

# Transport Theory in Dissipative Quantum Systems

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# Main References

D. SPEHNER, *Contributions à la théorie du transport électronique, dissipatif dans les solides aperiodiques*, Thèse, 13 mars 2000, Toulouse.

J. BELLISSARD, *Coherent and dissipative transport in aperiodic solids*, in *Dynamics of Dissipation*, pp. 413-486, Lecture Notes in Physics, 597, Springer (2002).  
P. Garbaczewski, R. Olkiewicz (Eds.).

H. SPOHN, *Large Scale Dynamics of Interacting Particles*, Springer (1991).

S. ATTAL, A. JOYES, C.-A. PILLET, *Open Quantum Systems*,  
*Vol.I*, Lecture Notes in Physics, **1880**, (2006)  
*Vol.II*, Lecture Notes in Physics, **1881**, (2006)  
*Vol.III*, Lecture Notes in Physics, **1882**, (2006)

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# I - Why Revisiting Transport ?

- It is a very old problem  
*BOLTZMANN (1872-80) for classical systems;*  
*DRUDE (1900) for electrons.*
- It is treated in textbooks: phenomenology, perturbation theory, numerical calculations.

# Motivations

1. No mathematically rigorous proof of the Kubo formulæ for transport coefficients.  
( However substantial progress for classical systems (LEBOWITZ's school) and for quantum ones (PILLET-JAKSIC, FRÖHLICH *et. al.*) ).
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,  $\sigma(T)$  increases as temperature decreases

$$\sigma(T) \stackrel{T \downarrow 0}{\sim} T^{-2}, \quad (\text{Fermi liquid theory}).$$

2. For a thermally activated process

$$\sigma(T) \stackrel{T \downarrow 0}{\sim} e^{-\Delta/T} \quad (\text{If a gap holds at Fermi level}).$$

3. For weakly disordered systems

$$\sigma(T) \xrightarrow{T \downarrow 0} \sigma(0) > 0 \quad (\text{residual conductivity}).$$

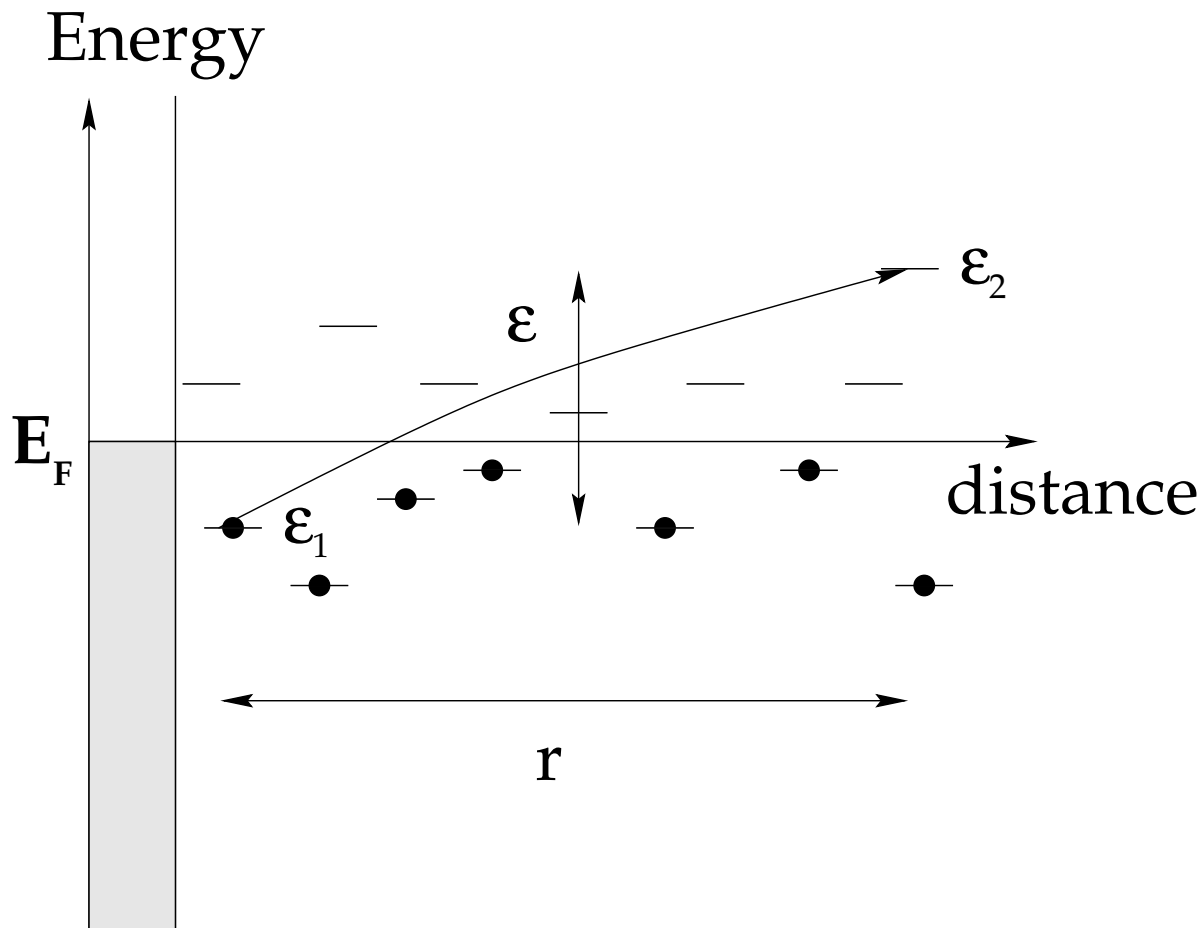
4. For strongly disordered systems in  $3D$

