KINETIC MODELS
for
QUANTUM TRANSPORT:
Anomalous Transport

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WHY REVISITING ELECTRONIC TRANSPORT AGAIN ?

- It is a very old problem (*Boltzmann* (ca. 1880) for classical systems; *Drude* (1900) for electrons)
- It is treated in textbooks: phenomenology, perturbation theory, numerical calculations.

However:

1. No mathematically rigorous proof of the Kubo formulæ for transport coefficients.
   (However substantial progress for classical systems (*Lebowitz*'s school))
2. Low temperature effects are difficult to describe
   ex. : Mott's variable range hopping
   (see e.g. *Efros & Schklovsky*)
3. Aperiodic materials escape Bloch theory : need for a more systematic treatment (**ex. :** quasicrystals)
4. Aperiodic media exhibit anomalous quantum diffusion

Transport is complex

- Thermodynamic quantities are much easier to measure: experiments are cleaner, easier to control.
  Ex. : *heat capacity, magnetic susceptibility, structure factors...*
  But they do not separate various mechanisms.

- Transport measurements are mostly indirect: harder to interpret (especially at low temperature). Too many mechanisms occur at once.

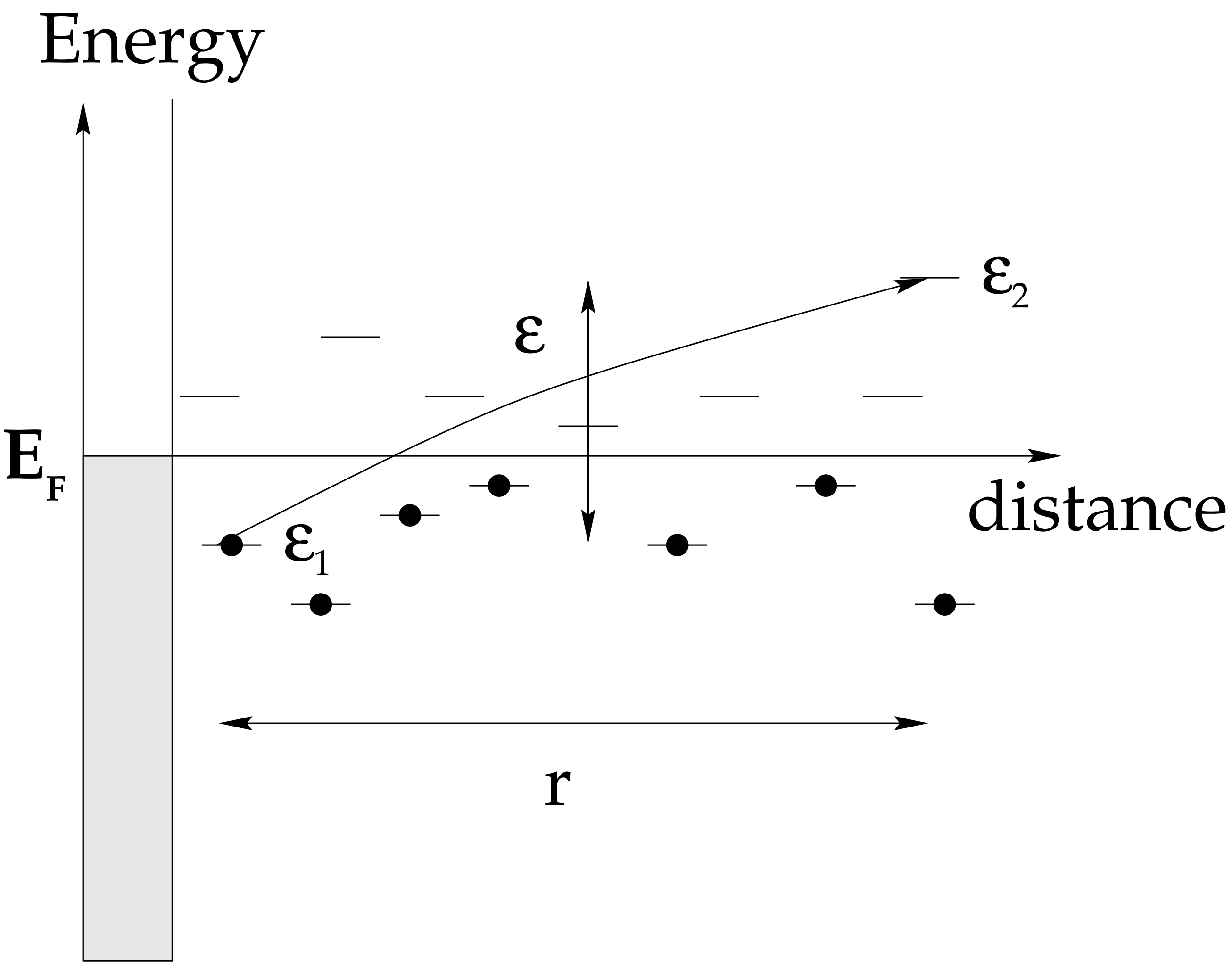
Few mechanisms

1. For metals, $\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{T^{-2}}$,
   $\sigma(\mathbf{T})$ increases as temperature decreases
   (*Fermi liquid theory*).

2. For thermally activated process
   $$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{e^{-\Delta/T}}$$ (*If a gap holds at Fermi level*).

3. For weakly disordered systems:
   $$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\to} \sigma(\mathbf{0}) > \mathbf{0}$$ (*residual conductivity*).

4. For strongly disordered systems in $3D$:
   $$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{e^{-(T_0/T)^{1/4}}}$$ (*variable range hopping*).



Mott's Variable Range Hopping

MOTT's VARIABLE RANGE HOPPING

1. N. Mott, (1968); see B. Shklovskii, A. L. Effros, *Electronic Properties of Doped Semiconductors*, (Springer-Verlag, Berlin, 1984).

