COHERENT & DISSIPATIVE TRANSPORT in APERIODIC MEDIA

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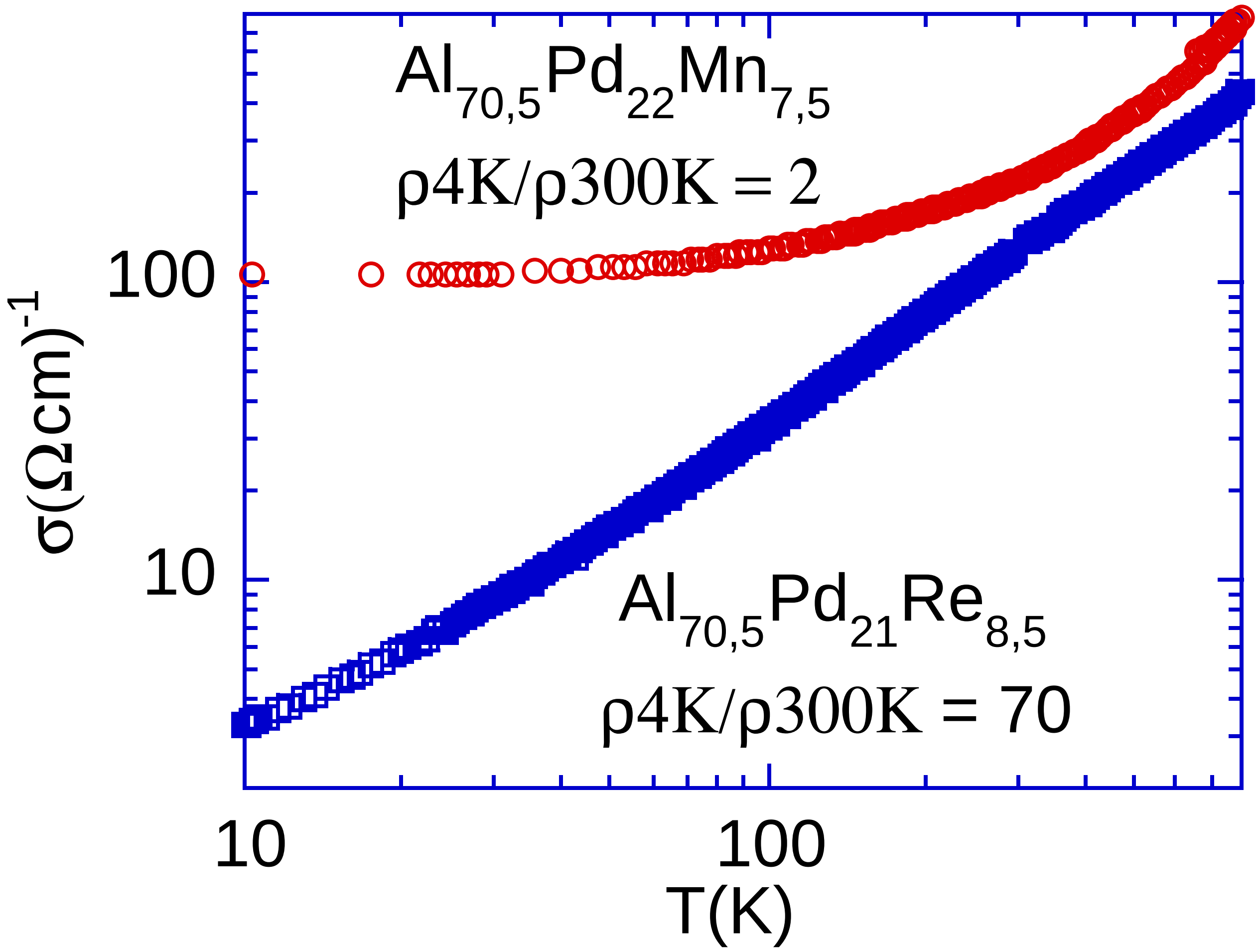
I)- Aperiodic media :

Examples

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) $\mathbf{Al_{62.5}Cu_{25}Fe_{12.5}}$;
   (b) $\mathbf{Al_{70}Pd_{22}Mn_{8}}$;
   (c) $\mathbf{Al_{70}Pd_{22}Re_{8}}$;

3. *Disordered media*: random atomic positions
   (a) Normal metals (with defects or impurities);
   (b) Doped semiconductors (**Si**, **AsGa**, ...);



Conductivity of Quasicrystals vs Temperature

$$\sigma \approx \sigma_0 + a\,T^{\gamma} \text{ with } 1 < \gamma < 1.5$$

$$\text{for } 1\,K \leq T \leq 1000\,K$$

Mathematical Description

1. Closing suitably the set of translated of the set of atomic positions leads to the *Hull* : it is a compact metrizable space Ω endowed with an $\mathbb{R}^d$-action.