$$\sigma(T) \stackrel{T \downarrow 0}{\sim} e^{-(T_0/T)^{1/4}} \quad (\text{variable range hopping}).$$

# Mott's variable range hopping

N. MOTT, (1968).

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  $\varepsilon$

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

- Tunnelling probability at distance  $r$

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

- Density of state at Fermi level  $n_F$ ,

$$\varepsilon n_F r^d \approx 1$$

- Optimizing, the conductivity satisfies

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

- Optimal energy  $\varepsilon_{opt} \sim T^{d/(d+1)} \gg T$

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

# Quasicrystalline Alloys

*Lectures on Quasicrystals,*

F. Hippert & D. Gratias Eds., Editions de Physique, Les Ulis, (1994),

S. ROCHE, D. MAYOU AND G. TRAMBLY DE LAISSARDIÈRE,

*Electronic transport properties of quasicrystals*, J. Math. Phys., **38**, 1794-1822 (1997).

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** (*Sainfort-Dubost, (1986)*)

**GaMgZn** (*Holzen et al., (1989)*)

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

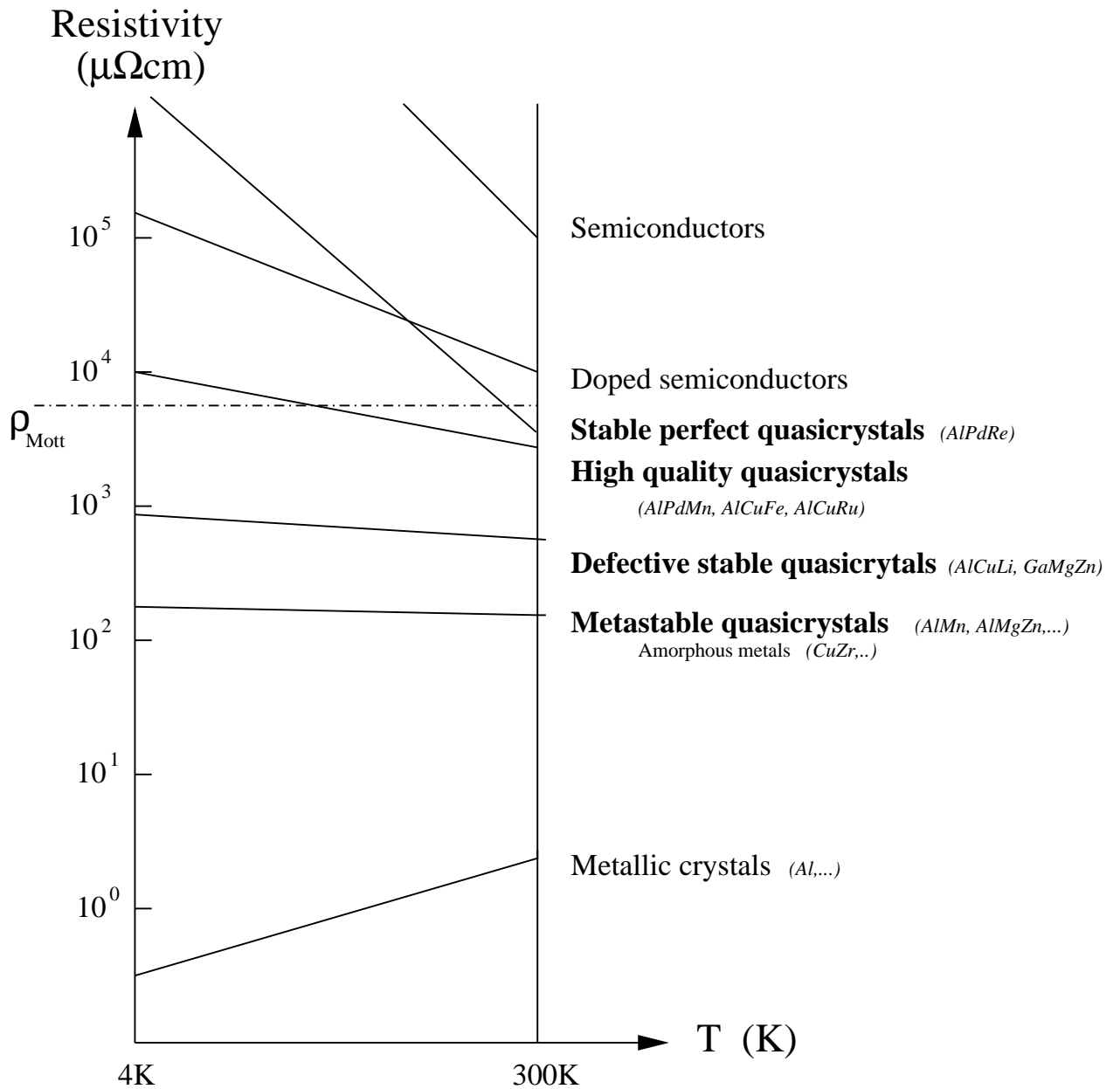
(*Hiraga, Zhang, Hirakoyashi, Inoue, (1988); Gurnan et al., Inoue et al., (1989);*

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

“Perfect” QC's:

