# Algebraic Approach to Localization

Jean BELLISSARD

*Westfälische Wilhelms-Universität, Münster*
*Department of Mathematics*

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

Sponsoring

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE

UNIVERSITÉ DE PROVENCE Aix-Marseille I

*SFB 878, Münster, Germany*

WESTFÄLISCHE WILHELMS-UNIVERSITÄT MÜNSTER

IRMA Strasbourg
*October 31, 2019*

# Contributors

H. SCHULZ-BALDES, *Department Mathematik*, Erlangen-Nürnberg, Germany

# Main References

J. Bellissard,
*Non Commutative Methods in Semiclassical Analysis*,
Lecture Notes in Mathematics, **1589**, Springer, (1994).

J. Bellissard, H. Schulz-Baldes, A. van Elst,
*The Non Commutative Geometry of the Quantum Hall Effect*,
J. Math. Phys., **35**, 5373-5471, (1994).

J. Bellissard,
*The Non Commutative Geometry of the Quantum Hall Effect*,
Proc. I.C.M. (Zürich 94), Birkhäuser (1995)

H. Schulz-Baldes, J. Bellissard,
*Anomalous transport: a mathematical framework*,
Rev. Math. Phys., **10**, 1-46, (1998).

# Content

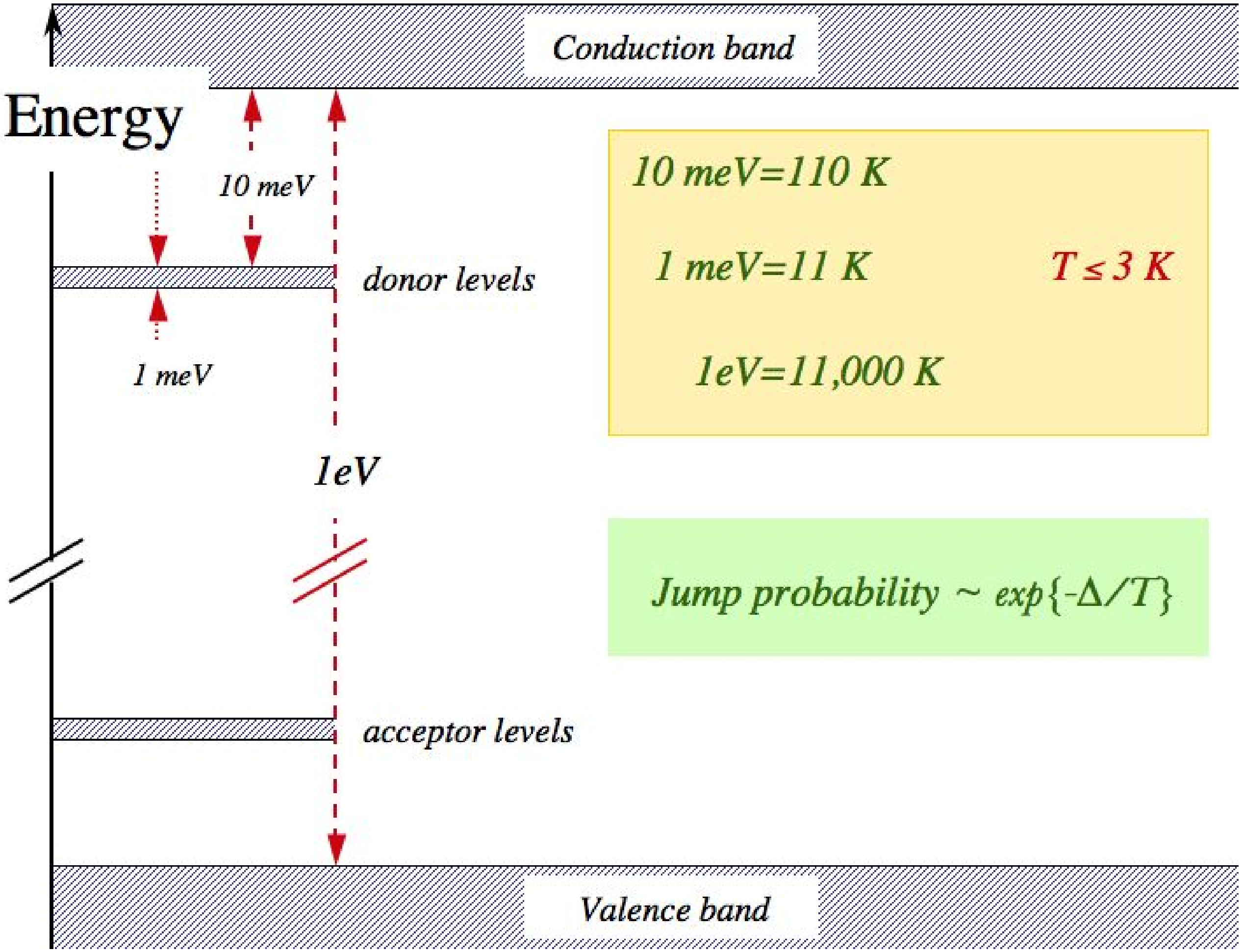
1. What is Localization ?
2. The Toolbox: Algebra.
3. Localization Length.