2. An invariant ergodic probability measure $\mathbb{P}$ is provided by the Gibbs state at zero temperature.

3. Observables are *random operators* $A = (A_\omega)_{\omega \in \Omega}$ acting on the Hilbert space $\mathcal{H}$ of quantum states (such as $L^2(\mathbb{R}^d)$ for spinless electrons) with:

   (a) Covariance : $T(a) A_\omega T(a)^{-1} = A_{\mathcal{T}^{-a}\omega}$.

   (b) $\omega \mapsto A_\omega$ is strongly continuous.

4. The trace per unit volume, defined by $\mathbb{P}$, exists:

$$\mathcal{T}_{\mathbb{P}}(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \mathrm{Tr}(A_\omega \restriction_\Lambda) = \int_\Omega d\mathbb{P}(\omega) \langle x | A_\omega | x \rangle$$

5. Differential: $(\vec{\nabla} A)_\omega = -\imath [\vec{X}, A_\omega]$

II)- Coherent Transport :

Local Exponents

Given a positive measure μ on $\mathbb{R}$:

$$\alpha_\mu^\pm(E) \;=\; \lim \left\{ \begin{array}{c} \sup \\ \inf \end{array} \right\}_{\varepsilon \downarrow 0} \frac{\ln \int_{E-\varepsilon}^{E+\varepsilon} d\mu}{\ln \varepsilon}$$

For Δ a Borel subset of $\mathbb{R}$:

$$\alpha_\mu^\pm(\Delta) \;=\; \mu - \mathrm{ess} \left\{ \begin{array}{c} \sup \\ \inf \end{array} \right\}_{E \in \Delta} \alpha_\mu^\pm(E)$$

1. For all E, $\alpha_\mu^\pm(E) \geq 0$.
   $\alpha_\mu^\pm(E) \leq 1$ for μ-almost all E.
2. If μ is *ac* on Δ then $\alpha_\mu^\pm(\Delta) = 1$,
   if μ is *pp* on Δ then $\alpha_\mu^\pm(\Delta) = 0$.
3. If μ and ν are equivalent measures on Δ, then
   $\alpha_\mu^\pm(E) = \alpha_\nu^\pm(E)$ μ-almost surely.
4. α_μ^+ coincides with the *packing dimension.*
   α_μ^- coincides with the *Hausdorff dimension.*

Fractal Exponents

For $p \in \mathbb{R}$:

$$D^{\pm}_{\mu,\Delta}(q) \;=\; \lim_{q'\to q} \frac{1}{q'-1} \lim_{\varepsilon\downarrow 0} \left\{ \begin{array}{c} \sup \\ \inf \end{array} \right\} \frac{\ln\left(\int_{\Delta} d\mu(E) \left\{ \int_{E-\varepsilon}^{E+\varepsilon} d\mu \right\}^{q'-1} \right)}{\ln \varepsilon}$$

1. $D^{\pm}_{\mu,\Delta}(q)$ is a non decreasing function of q.

2. $D^{\pm}_{\mu,\Delta}(q)$ is **not** an invariant of the measure class, in general.

3.(a) If μ is *ac* on Δ then $D^{\pm}_{\mu,\Delta}(q) = 1$.

(b) If μ is *pp* on Δ then $D^{\pm}_{\mu,\Delta}(q) = 0$.