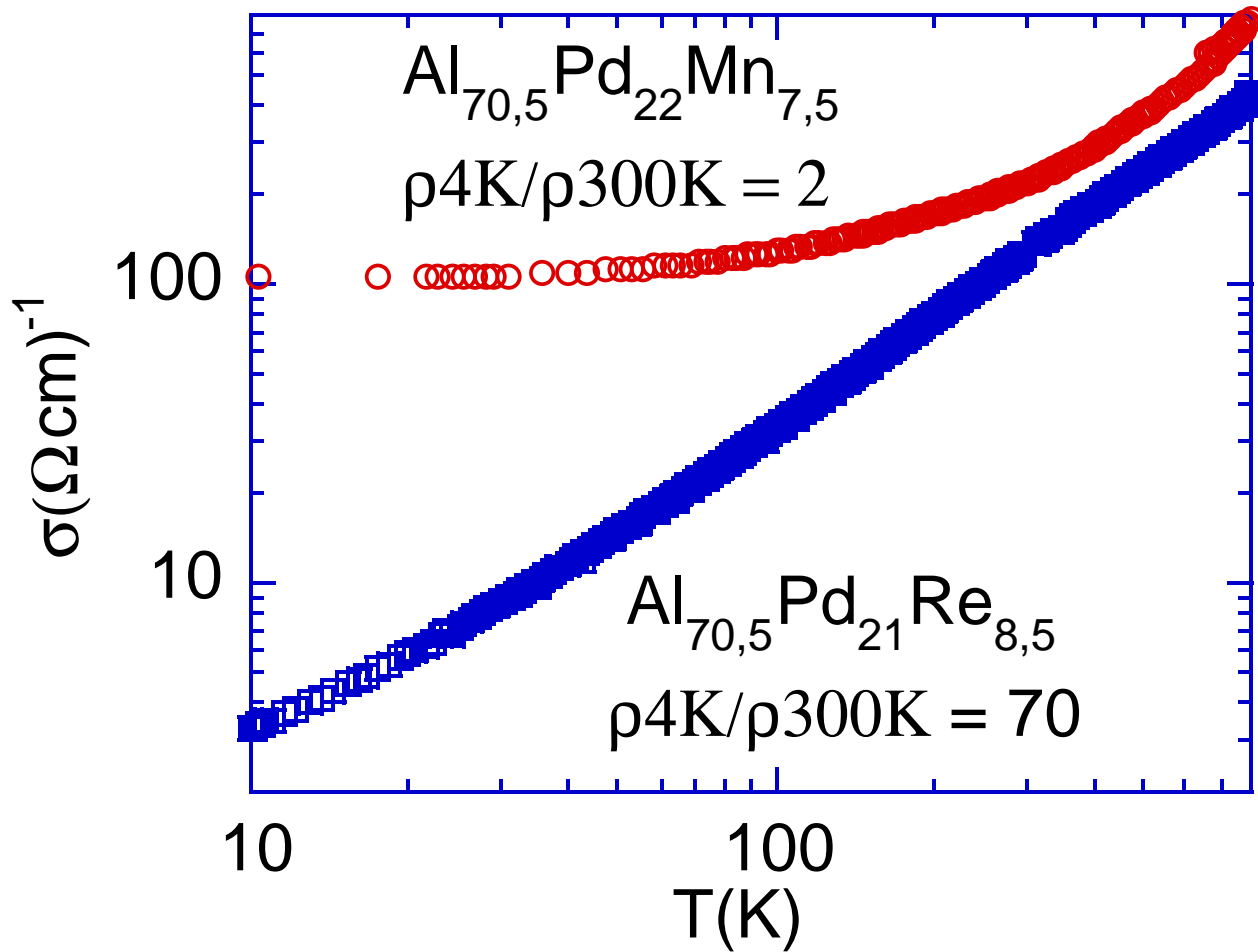
**AlPdMn**

**AlPdRe**



### Typical values of the resistivity

(Taken from *C. Berger* in ref. *Lectures on Quasicrystals*)



### Conductivity of Quasicrystals vs Temperature

$$\sigma \approx \sigma_0 + aT^\gamma \text{ with } 1 < \gamma < 1.5$$

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

## 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

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

*There is a new mechanism here!*

3. At low temperature for **Al<sub>70.5</sub>Pd<sub>22</sub>Mn<sub>7.5</sub>**,

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

4. At low temperature for **Al<sub>70.5</sub>Pd<sub>21</sub>Re<sub>8.5</sub>**,

$$\sigma \propto e^{-(T_0/T)^{1/4}} \quad \text{C. BERGER } et \text{ al. (1998)}$$

## II - Phenomenology

H. J. KREUZER, *Nonequilibrium Thermodynamics and its Statistical Foundations*, Clarendon Press Ed., Oxford, (1981).

G. H. WANNIER, *Statistical Physics*, Dover Pub. Inc., New-York, (1966).

# Linear Response

Experiments show that if a *force*  $\vec{F}$  is imposed to a system, its response is a *current*  $\vec{j}$  vanishing as the force vanishes. Thus for  $\vec{F}$  small

$$\vec{j} = L \cdot \vec{F} + O(\vec{F}^2),$$

Here  $L$  is a matrix of *transport coefficients*.