# I - What Is Localization ?

# Semi-conductors

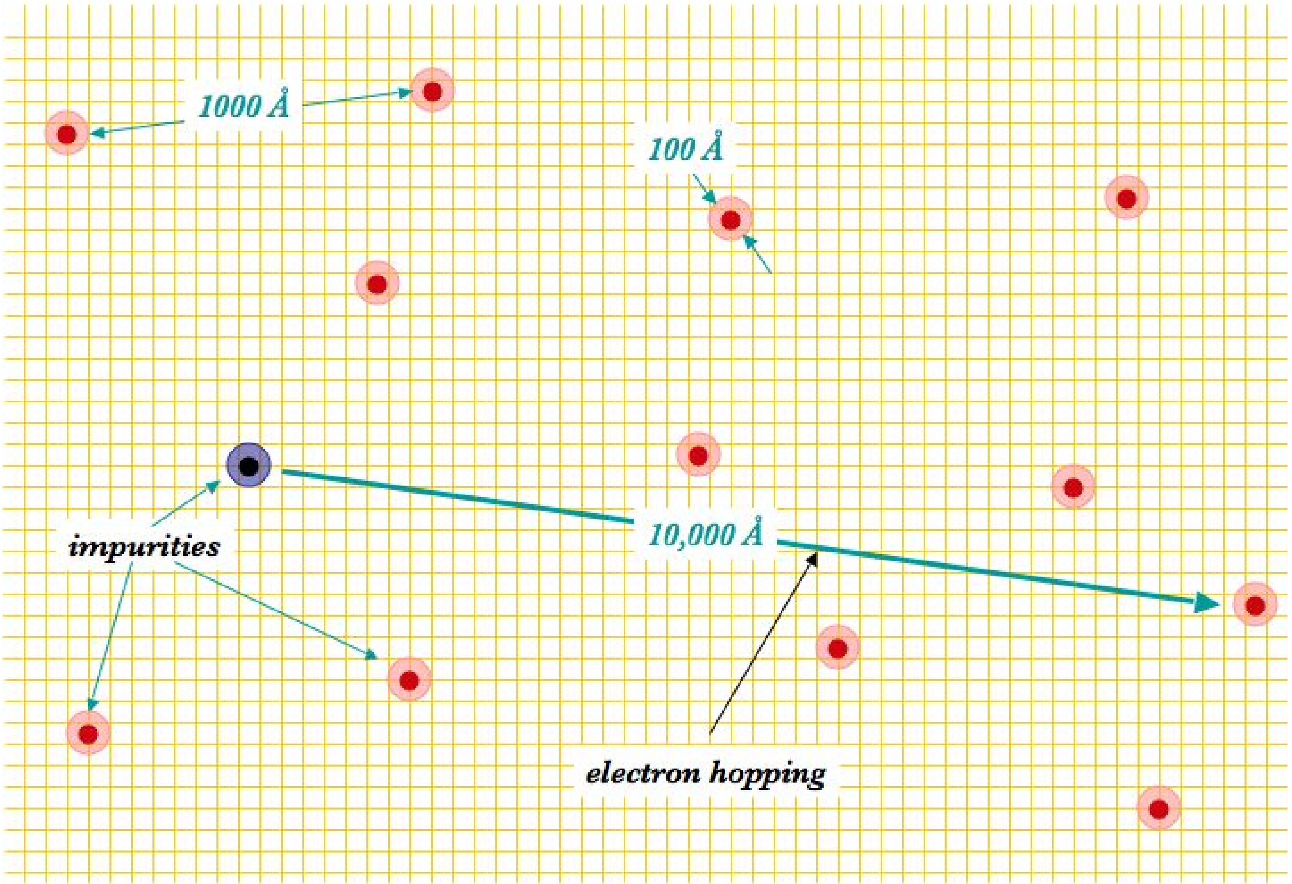
- Semi-conductors like $Si, Ga\,As$, have a diamond crystal structure: atoms are located on a *perfectly periodic lattice* $\mathcal{L}$.
- Electron-electron interaction on site induces a large gap at the Fermi level: *without impurities, perfect insulators*.
- Doping: according to a Poisson Law (thermal effects) with *concentration* of
  - $O(10^{-9})$ for Light doping,
  - $O(10^{-6})$ for Strong doping:
- At room temperature, impurity electrons jump in the conduction band leading to *"large" conductivity*.
- At very low temperature, electrons are confined on the impurity sites: electrons see only a *random sub-lattice* $\mathcal{L}_\omega \subset \mathcal{L}$.

# Semi-conductors




- Bands and gaps in semi-conductors -

# Semi-conductors




- Typical length scales for electron hopping -

# Doping

- Each *impurity* has been shown *(Slater '49)* to behave like an *hydrogen atom* for the electron in excess. Its *Bohr radius* is typically $a \sim 100\text{Å}$.

- Let $W$ denote the *impurity band width*. Hence $W \sim 1meV$.

- The *hoping terms* between two impurity sites can be estimated by tunneling effect. Typically, it is given by $t \simeq t_0 e^{-\ell/a}$ if $\ell$ is the distance between two impurities. Typically $t_0 \sim 1 - 6eV$.

- – **Light doping:** the average distance of impurities free of electron in excess is $\ell \sim 100a$. Thus $t \ll W$ *strong localization*.
  – **Strong doping:** $\ell \sim a$, then $t \geq W$ *weak localization*.