- Strongly localized regime, dimension d
- Low electronic DOS, Low temperature
- Absorption-emission of a phonon of energy ε

$$\mathbf{Prob} \propto \mathbf{e}^{-\varepsilon/\mathbf{k_B T}}$$

- Tunnelling probability at distance $\mathbf{r}$

$$\mathbf{Prob} \propto \mathbf{e}^{-\mathbf{r}/\xi}$$

- Density of state at Fermi level n_F,

$$\varepsilon\, \mathbf{n_F}\, \mathbf{r^d} \approx \mathbf{1}$$

Optimizing, the conductivity satisfies

$$\sigma \propto \mathbf{e}^{-(\mathbf{T_0}/\mathbf{T})^{\mathbf{1/d+1}}} \qquad \textit{Mott's law}$$

Optimal energy $\varepsilon_{\mathbf{opt}} \sim \mathbf{T}^{\mathbf{d}/(\mathbf{d+1})} \gg \mathbf{T}$
Optimal distance $\mathbf{r_{opt}} \sim \mathbf{1}/\mathbf{T}^{\mathbf{1}/(\mathbf{d+1})} \gg \xi$

TRANSPORT in QUASICRYSTALS (QC)

2. *Lectures on Quasicrystals*, F. Hippert & D. Gratias Eds.,
Editions de Physique, Les Ulis, (1994),

3. S. Roche, D. Mayou and G. Trambly de Laissardière, *Electronic transport properties of quasicrystals*, J. Math. Phys., **38**, 1794-1822 (1997),

Quasicrystalline alloys :

Metastable QC's: **AlMn**
(*Shechtman D., Blech I., Gratias D. & Cahn J., PRL* **53**, *1951 (1984)*)