## Examples:

1. **FOURIER**'s law: a temperature gradient produces a heat current  $\vec{j}_{heat} = -\lambda \vec{\nabla} T$ .
2. **OHM**'s law: a potential gradient (electric field) produces an electric current  $\vec{j}_{el} = -\sigma \vec{\nabla} V$ .
3. **FICK**'s law: a density gradient produce a flow of matter  $\vec{j}_{matter} = -\kappa \vec{\nabla} \rho$ .

- *What is the domain of validity ?*

- *What happens for quantum systems ?*

# Domain of study

Quantum dissipative phenomenon occurs in

1. *Cold atoms interacting with light*  
(*Quantum Optic*)
2. *Molecules (Quantum Chemistry)*
3. *Electrons and phonons in solids*  
(*Solid State Physics*)

Quantum dissipative transport occurs in Solids

1. *Periodic Crystals*
2. *Quasicrystals*
3. *Amorphous materials*  
(*Silicon, metallic glasses, alloys*)
4. *Periodic crystals in Magnetic Fields*

Degrees of freedom involved are *electrons, phonons, atomic diffusion, spin current.*



# A No-Go Theorem: Bloch's oscillations

If  $H = H^*$ , the *one-electron* Hamiltonian, is *bounded* and if  $\vec{R} = (R_1, \dots, R_d)$  is the *position* operator (self-adjoint, commuting coordinates), the *current* is

$$\vec{J} = \text{const.} \frac{i}{\hbar} [H, \vec{R}],$$

Adding a force  $\vec{F}$  at time  $t = 0$  leads to a new evolution with Hamiltonian  $H_F = H - \vec{F} \cdot \vec{R}$ . The 0-frequency component of the current is

$$\vec{j} = \lim_{t \rightarrow \infty} \int_0^t \frac{ds}{t} e^{i s H_F / \hbar} \vec{J} e^{-i s H_F / \hbar},$$

Simple algebra shows that (since  $\|H\| < \infty$ )

$$\vec{F} \cdot \vec{j} = \text{const.} \lim_{t \rightarrow \infty} \frac{H(t) - H}{t} = 0,$$

**WHY?**

This is called *Bloch's Oscillations*

# Dissipation

Dissipation is the *loss of information* experienced by the system observed as the time goes on

## SECOND LAW OF THERMODYNAMICS

### *Clausius-Boltzman entropy*

*The sources of dissipation can have various aspects*

1. External noise random in time
2. Exchange with a thermal bath  
(reservoir with infinite energy)
3. Collisions/interactions with other particles
4. Loss of energy at infinity (infinite volumes)
5. Chaotic motion: sensitivity to initial conditions  
*Kolmogorov-Sinai entropy*
6. Quantum measurement (wave function collapse)
7. Quantum Chaos: the Hamiltonian behaves like a random matrix. *Voiculescu entropy* .

# Length, Time & Energy Scales

## 1. Length scales:

- *Scattering length*: range of interactions between colliding particles.
- *Mean free path*: minimum distance between collisions
- *Mesoscopic scale*: minimum size for the system to reach a local thermodynamical equilibrium.
- *Sample size*

## 2. Times scales:

- *Scattering time*
- *Collision time*: time between two consecutive collisions
- *Relaxation time*: time for a mesoscopic size to relax to equilibrium
- *Measurement time*
- Other times: Heisenberg times  $\hbar/\Delta E$ ,  $\dots$

## 3. Energy scales

# Exchanges of Limits

1. *Infinite volume* limit & *low dissipation* limit:

- Usually

$$\text{mean free path} \ll \text{sample size}$$

(i) infinite volume limit (ii) low dissipation limit.