# Anderson's Model

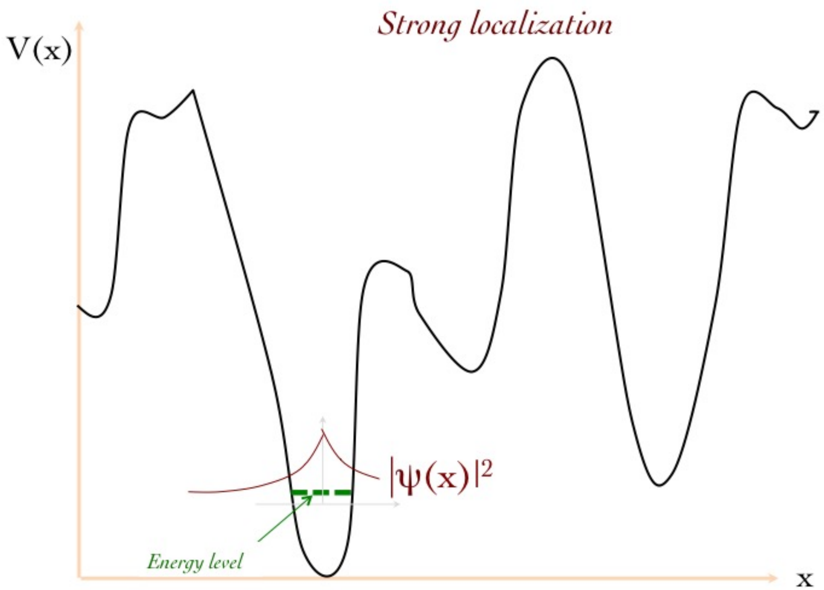
- This led Anderson to propose a simplified model, a discrete Schrödinger operator, in which the impurities are located on a *cubic lattice* $\mathbb{Z}^d$.

- The potential $V(x)$ at site $x$ is a random variable uniformly distributed in an interval $[-W, W]$ (with $W$ being the impurity band width).

- This leads to

$$H\psi(x) = t \sum_{|x-y|=1} \{\psi(x) - \psi(y)\} + V(x)\psi(x) \qquad \psi \in \ell^2(\mathbb{Z}^d)\,.$$

# Localization is Interference



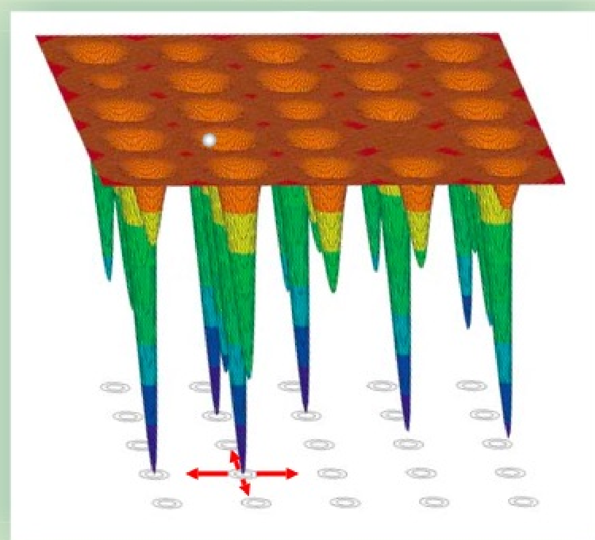



**Figure 3. The Anderson model.** Imagine an electron (silver) hopping on a two-dimensional lattice with random potential energies at each site. Quantum mechanics allows the electron to tunnel from one site to another through large energy barriers as depicted by the red arrows. The electron's energy thus changes randomly, although at each lattice site the spatial extent of its wavefunction (sketched below the potential) is assumed constant, leading to a constant tunneling rate. On an ordered lattice with all wells the same depth, the electron would be completely mobile for a range of energies. But here, a critical amount of randomness in the well depths localizes the electron, although on a scale larger than the lattice constant. For another perspective of what occurs as a lattice changes from perfect to disordered, see this month's cover.

**26** August 2009 Physics Today

STRONG LOCALIZATION: *Interferences on the electron wave build up constructively to trap the electrons in deep wells of the Anderson random potential.*

# Localization is Interference

PHYSICS REPORTS (Review Section of Physics Letters) 107, No. 1 (1984) 1–58. North-Holland, Amsterdam

**WEAK LOCALIZATION IN THIN FILMS**
**a time-of-flight experiment with conduction electrons**

Gerd BERGMANN

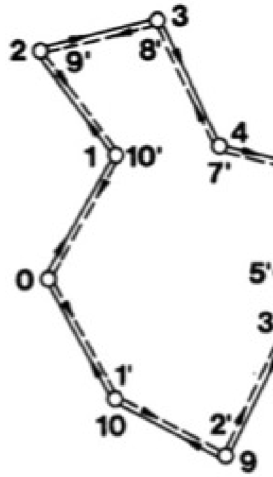



Fig. 2.5. Diffusion path of the conduction electron in the disordered system. The electron propagates in both directions (full and dashed lines). In the case of quantum diffusion the probability to return to the origin is twice as great as in classical diffusion since the amplitudes add coherently.

