\iota[X_i, \pi_{\xi}(A)]$

 ∂_i is is differentiation w.r.t quasi-momentum

Thanks for listening !