- In nanoscopic systems linear response may fail !  
The *resistivity* of a molecule is meaningless !

2. *Zero external force* limit & *large time measurement* limit:

- in solids

$$\frac{\hbar}{eV} \approx 10^{-12} - 10^{-15} \text{ s.} \ll \text{measurement time}$$

(i) infinite measurement time limit

(ii) low external field.

- In *pico-femtosecond* laser experiments, failures of linear response theory are observed.

# Approximations

1. Local Equilibrium Approximation
2. Markov approximation
3. Adiabatic Approximation
4. Detailed Balance Condition
5. Relaxation Time Approximation
6. Independant Electrons Approximation

# III - Transport Coefficients

# Local Equilibrium Approximation

- **Length Scales:**

$$\ell \ll \delta L \ll L$$

$\ell$  is a typical *microscopic* length scale  
 $L$  the typical *macroscopic* length scale.  
 Then  $\delta L$  is called *mesoscopic*.

- **Time Scales:**

$$\tau_{rel} \ll \delta t \ll t$$

$\tau_{rel}$  is a typical *microscopic* time scale  
 $t$  the typical *macroscopic* time scale.  
 Then  $\delta t$  is called *mesoscopic*.

- The system is partitioned into *mesoscopic cells*  
 the time is partitioned into *mesoscopic intervals*.
- Mesoscopic cells are *completely open* systems  
 After a time  $O(\delta t)$  they return to *equilibrium*.

- Let  $H$  be the Hamiltonian of the part of the subsystem contained in the mesoscopic cell located at  $\vec{x}$  at time  $t$ .
- Let  $\hat{X}_1 = H, \hat{X}_2 \cdots, \hat{X}_K$  be a complete family of first integral, namely observables commuting with the Hamiltonian.
- Let  $\mathcal{Q}(\vec{x}, t)$  be the set of indices labeling a common eigenbasis of the  $\hat{X}_\alpha$ 's: it is the set of *microstates* of the system contained in the mesoscopic cell.
- If  $\mathbb{P}_{(\vec{x}, t)}(q)$  denotes the Gibbs probability of the microstate  $q \in \mathcal{Q}(\vec{x}, t)$ , its *Boltzman entropy* is given by

$$S(\mathbb{P}) = -k_B \sum_{q \in \mathcal{Q}(\vec{x}, t)} \mathbb{P}_{(\vec{x}, t)}(q) \ln \mathbb{P}_{(\vec{x}, t)}(q)$$

- The *maximum entropy principle* gives *Lagrange multipliers*  $T(\vec{x}, t), F_2(\vec{x}, t), \cdots, F_K(\vec{x}, t)$  called *conjugate variables*. (In the following  $F_1 = 1$ )



- The Gibbs state for the mesoscopic cell centered at  $\vec{x} \in \mathbb{R}^d$  at time  $t$  is:

$$\mathbb{P}_{(\vec{x},t)}(q) = \frac{1}{\mathcal{Z}(\vec{x},t)} e^{-\frac{\sum_{\alpha=1}^K F_{\alpha}(\vec{x},t) \hat{X}_{\alpha}(q)}{k_B T(\vec{x},t)}}$$