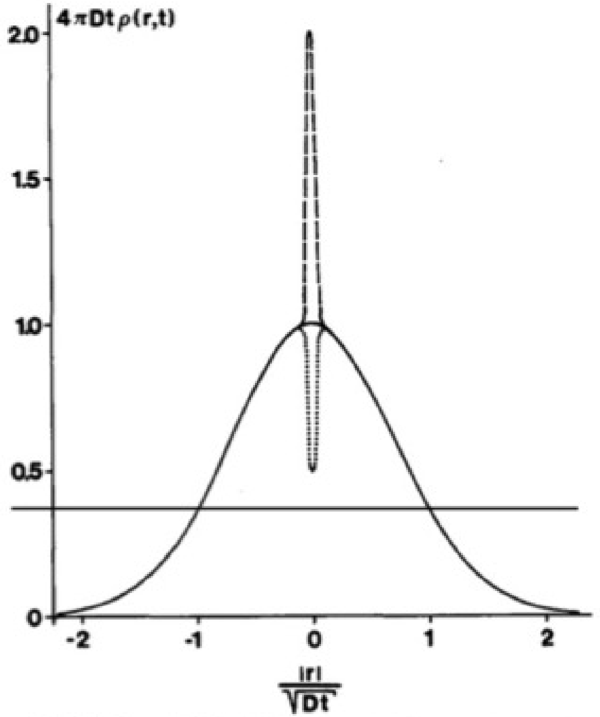



Fig. 2.6. The probability distribution of a diffusing electron which starts at $r = 0$ at the time $t = 0$. In quantum diffusion (dashed peak) the probability to return to the origin is twice as great as in classical diffusion (full curve). Large spin–orbit scattering reduces the probability by a factor of two (dotted peak) and yields a weak anti-localization.

Weak Localization: *electron diffusion, enhanced backscattering.*

# Localization Length

- For $\psi \in \ell^2(\mathbb{Z}^d)$ with $\|\psi\| = 1$, its *localization length* is defined as

$$\ell_2(\psi)^2 = \|(X - \langle X \rangle)\psi\|^2 = \sum_{x \in \mathbb{Z}^d} |x - \langle X \rangle|^2 \, |\psi(x)|^2$$

$$\langle X \rangle = \langle \psi | X \psi \rangle = \sum_{x \in \mathbb{Z}^d} x \, |\psi(x)|^2$$

- However, in the Anderson model, the *potential is random*, so are its eigenfunctions !!
  Hence this concept of *localization length* is a *random variable*.
- In addition, the eigenvalue (the *energy*) is *never strictly defined* in practice, and the localization length depends on it.
  *How to take this fact into account ?*

# II - The Toolbox: Algebra

# Randomness

- In *Anderson's model* the potential $V = (V(x))_{x\in\mathbb{Z}^d}$ has each of its components being *i.i.d* random variables with values in the interval $[-W, W]$. Hence $V \in \Omega = [-W, W]^{\mathbb{Z}^d}$.

- The space $\Omega$ is *compact* with its product topology and $\mathbb{Z}^d$ acts as a *shift* on it:

$$\tau^a\omega(x) = \omega(x-a)\,, \qquad\qquad \omega \in \Omega\,.$$

- The probability measure $\mathbb{P}$ defining the distribution of random potential is both *shift invariant* and *ergodic*.

# Randomness & Aperiodicity

- Actually $\Omega$ can be replaced by any *compact Hausdorff metrizable* space equipped with an *action* of $\mathbb{Z}^d$ by homeomorphisms.

- *Any configuration* of atoms in $\mathbb{R}^d$, with a *minimum distance* between atoms and *size-limited holes*, can be represented by such a dynamical system where the translation group is $\mathbb{R}^d$.

# Random Operators

- Both the *potential* and the *Anderson Hamiltonian* are *self-adjoint bounded* operators acting on the Hilbert space of states $\mathcal{H} = \ell^2(\mathbb{Z}^d)$. Both have the following property
  - they are short range, namely their matrix elements $\langle y|A_\omega|x\rangle$ vanish for $|x - y|$ large.
  - they are *strongly continuous* in the parameter $\omega \in \Omega$
  - they are *covariant* under the $\mathbb{Z}^d$-action, namely

$$U(a)A_\omega U(a)^{-1} = A_{\mathrm{T}^a\omega}\,, \qquad (U(a)\psi)\,(x) = \psi(x-a) \quad \psi \in \mathcal{H}$$

- Let $\mathcal{A}_0$ denote the *observable algebra*, namely the space of all such operators on $\mathcal{H}$.

# Random Operators

- If $A \in \mathcal{A}_0$ it has *matrix elements* defined by $a(\omega, x) = \langle 0|A_\omega|x\rangle$ since, by *covariance*,

$$\langle y|A_\omega|x\rangle = \langle 0|A_{\mathrm{T}^{-y}\omega}|x-y\rangle = A(\mathrm{T}^{-y}\omega, x-y)$$

- The function $(\omega, x) \in \Omega \times \mathbb{Z}^d \to A(\omega, x)$ is *continuous* with *compact support*.
- The *adjoint* is given by the function $A^*(\omega, x) = \overline{A(\mathrm{T}^{-x}\omega, -x)}$.
- Let $\|A\|_{\infty,1} = \sup_{\omega\in\Omega} \sum_{x\in\mathbb{Z}^d} |A(\omega, x)|$ then

$$\sup_{\omega\in\Omega} \|A_\omega\| \leq \max\{\|A\|_{\infty,1}, \|A^*\|_{\infty,1}\}$$

# Random Operators

The space $\mathcal{A}_0$ is invariant by the operator product and the adjoint. Its is a $*$-algebra over the complex field.