AlMnSi

AlMgT $(T = Ag, Cu, Zn)$

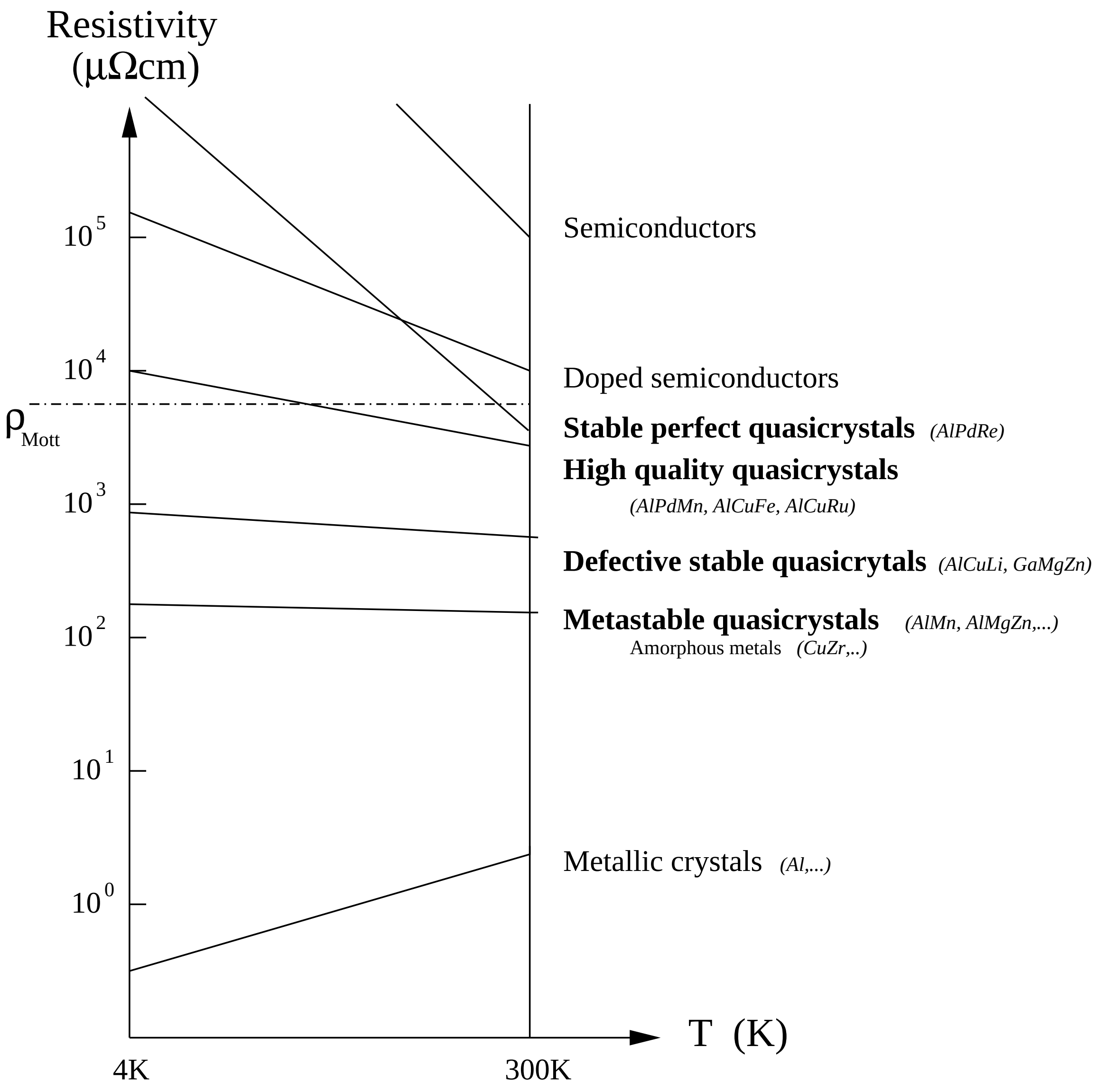
Defective stable QC's: **AlLiCu**

GaMgZn

High quality QC's: **AlCuT** $(T = Fe, Ru, Os)$

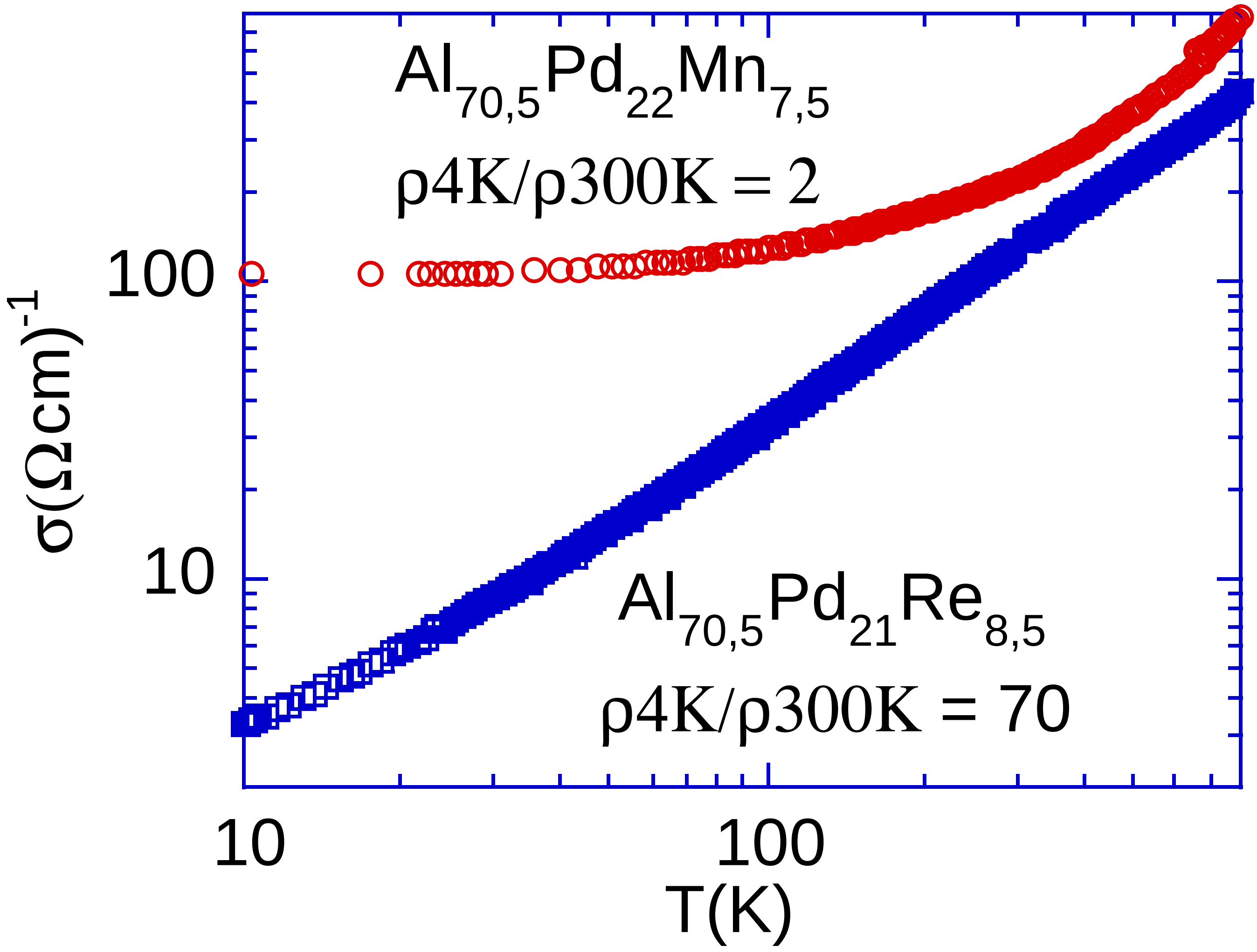
"Perfect" QC's: **AlPdMn**

AlPdRe



Typical values of the resistivity

(Taken from *C. Berger* in ref. [2])



Conductivity of two QC's

For QC's

1. Al, Fe, Cu, Pd are very good metals : why is the conductivity of quasicrystalline alloys so low ?
   Why is it decreasing ?
2. At high enough temperature

$$\sigma \propto \mathbf{T}^{\gamma} \qquad \mathbf{1} < \gamma < \mathbf{1.5}$$

   There is a new mechanism here!

3. At low temperature for $\mathbf{Al_{70.5}Pd_{22}Mn_{7.5}}$,

$$\sigma \approx \sigma(\mathbf{0}) > \mathbf{0}$$

4. At low temperature for $\mathbf{Al_{70.5}Pd_{21}Re_{8.5}}$,

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

   C. Berger et al. (1998)

Some disorder takes place in both alloys and dominates at very low temperature.

APERIODIC MEDIA and NON COMMUTATIVE GEOMETRY

4. J. Bellissard, *Gap Labelling theorems for Schrödinger Operators*, in *From Number Theory to Physics* Springer-Verlag, Berlin, (1992).

Schrödinger's equation (ignoring interactions)

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{r=1}^{K} \sum_{y \in L_r} v_r(. - y) \ .$$

acting on $\mathcal{H} = L^2(\mathbf{R}^d)$.

- d is the physical space dimension
- $r = 1, \ldots, K$ labels the atomic species
- L_r set of positions of atoms of type r
- v_r effective potential for valence electrons near an atome of type r.

Ideal Crystals

- $\mathcal{L}$ = lattice of periods
- For $a \in \mathcal{L}$ let $T(a)$ be translation by a in $\mathcal{H} = L^2(\mathbf{R}^d)$
- $T(a) H T(a)^{-1} = H$ *translation invariance*
- $\mathbf{B} = \hat{\mathbf{R}}^d / \mathcal{L}^*$ *Brillouin zone*

Then

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

with

$$H_k = \frac{1}{2m} \left(\frac{\hbar}{\imath} \vec{\nabla} + k \right)^2 + V(.) \qquad \textit{acting on } L^2(\mathbf{R}^d / \mathcal{L})$$

Theorem 1 (Bloch theorem) *Assume V smooth enough*

1. *for any $k \in \mathbf{B}$, H_k has compact resolvent,*
2. *Eigenvalues $E_n(k)$ are continuous (analytic) functions of $k \in \mathbf{B}$*
3. $\sigma(H) = \cup_n B_n$, $B_n = \{E_n(k); k \in \mathbf{B}\}$ *(bands)*

- A **gap** is a connected component of $\mathbf{R} \backslash \sigma(H)$.
- If $d = 1$, for *generic* V's, every possible gap occurs (an infinite number). If $d \geq 2$ only finitely many gaps (proved in $d = 2, 3$ by *Skriganov*).
- A typical observable is represented by a (continuous) function $k \in \mathbf{B} \mapsto ((A(k)_{n,n'}))$ where n, n' are band indices and $A(k) \in \mathcal{K}$ is a compact operator.
- Integration is given by

$$\mathcal{T}(A) = \int_{\mathbf{B}} \frac{d^d k}{|\mathbf{B}|} \mathrm{Tr}(A(k))$$

- Derivatives are $\partial / \partial k_i$ $(i = 1, \ldots, d)$

Question: Can one generalize Bloch's theory to non periodic point sets of atoms ?

Answer: YES ! But the price to be paid is to use NON COMMUTATIVE GEOMETRY !