- The average values of the first integrals are

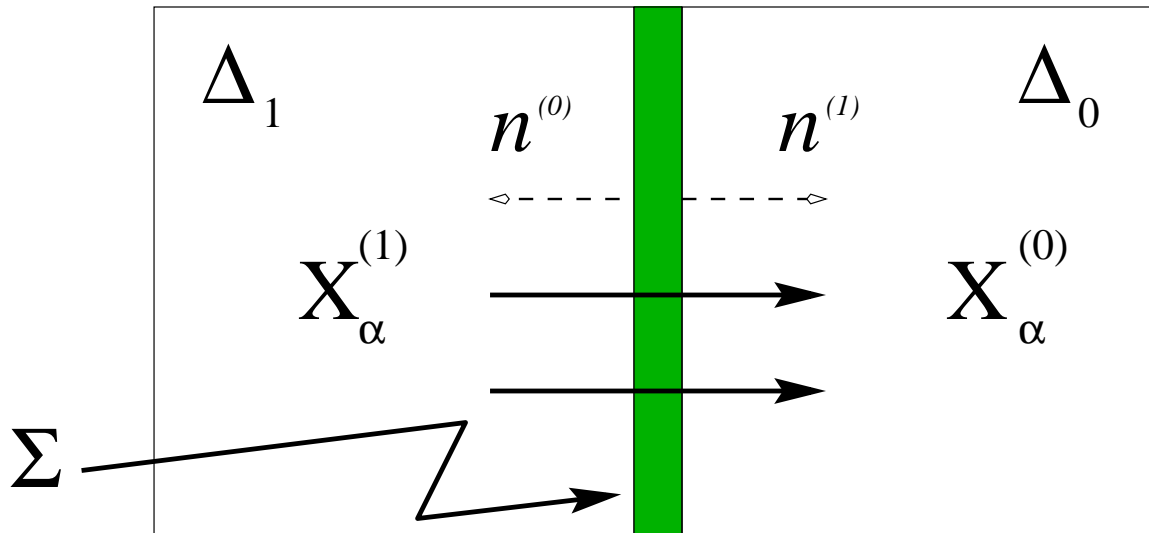
$$\delta X_{\alpha}(\vec{x},t) = \sum_{q \in \mathcal{Q}(\vec{x},t)} \mathbb{P}_{(\vec{x},t)}(q) \hat{X}_{\alpha}(q).$$

- The *volume* of the cell  $\delta V(\vec{x},t) = \delta V$  is mesoscopic and chosen constant in space and time.
- Then  $\delta X_{\alpha}(\vec{x},t) = O(\delta V)$  and the *local density* of  $X_{\alpha}$  is

$$\rho_{\alpha}(\vec{x},t) = \frac{\delta X_{\alpha}(\vec{x},t)}{\delta V}.$$

- Under an infinitesimal change of equilibrium the entropy changes as  $TdS = \sum_{\alpha} F_{\alpha} d\delta X_{\alpha}$

# Fluxes & Currents



- Transfer of  $X_\alpha$  from cell  $\Delta^{(1)}$  to cell  $\Delta^{(0)}$  across area  $\delta\Sigma$  during time  $\delta t$  gives a variation in time

$$\delta X_\alpha(\vec{x}, t) = -\vec{j}_\alpha(\vec{x}, t) \cdot \vec{n}^{(1)} \delta\Sigma \delta t.$$

where  $\vec{n}^{(1)}$  is the normal to area oriented from  $\Delta^{(1)}$  to  $\Delta^{(0)}$ .

- $\vec{j}_\alpha(\vec{x}, t)$  is the *local current* associated with  $X_\alpha$ . It is *mesoscopic* rather than *microscopic*.

- Since  $X_\alpha$  is conserved under evolution the balance leads to the *continuity equation*

$$\frac{\partial \rho_\alpha}{\partial t}(\vec{x}, t) + \vec{\nabla} \cdot \vec{j}_\alpha(\vec{x}, t) = 0.$$

- The *entropy density* is  $s = \frac{\delta S}{\delta V}$   
The entropy variation is then given by

$$\frac{\partial s}{\partial t} = \sum_{\alpha=1}^K \frac{F_\alpha}{T} \frac{\partial \rho_\alpha}{\partial t}.$$

- The *current entropy* is define through

$$\vec{j}_s(\vec{x}, t) = \sum_{\alpha=1}^K \frac{F_\alpha}{T} \vec{j}_\alpha(\vec{x}, t).$$

- The *entropy production rate* is then

$$\frac{ds}{dt} = \frac{\partial s}{\partial t} + \vec{\nabla} \cdot \vec{j}_s = \sum_{\alpha=1}^K \vec{\nabla} \cdot \left( \frac{F_\alpha}{T} \right) \vec{j}_\alpha(\vec{x}, t).$$

and is *positive* thanks to the 2nd Law.