**Definition** *The observable algebra $\mathcal{A}$ is the operator norm completion of $\mathcal{A}_0$. It is a $C^*$-algebra.*

**Remark:** It can be shown that, for Anderson like models $\mathcal{A}$ is the *smallest $C^*$-algebra* containing the *Hamiltonian (energy)* and the action of the *translations*. In particular $H \in \mathcal{A}$

# Trace per Unit Volume

- Since $\langle x|A_\omega|x\rangle = a(\tau^{-x}\omega, 0)$, the *Birkhoff Ergodic Theorem* implies that with *probability one* on $\omega$, the *trace per unit volume* is given by

$$\lim_{\Lambda\uparrow\mathbb{Z}^d} \frac{1}{|\Lambda|} \sum_{x\in\Lambda} \langle x|A_\omega|x\rangle = \int_\Omega A(\omega, 0)\, d\mathbb{P}(\omega) = \mathcal{T}_{\mathbb{P}}(A)\,.$$

- Then $\mathcal{T}_{\mathbb{P}} : \mathcal{A} \to \mathbb{C}$ is a *linear continuous* map such that

$$A \in \mathcal{A}, \quad A \neq 0 \;\Rightarrow\; \mathcal{T}_{\mathbb{P}}(A^*A) > 0 \qquad\qquad \mathcal{T}_{\mathbb{P}}(1) = 1$$

$$\mathcal{T}_{\mathbb{P}}(AB) = \mathcal{T}_{\mathbb{P}}(BA) \qquad\qquad A, B \in \mathcal{A}$$

Hence $\mathcal{T}_{\mathbb{P}}$ is a *tracial state* on $\mathcal{A}$.

# Density of States

- The *number of eigenstates* of energy less than or equal to $E$ in a finite volume $\Lambda \subset \mathbb{Z}^d$ is given by

$$N_\Lambda(E, \omega) = \{E' \in \mathrm{Spec}(H_\omega \restriction_\Lambda) \,;\, E' < E\}$$

- Let $P_H(E)$ be the *spectral projection* of $H \in \mathcal{A}$ corresponding to the interval of energies $(-\infty, E]$.
- **Shubin's Formula:** *there is a probability measure $\mathcal{N}$ on $\mathbb{R}$, called the* density of states *with support in* $\mathrm{Spec}(H)$ *such that, for $\mathbb{P}$-almost every $\omega \in \Omega$, the following holds*

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{N_\Lambda(E, \omega)}{|\Lambda|} = \mathcal{T}_{\mathbb{P}}(P_H(E)) = \int_{-\infty}^{E} d\mathcal{N}(E)$$

# Density of States

**Theorem:** *In the Anderson's model*

1. *The spectrum coincides with the interval* $[-(2d+W),+(2d+W)]$
2. *The density of state is absolutely continuous*

**Remark:** In the analogous model on the *Penrose lattice* instead, *without disorder*, there is an *isolated eigenvalue* at $E = 0$ of infinite multiplicity *(Kohmoto, Sutherland, 1986) (Lenz et al.)* and the spectrum is conjectured to be *singular continuous* for any potential strength.

# Trace per Unit Volume

**Remark:** the *trace per unit volume* $\mathcal{T}_{\mathbb{P}}$ defines a Hilbert space denoted by $L^2(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$ *(Gelfand-Naĭmark-Segal construction)*. The C*-algebra $\mathcal{A}$ acts on this space *(GNS representation)*. Then $L^\infty(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$ is defined as the *von Neumann Algebra* (namely the weak closure) generated by this representation on this space. Then

- The trace per unit volume $\mathcal{T}_{\mathbb{P}}$ extends as a *normal state* (monotone convergence property) on $L^\infty(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$.

- The *spectral projections* are well defined in $L^\infty(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$ *(Measurable Functional Calculus)*.

# Derivation

- Let $X = (X_1, \cdots, X_d)$ denotes the (self-adjoint) *position operator* defined by

$$X\psi(x) = x\psi(x)\,, \qquad\qquad \psi \in \ell^2(\mathbb{Z}^d)$$

- For $A \in \mathcal{A}_0$ the commutator with $X$ satisfies

$$\langle 0|\imath[X, A_\omega]|x\rangle = -\imath x\, A(\omega, x) \stackrel{def}{=} -(\partial A)(\omega, x)$$

- Then $\partial A \in \mathcal{A}_0$ and $\partial : \mathcal{A}_0 \to \mathcal{A}_0$ is a *$*$-derivation* namely a *linear* map such that *(Leibniz rule)*

$$\partial A^* = (\partial A)^*\,, \qquad \partial(AB) = (\partial A)\,B + A\,(\partial B)$$

# III - Localization Length

# The Wiener Criterion

**Wiener' Criterion:** *Let $\mu$ be a finite complex valued measure on the real line. Let $F_\mu$ denote its Fourier transform $\int_{\mathbb{R}} e^{\imath t x}\, d\mu(x)$. Then*

$$\lim_{T\to+\infty} \frac{1}{T} \int_0^T \left|F_\mu(t)\right|^2 = \sum_{e\in\mathbb{R}} \left|\mu(\{E\})\right|^2 .$$

# Inverse Participation Ratio

- If $\psi \in \ell^2(\mathbb{Z}^d)$, its *participation ratio* is defined by

$$p(\psi) = \frac{\sum_{x\in\mathbb{Z}^d} |\psi(x)|^4}{\left(\sum_{x\in\mathbb{Z}^d} |\psi(x)|^2\right)^2}$$

- **Examples:** if $\psi(x) = 1/\sqrt{N}$ on a finite subset of $N$ sites in $\mathbb{Z}^d$, then $1/p(\psi) = N$. In particular this *inverse participation ratio* gives a measure of how many sites are really contributing to $\psi$. Hence it could be used as a measure of how much $\psi$ is *localized*.