Fourier analysis $\Longleftrightarrow$ C^*-algebras

The Hull

- The set $\{H_a = T(a)HT(a)^{-1}; a \in \mathbf{R}^d\}$ of translated of H, is endowed with the strong-resolvent topology.
- Let Ω be its closure and $\omega^{(0)}$ be the representative of H.

Definition 1 *The operator H is homogeneous if Ω is compact.*

- $(\Omega, \mathbf{R}^d)$ becomes a dynamical system called **the Hull** of H.
  It is topologically transitive (one dense orbit). The action is denoted $\omega \mapsto \tau^a\omega$ $(a \in \mathbf{R}^d)$.
- If the potential V is continuous, there is a continuous function $\hat{v}$ on Ω such that if $\omega \in \Omega$ the corresponding operator H_ω is a Schrödinger operator with potential $V_\omega(x) = \hat{v}(\tau^{-x}\omega)$.
- *covariance* $T(a)H_\omega T(a)^{-1} = H_{\tau^a\omega}$
- The observable algebra $\mathcal{A}_H$ is the C^*-algebra generated by bounded functions of the H_a's. It is related to the *crossed product* $\mathcal{C}(\Omega) \times \mathbf{R}^d$.

The C^*-algebra $\mathcal{C}(\Omega) \times \mathbf{R}^d$

Endow $\mathcal{A}_0 = \mathcal{C}_c(\Omega \times \mathbf{R}^d)$ with the following $*$-algebraic structure ($A, B \in \mathcal{A}_0$):

PRODUCT

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

INVOLUTION

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

A faithfull family of $*$-representations in $\mathcal{H} = L^2(\mathbf{R}^d)$ is given by:

$$\pi_\omega(A)\psi(x) = \int_{\mathbf{R}^d} A(\tau^{-x}\omega, y - x)\psi(y)$$

if $A \in \mathcal{A}_0$, $\psi \in \mathcal{H}$.

C^*-NORM

$$||A|| = \sup_{\omega \in \Omega} ||\pi_\omega(A)||$$

Definition 2 *The C^*-algebra $\mathcal{A} = \mathcal{C}(\Omega) \times \mathbf{R}^d$ is the completion of $\mathcal{A}_0$ under this norm.*

Tight-Binding Representation

1. If $\mathcal{L}$ is the original set of atomic positions, let Σ be the closure of the set of $\tau^{-x}\omega^{(0)}$'s $x \in \mathcal{L}$. Σ is a *transversal.* It is called *the atomic surface* in QC's.

2. Replace $\Omega \times \mathbf{R}^d$ by $\Gamma = \{(\omega, x) \in \Omega \times \mathbf{R}^d\,; \omega \in \Sigma\,, \tau^{-x}\omega \in \Sigma\,\}$. Γ is a *groupoid.*

3. Replace integral over $\mathbf{R}^d$ by discrete sum over x.

4. Replace $\mathcal{A}_0$ by $\mathcal{C}_c(\Gamma)$, the space of continuous function with compact support on Γ. Then proceed as before to get $C^*(\Gamma)$.

5. $C^*(\Gamma)$ is unital. The trace induced by $\mathcal{T}$ on $C^*(\Gamma)$ is a state.

6. One can restrict the original Hamiltonian H to a spectral bounded interval (in practice near the Fermi level), so as to get an *effective* Hamiltonian H_{eff} in $C^*(\Gamma)$. Thus H_{eff} is bounded.

Calculus

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

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

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

- This is a *trace per unit volume* namely, thanks to Birkhoff's theorem:

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

- A commuting set of $*$-derivations is given by

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

defined on $\mathcal{A}_0$.
It satisfies $\pi_\omega(\partial_i A) = \imath[X_i, \pi_\omega(A)]$ where $\vec{X} = (X_1, \cdots, X_d)$ are the coordinates of the position operator.

Properties of $\mathcal{A}$

Theorem 2 *Let $\mathcal{L}$ be a lattice in $\mathbf{R}^d$. If H is $\mathcal{L}$-invariant, $\mathcal{A}$ is isomorphic to $\mathcal{C}(\mathbf{B}) \otimes \mathcal{K}$, where $\mathbf{B}$ is the Brillouin zone and $\mathcal{K}$ is the C^*-algebra of compact operators.*

$\mathcal{A}$ is thus the non commutative analog of the space of continuous functions on the Brillouin zone : it will be called

the Non Commutative Brillouin zone

Theorem 3 *Let H be a homogeneous Schrödinger operator with hull Ω, then for any $z \in \mathbf{C} \backslash \sigma(H)$ there is an element $R(z) \in \mathcal{A}$ (which is C^∞), such that*

$$\pi_\omega(R(z)) = (z\mathbf{1} - H_\omega)^{-1}$$

for all $\omega \in \Omega$.

Moreover, the spectrum of $R(z)$ is given by

$$\sigma(R(z)) = \{(z - \zeta)^{-1}; \zeta \in \Sigma\}, \ \Sigma = \cup_{\omega \in \Omega} \sigma(H_\omega)$$

IDoS and Shubin's formula

- Let $\mathbf{P}$ be an invariant ergodic probability on Ω. Let

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

  It is called the **Integrated Density of states** or **IDoS**.

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

$$\mathcal{N}(E) = \mathcal{T}(\chi(H \leq E)) \qquad \textbf{Shubin}$$

  $\chi(H \leq E)$ 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 $E < \inf \Sigma$. For $E \to \infty$ $\mathcal{N}(E) \sim \mathcal{N}_0(E)$ where $\mathcal{N}_0$ is the IDS of the free case (namely $V = 0$).

- $d\mathcal{N}/dE = n_{\text{DOS}}$ defines a Stieljes measure called the **Density of States** or **DOS**.