Spectral Exponents

Given a Hamiltonian $H = (H_\omega)_{\omega\in\Omega}$, namely a selfadjoint observable, we define:

1. The *local density of state* (LDOS) is the spectral measure of H_ω relative to a vector $\varphi \in \mathcal{H}$.
2. The corresponding local exponent is obtained after maximizing (+) or minimizing (-) over φ. It is denoted $\alpha^{\pm}_{\text{LDOS}}$. It is $\mathbb{P} - a.s.$ independent of ω.
3. The *density of states* (DOS) as the measure defined by
$$\int d\mathcal{N}_{\mathbb{P}}(E) f(E) \; = \; \mathcal{T}_{\mathbb{P}}(f(H))$$
4. The local exponent associated with the DOS is denoted by $\alpha^{\pm}_{\text{DOS}}$.
5. Inequality : $\quad \alpha^{\pm}_{\text{LDOS}}(\Delta) \leq \alpha^{\pm}_{\text{DOS}}(\Delta)$.
6. The fractal exponents for the LDOS are defined in the same way, provided we consider the average over ω before taking the logarithm and the limit $\varepsilon \downarrow 0$.

Transport Exponents

1. For $\Delta \subset \mathbb{R}$ Borel, let $P_{\Delta,\omega}$ be the corresponding spectral projection of H_ω. Set:
$$\vec{X}_\omega(t) \;=\; e^{\imath t H_\omega}\, \vec{X}\, e^{-\imath t H_\omega}$$
2. The averaged spread of a typical wave packet with energy in Δ is measured by:
$$L_\Delta^{(p)}(t) \;=\; \left(\int_0^t \frac{ds}{t} \int_\Omega d\mathbb{P}\, \langle x | P_{\Delta,\omega} | \vec{X}_\omega(t) - \vec{X} |^p P_{\Delta,\omega} | x \rangle \right)^{1/p}$$
3. Define $\beta = \beta_p^\pm(\Delta)$ similarly so that $L_\Delta^{(p)}(t) \sim t^\beta$.
4. $\beta_p^-(\Delta) \leq \beta_p^+(\Delta)$.
$\beta_p^\pm(\Delta)$ are non decreasing in p.
5. *Heuristic*
$\beta = 0 \longrightarrow$ absence of diffusion (*ex: localization*),
$\beta = 1 \longrightarrow$ ballistic motion (*ex: in crystals*),
$\beta = 1/2 \longrightarrow$ quantum diffusion
(*ex: weak localization*).
$\beta < 1 \longrightarrow$ subballistic regime,
$\beta < 1/2 \longrightarrow$ subdiffusive regime
(*ex: in quasicrystals*).

Inequalities

1. *Guarneri's inequality:* (*Guarneri '89, Combes , Last '96*)

$$\beta_p^{\pm}(\Delta) \;\geq\; \frac{\alpha^{\pm}_{\mathrm{LDOS}}(\Delta)}{d}$$

2. *BGT inequalities:* (*Barbaroux, Germinet, Tcheremchantsev '00*)

$$\beta_p^{\pm}(\Delta) \;\geq\; \frac{1}{d}\, D^{\pm}_{\mathrm{LDOS},\Delta}\left(\frac{d}{d+p}\right)$$

3. *Heuristics:*
   (a) *ac* spectrum implies $\beta \geq 1/d$.
   (b) *ac* spectrum implies ballistic motion in $d = 1$
   (c) *ac* spectrum is compatible with quantum diffusion in $d = 2$. This is expected in weak localization regime.
   (d) *ac* spectrum is compatible with subdiffusion for $d \geq 3$.

Results for Models

1. For Jacobi matrices (1D chains), the position operator is defined by the spectral measure (orthogonal polynomials) $\Rightarrow$ transport exponents should be defined through the spectral ones.

2. For Jacobi matrices of a Julia set, with μ the σ-balanced measure (*Barbaroux, Schulz-Baldes '99*)
$$\beta_p^+ \;\leq\; D_\mu(1-p) \qquad \text{for all} \quad 0 \leq p \leq 2$$

3. If $H_1, \cdots, H_d$ are Jacobi matrices, $\eta_1, \cdots, \eta_d$ are positive numbers and if
$$H^{(\eta)} \;=\; \sum_{j=1}^{d} \eta_j \, \mathbf{1} \otimes \cdots \otimes \mathbf{H_j} \otimes \cdots \otimes \mathbf{1}$$
Then (*Schulz-Baldes, Bellissard '00*)
$$\beta_p^+(H^{(\eta)}) = \max_j \beta_p^+(H_j)$$
$$\alpha_{\text{LDOS}}(H^{(\eta)}) = \min\{1, \sum_j \alpha_{\text{LDOS}}(H_j)\}$$
for a.e. η. In addition if $\sum_j \alpha_{\text{LDOS}}(H_j) > 1$, $H^{(\eta)}$ has *a.c.* spectrum.