# Return Probability

For $\Delta \subset \mathbb{R}$ a Borel set, let $P_\omega(\Delta)$ denote the eigenprojector of the covariant self-adjoint operator $H_\omega$ acting on $\mathcal{H} = \ell^2(\mathbb{Z}^d)$.

- The *quantum probability amplitude* for vectors starting at site $x \in \mathbb{Z}^d$ at time $t = 0$ to belong to the subspace $P_\omega(\Delta)\mathcal{H}$ and to return to the site $x$ after time $t$ is

$$\langle x | e^{\imath t H_\omega} P_\omega(\Delta) | x \rangle \,.$$

- Therefore the corresponding *time average probability* is defined as

$$A_x(\Delta, \omega) = \lim_{T \to +\infty} \int_0^T \frac{dt}{T} \, \left| \langle x | e^{\imath t H_\omega} P_\omega(\Delta) | x \rangle \right|^2$$

# Return Probability

- By covariance $A_x(\Delta,\omega) = A_0(\Delta, \mathrm{T}^{-x}\omega)$ so that averaging over the disorder leads to the *time and disorder average probability of return*

$$\xi(\Delta) = \int_\Omega d\mathbb{P}(\omega)\, A_0(\Delta,\omega)$$

- This can also be expressed *algebraically* as

$$\xi(\Delta) = \lim_{T\to+\infty} \int_0^T \frac{dt}{T} \int_{\mathbb{T}^d} \frac{d\theta^d}{(2\pi)^d}\, \mathcal{T}_{\mathbb{P}}\Big( (e^{-\imath tH} P(\Delta))\, e^{\imath\theta\cdot\partial}\, (e^{+\imath tH} P(\Delta)) \Big)\,.$$

# Return Probability

Let $\sigma_{pp}(\omega)$ denote the set of *eigenvalues* of $H_\omega$. For $E \in \sigma_{pp}(\omega)$ let $\psi_{\omega,E}$ denotes the corresponding *normalized eigenstate*. Using the Wiener criterion and the *ergodicity* of $\mathbb{P}$ leads to

**Theorem:** *the "time and disorder average probability of return" satisfies*

$$\xi(\Delta) = \int_\Omega d\mathbb{P}(\omega) \sum_{E \in \sigma_{pp}(\omega) \cap \Delta} \left|\psi_{\omega,E}(0)\right|^4$$

In some sense, this formula provides an *average* over *energy* and *disorder* of the *participation ratio*.

In particular, with probability one, only a *finite number of eigenvalues* have a significant contribution near any given site.

# Localization Length

- The position at *time* $t$ is given by $X_\omega(t) = e^{\imath t H_\omega} X e^{-\imath t H_\omega}$, so that

$$X_\omega(t) - X_\omega(0) = \imath\, e^{\imath t H_\omega} \left(\partial e^{-\imath t H}\right)_\omega$$

- It follows that the *average distance* spanned by a state starting at the site $x$ at time $t = 0$ over the period of time $T$ is

$$\delta X_{\omega,x}(T) = \int_0^T \frac{dt}{T} \langle x | (X_\omega(t) - X_\omega(0))^2 | x \rangle$$

# Localization Length

- Averaging over the *disorder* leads to

$$\delta X(T) = \int_0^T \frac{dt}{T} \mathcal{T}_{\mathbb{P}}\left( \left| \partial (e^{-\imath t H}) \right|^2 \right)$$

- Localizing the evolution in a spectral set $\Delta$ leads to the following definition of the *energy dependent localization length*

$$l(\Delta)^2 = \limsup_{T \to +\infty} \int_0^T \frac{dt}{T} \mathcal{T}_{\mathbb{P}}\left( \left| \partial (e^{-\imath t H} P(\Delta)) \right|^2 \right)$$

# Localization Length

**Theorem** *If* $l(\Delta)^2 < \infty$ *then*

1. *the spectral measure of* $H_\omega$ *inside* $\Delta$ *is pure point for* $\mathbb{P}$*-almost every* $\omega$.
2. *If* $\mathcal{N}$ *denotes the density of state, then there is a measurable function* $l \in L^2(\Delta, \mathcal{N})$ *such that for* $\Delta' \subset \Delta$ *measurable*

$$l(\Delta')^2 = \int_{\Delta'} l(E)^2 \, d\mathcal{N}(E)$$

*and*

$$l(\Delta')^2 = \int_\Omega d\mathbb{P}(\omega) \sum_{x \in \mathbb{Z}^d} \sum_{E \in \sigma_{pp}(\omega) \cap \Delta'} |x|^2 \, |\psi_{\omega,E}(0)|^2 \, |\psi_{\omega,E}(x)|^2$$

# Current-Current Correlation

- From the *Riesz-Markov-Kakutani Theorem*, if $H$ is a covariant self-adjoint bounded operator such that $\|\partial H\| < \infty$, then there is a *matrix of complex valued bounded $\mathcal{N} \otimes \mathcal{N}$- integrable functions* $\mathcal{M} = (m_{ij})_{i,j\in[1,d]}$ on $\mathbb{R}^2$ satisfying for any pair of continuous functions $f$ and $g$ on $\mathbb{R}$ vanishing at infinity

$$\mathcal{T}_{\mathbb{P}}\Big(f(H)\partial_i H g(H)\partial_j H\Big) = \int_{\mathbb{R}^2} f(E)\, g(E')\, m_{ij}(E,E')\, d\mathcal{N}(E)\, d\mathcal{N}(E')\,.$$

- The function $m = \sum_{i=1}^{d} m_{ii}$ is *nonnegative and integrable*.