States

We will consider states on $\mathcal{A}$ of the form

$$A \in \mathcal{A} \to \mathcal{T}\{\rho A\} \ ,$$

with $\rho \geq 0$ and $\mathcal{T}\{\rho\} = n$ if n is the charge carrier density. Then

$$\rho \in L^1(\mathcal{A}, \mathcal{T})$$

One important example of such states is the **Fermi-Dirac** one, describing equilibrium of a fermion gas of independent particles at inverse temperature $\beta = 1/k_{\mathrm{B}}T$ and chemical potential μ:

$$\rho_{\beta,\,\mu} \ = \ \frac{1}{\mathbf{1} + e^{\beta(H-\mu)}}$$

with μ fixed by the normalization

$$\mathcal{T}\{\rho_{\beta,\,\mu}\} = n \ .$$

SPECTRAL and DIFFUSION EXPONENTS

5.C. A. Rodgers, *Hausdorff measures*, (Cambridge University Press, Cambridge, 1970).
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8. C. Sire, B. Passaro, V. Benza, Phys. Rev., **B46**, 137551 (1992).
9. J.X. Zhong, J. Bellissard, R. Mosseri, J. Phys.: Cond. Mat., **7**, 3507-3514 (1995).
10. J.M. Barbaroux, J.M. Combes, R. Montcho, J. Math. Anal. and Appl., **213**, 698-722 (1997).
11. H. Schulz-Baldes & J. Bellissard, *Anomalous transport: a mathematical framework*, Rev. Math. Phys., **10**, 1-46 (1998).

Local Exponent of a Measure

For $f \geq 0$ a Lebesgue-measurable functions on $(0, a]$

$$\mathbf{f}(\mathbf{x}) \underset{\mathbf{x}\downarrow 0}{\sim} \mathbf{x}^{\alpha}$$

means $\int_0^a dx \;\; f(x)/x^{1+\gamma}$ converges if $\gamma < \alpha$ and diverges if $\gamma > \alpha$.

For ν a Borel probability measure on $\mathbf{R}$, its **local exponents** is defined by:

$$\int_{E-\epsilon}^{E+\epsilon} d\nu(E') \;\; \underset{\epsilon\downarrow 0}{\sim} \;\; \epsilon^{\alpha_\nu(E)} \; .$$

Equivalently:

$$\alpha_\nu(E) \; = \; \sup\{\gamma \in \mathbf{R} \mid \;\; \int d\nu(E') \frac{1}{|E - E'|^{\gamma}} \; < \; \infty\} \; .$$

Theorem 4 *Let $\mathcal{M}$ be the space of Borel probability measures on $\mathbf{R}$, endowed with the vague topology. Let $\nu, \mu \in \mathcal{M}$.*

i) *For ν-almost all E, $0 \leq \alpha_\nu(E) \leq 1$.*

ii) *If μ dominates ν, then $\alpha_\mu(E) \leq \alpha_\nu(E)$ μ-almost surely and $\alpha_\nu(E) = \alpha_\mu(E)$ ν-almost surely.*

iii) *If ν is pure-point, then $\alpha_\nu(E) = 0$ ν-almost surely .*

iv) *If ν is absolutely continuous, then $\alpha_\nu(E) = 1$ ν-almost surely.*

v) *$(\nu, E) \in \mathcal{M} \times \mathbf{R} \mapsto \alpha_\nu(E)$ is a Borel function.*

The Green function behaves as *(Zhong, Mosseri, Bellissard (1995))*

$$G_\nu(E + \imath\epsilon) \;=\; \int_{\mathbf{R}} \frac{d\nu(E')}{E + \imath\epsilon - E'} \;\; \underset{\epsilon\downarrow 0}{\sim} \;\; \epsilon^{\alpha_\nu(E)-1} \qquad 0 \leq \alpha_\nu(E) \leq 2$$

The **upper exponent** on the Borel set Δ is *(Rodgers & Taylor (1970))*

$$\alpha_\nu^+(\mathbf{\Delta}) \;=\; \nu-\underset{\mathbf{E}\in\mathbf{\Delta}}{\text{esssup}}\, \alpha_\nu(\mathbf{E}) \;=\; \dim_{\mathrm{H}}(\nu|_{\mathbf{\Delta}}) \quad \textit{Hausdorff dimension}$$

Spectral Exponents

Let $H = H^* \in \mathcal{A}$.

- For $\omega \in \Omega$ and $\phi \in \mathcal{H}$, let $\mu_{\omega,\phi}$ be the spectral measure of $\pi_\omega(H)$ associated to ϕ. We set

$$\alpha_\omega(E) = \inf_{\phi \in \mathcal{H}} \alpha_{\mu_{\omega,\phi}}(E) \ .$$

- For Δ a Borel subset of $\mathbf{R}$

$$\alpha_\omega^+(\Delta) = \sup_{\phi \in \mathcal{H}} \alpha^+_{\mu_{\omega,\phi}}(\Delta) \ .$$

- Then $\alpha_\omega(E) = \alpha_{\text{LDOS}}(E)$ and $\alpha_\omega^+(\Delta) = \alpha^+_{\text{LDOS}}(\Delta)$ are $\mathbf{P}$-almost surely independent of ω.
- If $\pi_\omega(H)$ is a. s. *pp* in Δ then $\alpha^+_{\text{LDOS}}(\Delta) = 0$.
- If $\pi_\omega(H)$ is a. s. *ac* in Δ then $\alpha^+_{\text{LDOS}}(\Delta) = 1$.
- Set $\alpha_{\mathcal{N}}(E) = \alpha_{\text{DOS}}(E)$ and $\alpha^+_{\mathcal{N}}(\Delta) = \alpha^+_{\text{DOS}}(\Delta)$. Then

$$\alpha_{\text{LDOS}}(E) \leq \alpha_{\text{DOS}}(E) \qquad \alpha^+_{\text{LDOS}}(\Delta) \leq \alpha^+_{\text{DOS}}(\Delta) \ .$$

Diffusion Exponents

- Set $\vec{X}_\omega(t) = e^{\imath t \pi_\omega(H)} \vec{X} e^{-\imath t \pi_\omega(H)}$.
  Mean square displacement for energies in Δ

$$\delta X^2_{\omega,\Delta}(T) = \int_0^T \frac{dt}{T} \, \Pi_\omega(\Delta)(\vec{X}_\omega(t) - \vec{X})^2 \Pi_\omega(\Delta) \; ,$$

where $\Pi_\omega(\Delta) = \chi_\Delta(\pi_\omega(H))$.