4. For any $\epsilon > 0$, there is a Jacobi matix H_0 such that if $H_j = H_0$, $\forall j$, $H^{(\eta)}$ has *a.c. spectrum* for $d \geq 3$ and spectral exponent $\leq 1/d - \epsilon$ for *a.e.* η.
   (*Schulz-Baldes, Bellissard '00*)

5. There is a class of models of Jacobi matrices on an infinite dimensional hypercube with *a.c. spectrum* and vanishing transport exponents.
   (*Vidal, Mosseri, Bellissard '99*)

III)- Dissipative Transport :

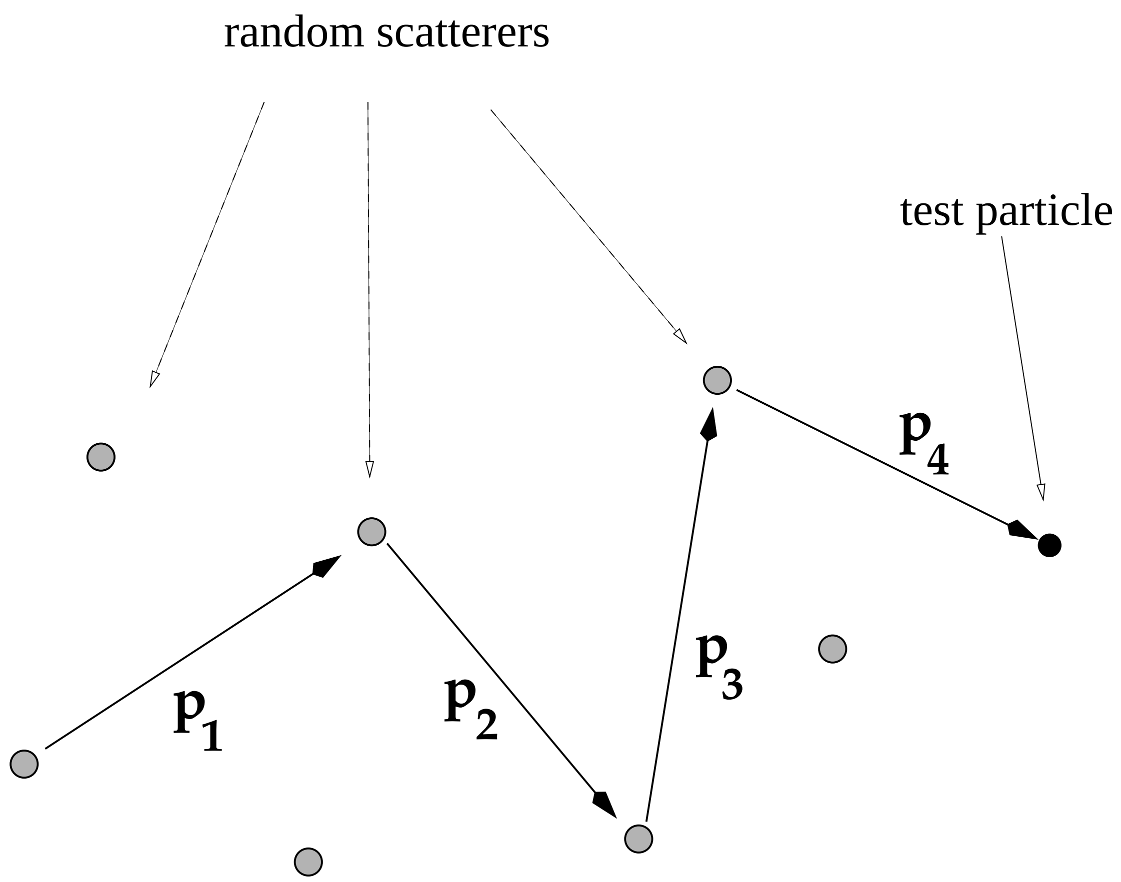
The Drude Model (1900)

Hypothesis :

1. Electrons in a metal are free classical particles of mass m_* and charge q.
2. They experience collisions at random poissonnian times $\cdots < t_n < t_{n+1} < \cdots$, with average relaxation time τ_{rel}.
3. 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*

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



The Drude Kinetic Model

Anomalous Drude formula (RTA)