**Definition:** *each $m_{ij}$ is called a* current-current correlation

# Current-Current Correlation

**Theorem:** *With the notation and the assumptions used previously, the localization length $l(E)$ is given by the following formula*

$$l(E)^2 = 2 \int_{\mathbb{R}} \frac{m(E,E')}{(E-E')^2}\, d\mathcal{N}(E')\,.$$

*for $\mathcal{N}$-almost every $E$.*

**Remarks:**

- A *finite localization length* implies that the current-current correlation must *vanish* on the *diagonal* $E = E'$ so as staying integrable as divided by $(E - E')^2$.
- For the *Anderson model*, this vanishing is expected to be of *infinite order* at large disorder.

# IV - Numerical Approach

E. PRODAN, "Quantum transport in disordered systems under magnetic fields: a study based on operator algebras", arXiv:1204.6490; Applied Math. Res. eXpress, **2013**(2), 176-265, (2013).

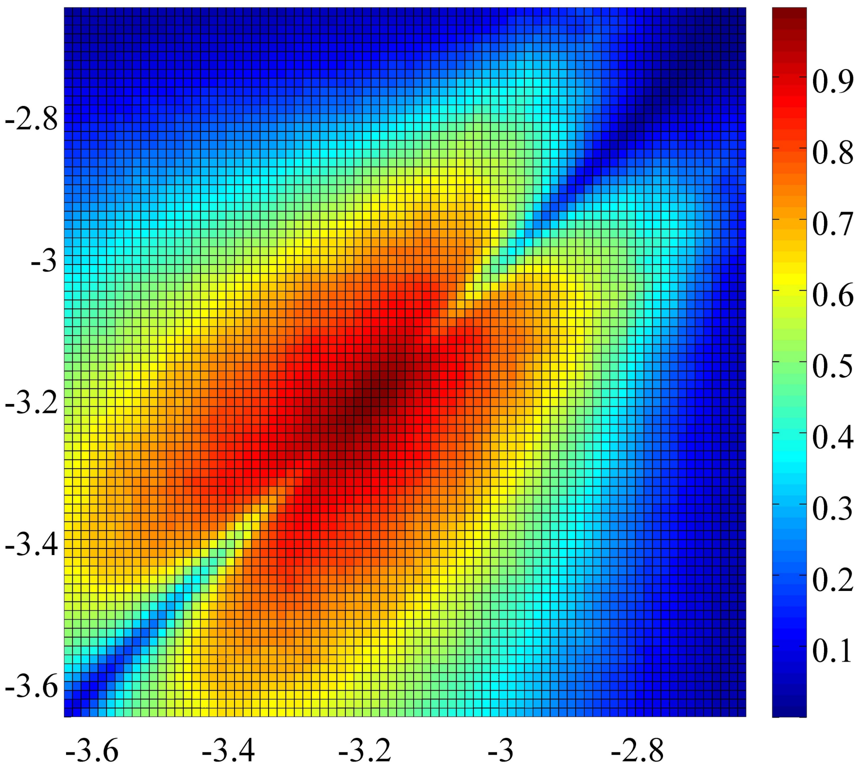
J. SONG, E. PRODAN, "Characterization of the quantized Hall insulator phase in the quantum critical regime", arXiv:1301.5305; Europhys. Lett., **105**(3), 37001, (2014).

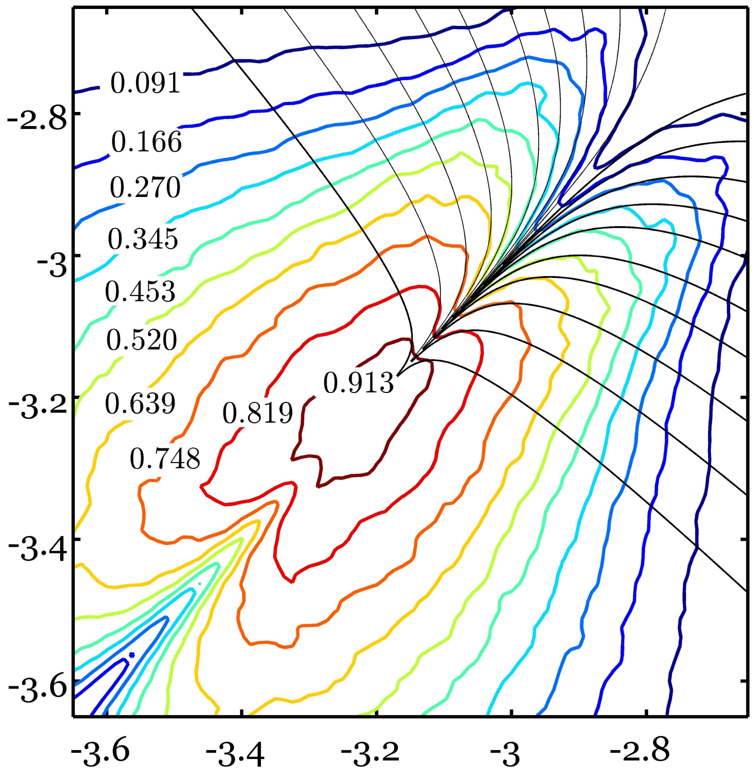
E. PRODAN, J. BELLISSARD, "Mapping the Current-Current Correlation Function Near a Quantum Critical Point", arXiv:1512.02476; Ann. of Phys., **368**, 1-15, (2016).