- The diffusion exponent $\sigma_{\text{diff}}(\Delta)$ is defined by

$$\int_\Omega d\mathbf{P}(\omega) \; \langle 0 | \delta X^2_{\omega,\Delta}(T) | 0 \rangle \;\; \underset{T \uparrow \infty}{\sim} \;\; T^{2\sigma_{\text{diff}}(\Delta)} \; .$$

- Remark 1: if $H \in \mathcal{C}^1(\mathcal{A})$, the l.h.s. is

$$\int_0^T \frac{dt}{T} \, \mathcal{T}(|\vec{\nabla}(e^{-\imath H t})|^2 \Pi(\Delta)) \; .$$

- Remark 2: localization holds in Δ (a.s. in ω) if

$$l^2(\Delta) \; = \; \limsup_{T \to \infty} \int_0^T \frac{dt}{T} \, \mathcal{T}(|\vec{\nabla} e^{-\imath H t}|^2 \, \Pi(\Delta)) \; < \; \infty \; .$$

Theorem 5 *Let $H \in \mathcal{C}^1(\mathcal{A})$. Then:*

i) $0 \leq \sigma_{\rm diff}(\Delta) \leq 1$.

ii) $\sigma_{\rm diff}(\Delta)$ *does not change by compact perturbation of* $\pi_\omega(H)$.

iii) Guarneri's bound

$$\alpha^{+}_{\rm LDOS}(\Delta) \ \leq \ d \cdot \sigma_{\rm diff}(\Delta) \ ,$$

if $\Delta \subset \mathbf{R}$ *is a bounded open interval and if* $H \in \mathcal{C}^k(\mathcal{A})$ $k > d/2$.

Consequences:

1. in 1D, a.c. spectrum $\Rightarrow \sigma_{\rm diff}(\Delta) = 1$.
2. For any d a.c. spectrum $\Rightarrow \sigma_{\rm diff}(\Delta) \geq 1/d$.
   Ex.: *weak disorder spin-orbit coupling in 2D*
3. For any $0 \leq \beta \leq 1$ there are models in $d = \infty$ with a.c. spectrum and $\sigma_{\rm diff}(\Delta) = \beta$
   (*J.Vidal, J. Bellissard, R. Mosseri*).

Current-current correlation measure

- The current operator is

$$\vec{J}_\omega \;=\; \imath \frac{q}{\hbar}[\pi_\omega(H), \vec{X}] \;=\; \pi_\omega(-\frac{q}{\hbar}\vec{\nabla} H) \ .$$

- The current-current correlation measure is defined by

$$\int_{\mathbf{R}^2} dm(E,E')\; f(E) g(E') \;=\; \mathcal{T}\left\{\vec{J} f(H) \vec{J} g(H)\right\}$$

for any $f, g \in \mathcal{C}_0(\mathbf{R}^d)$.

- The diffusion exponent is also given by

$$\int_{E,\,E' \in \Delta,\, |E-E'| \leq \epsilon} dm(E,E') \;\underset{\epsilon\downarrow 0}{\sim}\; \epsilon^{2(1-\sigma_{\rm diff}(\Delta))} \ .$$

Quantum Diffusion

- $\sigma_{\rm diff}(\Delta)) = 1$ ballistic motion
  ex. : *free motion in a perfect crystal.*

- $\sigma_{\rm diff}(\Delta)) = 0$ absence of diffusion
  ex. : *localization.*

- $\sigma_{\rm diff}(\Delta)) = 1/2$ quantum diffusion
  ex. : *weak localization, 2D Harper.*

- $0 < \sigma_{\rm diff}(\Delta)) < 1/2$ subdiffusion
  ex. : *3D quasicrystals at Fermi level.*

- $1/2 < \sigma_{\rm diff}(\Delta)) < 0$ overdiffusion
  ex. : *2D quasilattices.*

THE KUBO FORMULA

12. H. Schulz-Baldes & J. Bellissard, *A Kinetic Theory for Transport in Aperiodic Media*, J. Stat. Phys.,**91**, (1998), 991-1026.
13. D. Spenher & J. Bellissard,*in preparation.*

Bloch Oscillations

- To produce a non zero current turn on an electric field $\vec{\mathcal{E}}$. The new evolution is provided by

$$H_{\omega,\vec{\mathcal{E}}} = H_\omega - q\vec{\mathcal{E}}\vec{X}$$

- The unitary associated to $H_{\omega,\vec{\mathcal{E}}}$ implements an automorphism group on $\mathcal{A}$ (*see [12] above*).

Theorem 6 *If H is bounded, the time average of the component of the current along the electric field vanishes !!*

Because:

$$\int_0^t \frac{ds}{t}\vec{\mathcal{E}} \cdot \vec{J}(s) = \frac{H(t) - H(0)}{t} \xrightarrow{t\uparrow\infty} 0$$

No dissipation ⇒ No transport !!

The Drude Model (*Drude*, 1900)

- Electrons in a metal are free classical particles of mass $\mathbf{m_*}$ and charge $\mathbf{q}$.
- Electron density is $\mathbf{n}$.
- Collisions occur at random poissonian times $\cdots < t_{-1} < t_0 < \cdots < t_{n+1} < \cdots$ with