1. Replace the classical dynamics by the quantum one electron dynamic in the aperiodic solid.
2. At each collision, force the density matrix to come back to equilibrium. (*Relaxation time Approximation* or RTA).
3. There is then one *relaxation time* τ_{rel}. The electric conductivity is then given by Kubo's formula:
$$\sigma_{i,j} \;=\; \frac{q^2}{\hbar}\, \mathcal{T}_{\mathbb{P}} \left(\partial_j \left(\frac{1}{1 + e^{\beta(H-\mu)}} \right) \frac{1}{1/\tau_{rel} - \mathcal{L}_H}\, \partial_i H \right)$$
Here q is the charge of the carriers, $\beta = 1/k_B T$, μ is the chemical potential and $\mathcal{L}_H = \imath/\hbar\,[H, .]$.
4. For the Hilbert-Schmidt inner product defined by $\mathcal{T}_{\mathbb{P}}$, $\mathcal{L}_H$ is anti-selfadjoint. Thus as $\tau_{rel} \uparrow \infty$, the resolvent of $\mathcal{L}_H$ is evaluated closer to the spectrum near 0. Then (*Mayou '92, Sire '93 Bellissard, Schulz-Baldes '95*):
$$\sigma \quad \stackrel{\tau_{rel} \uparrow \infty}{\sim} \quad \tau_{rel}^{\,2\beta_F - 1}$$
where β_F is the transport exponent $\beta_2(E_F)$ evaluated at Fermi level.

Heuristic

1. In practice, $\tau_{rel} \uparrow \infty$ as $T \downarrow 0$.
2. If $\beta_F = 1$ (*ballistic motion*), $\sigma \sim \tau_{rel}$ (*Drude*). The system behaves as a conductor.
3. If $\beta_F = 0$ (*absence of diffusion*) $\sigma \sim 1/\tau_{rel}$. The system behaves as an insulator. The RTA is incorrect however at low temperature.
4. If $\beta_F = 1/2$ (*quantum diffusion*), $\sigma \sim$ *const.*: residual conductivity at low temperature.
5. For $1/2 < \beta_F \leq 1$, $\sigma \uparrow \infty$ as $T \downarrow 0$:the system behaves as a conductor.
6. For $0 \leq \beta_F < 1/2$, $\sigma \downarrow 0$ as $T \downarrow 0$: the system behaves as an insulator.
7. If we assume in addition that the Bloch law $\tau_{rel} \sim T^{-5}$ (*Roche, Fujiwara '98*), then σ follows a scaling law (compatible with the behaviour of quasicrystals).

Beyond the RTA

1. At low temperature, the RTA is invalid. There is a spectrum of relaxation times.
2. A kinetic model of *quantum jumps* has been proposed leading to the validity of linear response. (*Spehner, Bellissard '00, Bellissard, Rebolledo, Spehner, von Waldenfels '00*).
3. The current admits two parts : the coherent one, induced by $\vec{J} = \imath[\vec{X}, H]$, and a dissipative one including other effects like *phonon drag*, etc.
4. The Kubo formula becomes more involved and can be decomposed into five contributions in general.
5. Applied to strongly localized electrons, this formalism gives rise to a justification of the Abrahams and Miller random resistor network model (*Spehner, Thesis '00, Spehner, Bellissard, '00*).

   This model describes the *Mott variable range hopping* and leads to

$$\sigma \stackrel{T \downarrow 0}{\sim} e^{\left(-\frac{T_0}{T}\right)^{1/d+1}} \qquad \textit{(Mott '64)}$$

IV)- Conclusions :

1. The electron dynamics in an aperiodic solid can be described by using random operators and rules of Non Commutative Calculus.
2. The quantum evolution of a typical wave packet leads to anomalous diffusion, described through various spectral and transport exponents.
3. These exponents are related by inequalities that allow subdiffusion together with absolutely continuous spectrum for $d \geq 3$.
4. Dissipative mechanisms, such as electron-phonon interaction, may be described through kinetic models, generalizing the Drude model.
5. The interplay between coherent and dissipative transport is revealed at low temperature. Anomalous diffusion then leads to an anomalous Drude formula within the RTA.
6. The anomalous Drude formula may explain the behaviour of quasicrystals.
7. Beyond the RTA, the kinetic models are still valid but involve more conditions. One consequence is the justification of the Abraham-Miller random resistor network which usually leads to a better understanding of the Mott variable range hopping conductivity, in strongly disordered systems.