# Numerical Method

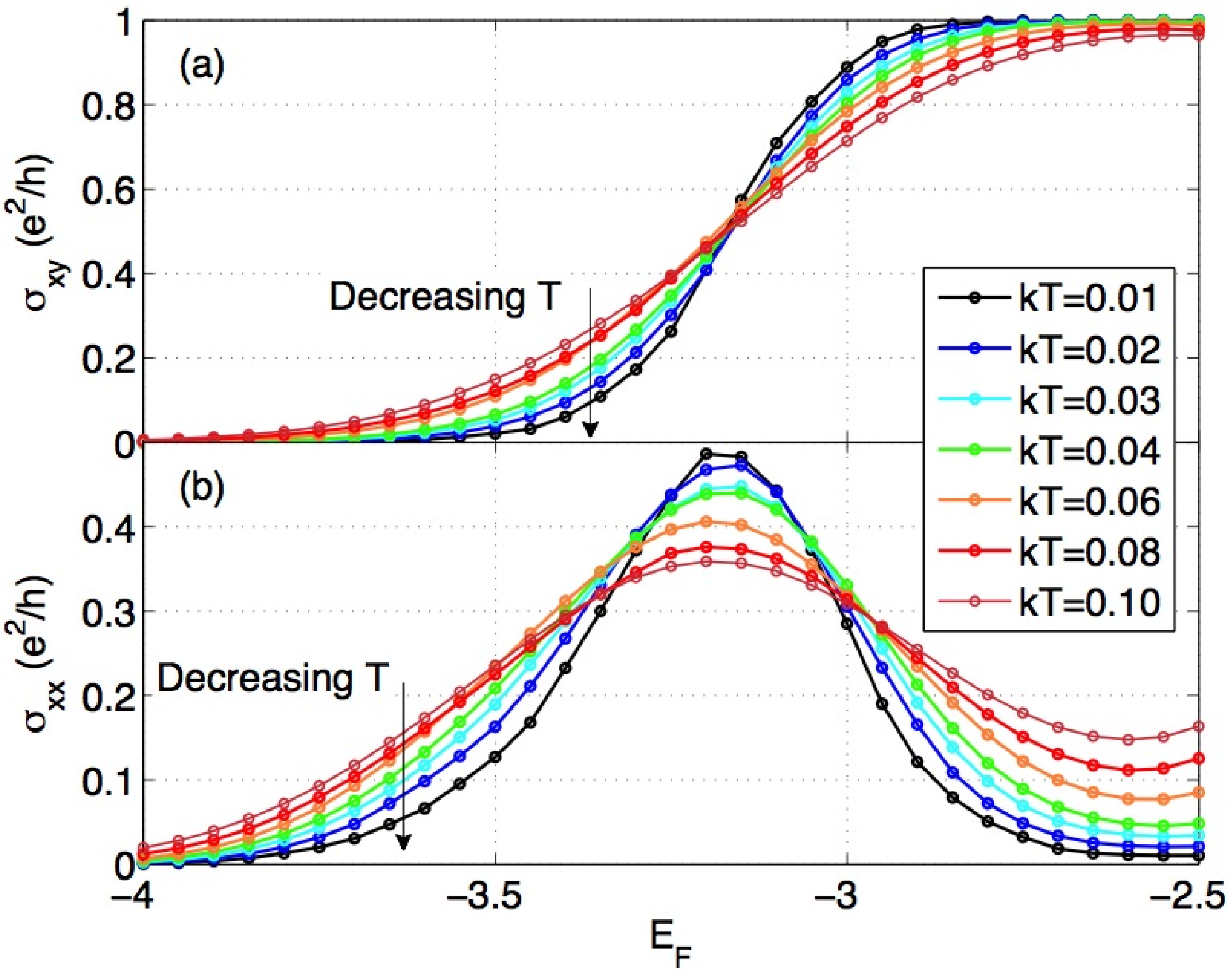
- In the early 2010's *Emil Prodan* found a way to approximate the C*-algebra by a *periodic approximation* liable to reduce the problem to a well-known method called *Floquet-Bloch Theory*.
- Using a formula for the *conductivity*, valid for *aperiodic media* *(JB, Schulz-Baldes '98)*, he could numerically computed it for the *Quantum Hall Effect*.
- From his numerical results, a *critical point* of the conductivity could be analyzed in terms of a *singularity* of the current-current correlation on the diagonal *(Prodan, JB '15)*.
- At this energy of this singularity, the *localization length diverges* leading to a change of *Chern Number* for the transverse conductivity.

# Numerical Method



# Numerical Method



Thanks for Listening!!