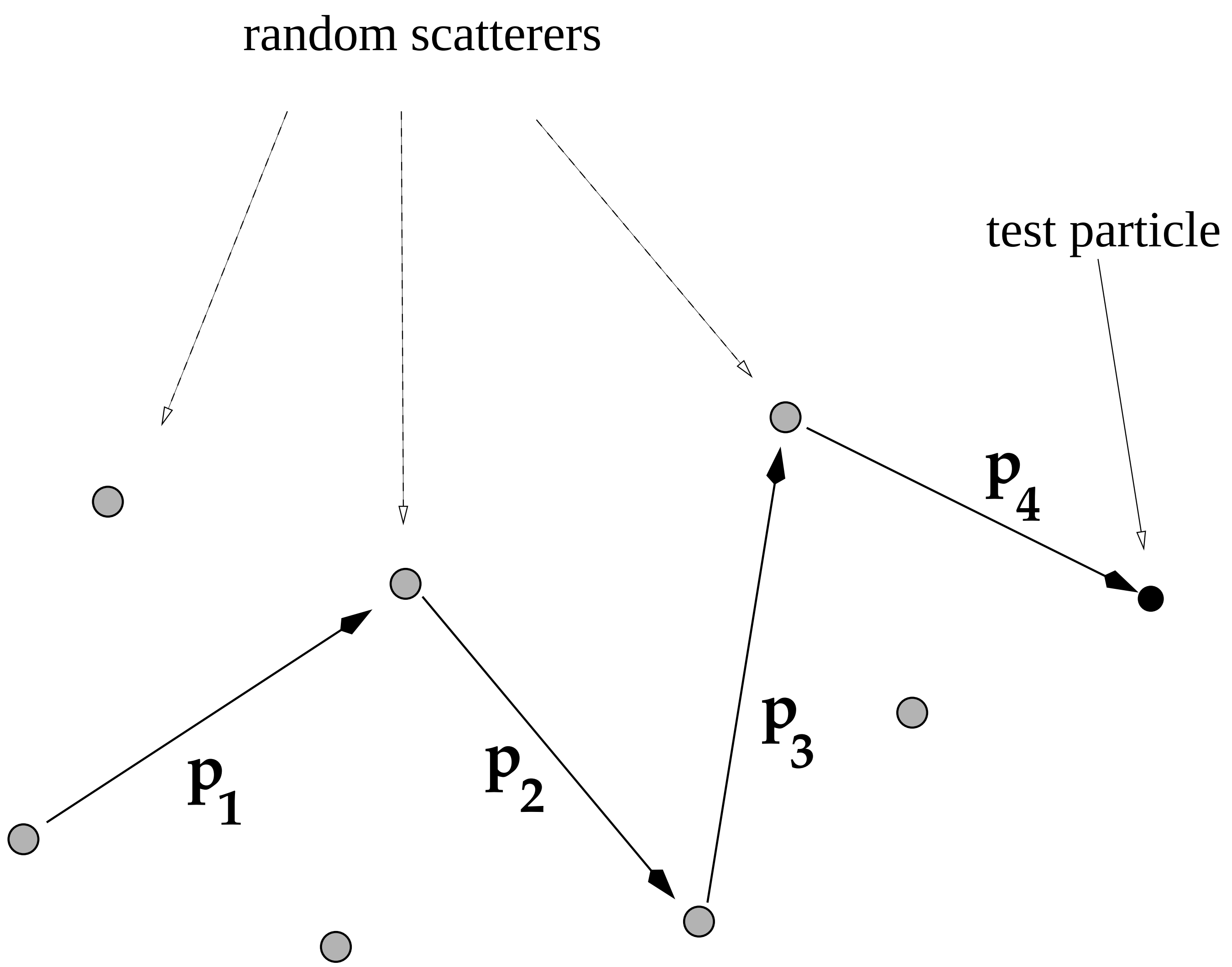
$$< \mathbf{t_{n+1}} - \mathbf{t_n} >= \tau_{\mathbf{rel}}$$

.

- If p_n is the electron momentum between times t_n and t_{n+1}, then the $p_{n+1} - p_n$'s are independent random variables distributed according to the Maxwell distribution at temperature T.

Then the conductivity follows the *Drude formula*

$$\sigma = \frac{\mathbf{q^2 n}}{\mathbf{m_*}} \tau_{\mathbf{rel}}$$



The Drude kinetic model

Quantum Drude Models

1. Replace the classical motion by the quantum one in the homogeneous system with Hamiltonian H.
2. Replace collisions by *quantum jumps* indexed by r at random poissonian times
   $\cdots < t^{(r)}_{-1} < t^{(r)}_{0} < \cdots < t^{(r)}_{n+1} < \cdots$ with
   $$< \mathbf{t^{(r)}_{n+1} - t^{(r)}_{n}} >= \mathbf{\Gamma_r^{-1}}$$
   .
3. At each collision of type r the density matrix ρ changes into $\mathcal{K}^*_r(\rho)$ for some operator $\mathcal{K}^*_r$.
4. The *dissipation operator* is
   $$C^*(\rho) \;=\; \Sigma_r \Gamma_r \left(\rho - \mathcal{K}^*_r(\rho)\right)$$
5. Assume:
   (a) If $\rho \in L^1(\mathcal{A}, \mathcal{T})$ then $C^*(\rho) \in L^1(\mathcal{A}, \mathcal{T})$,
   (b) $\exp\{-C^*\}(\rho) \geq 0$ if $\rho \geq 0$,
   (c) $\exp\{-C^*\}$ leaves $\mathcal{T}$ invariant.

Dissipative Evolution

The Liouville operator associated to $A = A^*$ is

$$\mathcal{L}_A = \frac{\imath}{\hbar}[A, \cdot]$$

The evolution of the density matrix is given by

$$\rho(t) = \eta^*_{t-t_n} \circ \mathcal{K}^*_{r_n} \circ \eta^*_{t_n - t_{n-1}} \circ \cdots \circ \mathcal{K}^*_{r_1} \circ \eta^*_{t_1}(\rho)$$

if

1. $t_0 \leq 0 < t_1 < \cdots < t_n \leq t < t_{n+1}$ are the collision times and $r_1, \cdots, r_n$ the corresponding quantum jumps.
2. η^*_t is the action on states of the quantum evolution associated to $H_{\omega,\vec{\mathcal{E}}}$.

Theorem 7 *The collision average evolution of an initial state $\rho \in L^1(\mathcal{A}, \mathcal{T})$ is given by :*

$$\frac{d\langle\rho\rangle}{dt} = \left\{-\mathcal{L}_H + \frac{q}{\hbar}\vec{\mathcal{E}} \cdot \vec{\nabla} - C^*\right\} \langle\rho\rangle$$

The Conductivity

Theorem 8 *The (time, thermal, quantum) averaged current obeys to the linear response theory. The corresponding AC-conductivity tensor at frequency ω_0 is given by the* **Kubo formula***:*

$$\sigma_{i,j} \;=\; \frac{q}{\hbar}\mathcal{T}\left\{\partial_i(\rho_{\beta,\mu})\,(C-\mathcal{L}_H-\imath\,\omega_0)^{-1}\,(J_j)\right\}$$

where $\rho_{\beta,\mu} = (\mathbf{1}+\exp\{\beta(H-\mu)\})^{-1}$ is the (Fermi-Dirac) equilibrium state at inverse temperature β and chemical potential μ and C is the dual action of C^* on $\mathcal{A}$.

□

The *Relaxation Time Approximation* (**RTA**), consists in setting $C^*(\rho) = \rho_{\beta,\mu}$ (immediate return to equilibrium after each collision) namely $C = \mathbf{1}/\tau$ where τ is the *relaxation time*.

In the limit of zero dissipation $\tau \to \infty$, the conductivity tests the spectral properties of $\mathcal{L}_H$ near $\imath\omega_0$ on the imaginary axis.

Anomalous Drude Formula in the RTA

14. *Lectures on Quasicrystals*, F. Hippert, D. Gratias Eds., Ed. de Physique, Les Ulis, (1994); (a) D. Mayou pp. 417-462, (b) C. Sire pp. 505-533.

15. J. Bellissard & H. Schulz-Baldes, in *Proceedings of the 5th International Conference on Quasicrystals*, C. Janot, R. Mosseri Eds., World Scientific, Singapore, (1995).

Theorem 9 *Assume that* $\tau \uparrow \infty$ *as the temperature* $T \downarrow 0$ *and let* $\sigma_F = \lim_{\epsilon \downarrow 0} \sigma_{\rm diff}([\mu - \epsilon, \mu + \epsilon])$, *where* $\mu = \mu(T)$ *is the chemical potential fixed by the charge carrier density* n. *Then the DC-conductivity (i.e.* $\omega_0 = 0$*) satisfies*

$$\sigma_{i,i}(T) \underset{T\downarrow 0}{\sim} \tau^{(2\sigma_F - 1)}$$

□

Comments:

1. if $\sigma_F = 1$ (ballistic) then $\sigma_{i,i} \underset{T\downarrow 0}{\sim} \tau$ (Drude);
2. if $\sigma_F = 0$ (localization) then $\sigma_{i,i} \underset{T\downarrow 0}{\sim} 1/\tau$ (anti-Drude);
3. if $\sigma_F = 1/2$ (diffusion) then $\sigma_{i,i} \underset{T\downarrow 0}{\sim}$ *const.* (residual conductivity);
4. if $0 < \sigma_F < 1/2$ (subdiffusion) then $\sigma_{i,i} \underset{T\downarrow 0}{\sim} 1/\tau^\alpha$ (insulator) (**ex.:** quasicrystals !!);
5. if $1/2 < \sigma_F < 1$ (overdiffusion) then $\sigma_{i,i} \underset{T\downarrow 0}{\sim} \tau^\alpha$ (conductor).

Variable Range Hopping

Under progress with D. Spenher

1. The RTA is not valid anymore!

2. There are infinitely many types of quantum jumps between impurity sites in the infinite volume limit.

3. Each quantum jump corresponds to a quantum resonance $\Rightarrow$ non unitary instantaneous evolution .

4. On has to prove that the instantaneous evolution converges in this limit. (*This is proved indeed !*)

5. Since C is "very small", one can expand the Kubo formula in powers of C. First order suffices. If C has the correct form, then one gets the Mott law.

APPLICATIONS

Conductivity in QC's

16. S. Roche & Fujiwara, Phys. Rev., **B58**, 11338-11396, (1998).

1. *ab initio* calculations using LMTO for $i - AlCuCo$ and taking orbitals hybridization gives $\sigma_F = .375$
2. If only collisions with phonons occur, Bloch's law implies $\tau \underset{T\uparrow\infty}{\sim} T^{-5}$.
3. Thus we get

$$\sigma_{i,i}(T) \underset{T\uparrow\infty}{\sim} T^{1.25}$$

   compatible with experiments !

4. At low temperature ($T \leq T_{\text{dis}}$), disorder dominates:
   (a) for $AlPdMn$, $T_{\text{dis}} \approx 300K$. There should be a *high density of defects*, leading to *weak localization* regime thus to *residual conductivity.*
   (b) for $AlPdRe$, $T_{\text{dis}} \approx 10K$. One expects a very *low density of defects* leading to *strong localization* regime thus to *Mott variable range hopping conductivity.*

2D Lattice Electrons in a Magnetic Field

A. Barelli, J. Bellissard and F. Claro, *Magnetic field induced directional localization in a 2D rectangular lattice*, sub to PRL (1998),

Anisotropic Harper model in 2D ($\mathbf{t_x} < \mathbf{t_y}$):

$$H = t_x(U_x + U_x^{-1}) + t_y(U_y + U_y^{-1}) \ ,$$

U_x, U_y = magnetic translation along x, y-axis;
ϕ= magnetic flux through unit cell
$\phi_0 = h/e$ is the flux quantum:

$$U_x \, U_y = e^{2\imath\pi\phi/\phi_0} \, U_y \, U_x \ ,$$

Aubry's duality: for $\phi/\phi_0 \notin \mathbf{Q}$,

S. Aubry, (1978)

- eigenstates are *localized* along the x-axis
- eigenstates are *plane wave-like* along the y-axis.

Result

In the *Relaxation Time Approximation* (RTA):

1. If $\phi = 0$, at low temperature (*Drude*)

$$\frac{\sigma_{xx}}{\sigma_{yy}} \approx const. \left(\frac{t_x}{t_y}\right)^2 \ , \tag{1}$$

2. If $\phi/\phi_0 \notin \mathbf{Q}$, at temperature T, relaxation time τ

$$\frac{\sigma_{xx}}{\sigma_{yy}} \approx const. \left(\frac{t_x}{t_y}\right)^2 (\max(k_B T, \hbar/\tau))^2 \ , \tag{2}$$

$\Rightarrow$ *Enhanced anisotropy at low temperature*

3. If $\phi/\phi_0 = p/q \in \mathbf{Q}$, there is a crossover temperature T_* depending on q with
   - Drude behaviour (1) at $T < T_*$
   - Enhanced anisotropy (2) at $T > T_*$
   - $T_* \downarrow 0$ as $q \uparrow \infty$

CONCLUSION

1. Non Commutative Geometry allows to treat aperiodic homogeneous media.
2. Spectral exponents describe singular continuous spectra.
3. Diffusion exponents describe non ballistic motions.
4. Guarneri's inequality between the spectral and the diffusion exponents is the only constraint. This constraint is mild in high dimension.

   (In particular for QC's one may have an a.c. spectrum near the Fermi level together with a quantum subdiffusion.)
5. A quantum kinetic theory permits to prove Kubo's formula. It is under control in the RTA. It is in progress in the general case.
6. Anomalous diffusion gives rise to an anomalous Drude formula with a scaling law w.r.t the relaxation time.
7. One expects to get the Mott law for variable range hopping as a by-product of this theory.
8. Applied to QC's this theory permits to understand qualitatively their transport properties.
9. Aubry's duality produces an enhanced conductivity anisotropy by the magnetic field for a 2D electron on an anisotropic lattice.