# Linear Response

- A variation of the  $F_\alpha/T$ 's produces currents.  
In the local equilibrium approximation

$$\vec{j}_\alpha = \sum_{\beta=1}^K L_{\alpha,\beta} \vec{\nabla} \left( \frac{F_\beta}{T} \right) + O \left\{ \left| \vec{\nabla} \left( \frac{F_\beta}{T} \right) \right|^2 \right\}$$

- The  $L_{\alpha,\beta}$ 's are  $d \times d$  matrices called *Onsager coefficients*.
- The gradient of  $F_\alpha/T$  is an *affinity*.  
It plays a role similar to *forces*.
- By 2nd Law, the positivity of entropy production rate implies

$$\mathbb{L} = ((L_{\alpha,\beta}))_{\alpha,\beta=1}^K \Rightarrow \mathbb{L} + \mathbb{L}^t \geq 0$$

- **Reciprocity Relations:** if, under time reversal symmetry,  $X_\alpha \xrightarrow{TR} \varepsilon_\alpha X_\alpha$  then

$$L_{\beta,\alpha}(\text{parameters}) = \varepsilon_\alpha \varepsilon_\beta L_{\alpha,\beta}^t(\text{TR-parameters}).$$

# Dissipative & Nondissipative Response

- **Dissipation = Loss of Information**

Dissipation contributes to entropy production.

Hence

$$\mathbb{L}^{(diss)} = \frac{1}{2} (\mathbb{L} + \mathbb{L}^t)$$

- The *nondissipative* part

$$\mathbb{L}^{(nondis)} = \frac{1}{2} (\mathbb{L} - \mathbb{L}^t)$$

contains quantities exhibiting *quantization*  
at very low temperature !

- The *Hall conductivity* is nondissipative.  
It is quantized at  $T = 0$ .
- Quantization of currents in superconductors.

# WARNING: Coherence vs. Dissipation !

In *mesoscopic* systems, the quantization of conductance, thermal conductance, mechanical response, is due to the lack of dissipation.

The system is too small for the local equilibrium approximation to hold. The quantum dynamics is *coherent* and the transport is the result of interference effect

However, due to presence of *quenched disorder* the quantum dynamics is *diffusive* and mimicks the effect of dissipation. This is why it is still possible to measure transport coefficients.

## IV - Kubo's Formula

# Quantum Evolution in Mesoscopic Cells

- *Observable algebra*  $\mathcal{A} = \mathcal{A}_S \otimes \mathcal{A}_E$   
( $S = \text{system}$ ,  $E = \text{environment}$ ).
- *Quantum evolution*  $\eta_t \in \text{Aut}(\mathcal{A})$ ,  
 $t \in \mathbb{R} \mapsto \eta_t(B) \in \mathcal{A}$  continuous  $\forall B \in \mathcal{A}$ .
- *Initial state*  $\rho \otimes \rho_E$
- *System evolution*

$$\rho(\Phi_t(A)) = \rho_t(A) = \rho \otimes \rho_E (\eta_t(A \otimes \mathbf{1}))$$

$\Phi_t : \mathcal{A}_S \mapsto \mathcal{A}_S$  is *completely positive*,  
 $\Phi_t(\mathbf{1}) = \mathbf{1}$  and  $t \mapsto \Phi_t(A) \in \mathcal{A}_S$  is continuous.

- *Markov approximation*: for  $\delta t$  mesoscopic

$$\Phi_{t+\delta t} \approx \Phi_t \circ \Phi_{\delta t} \approx \Phi_{\delta t} \circ \Phi_t$$

Then

$$\frac{\delta \Phi_t}{\delta t} = \mathfrak{L} \circ \Phi_t = \Phi_t \circ \mathfrak{L}$$

$\mathfrak{L}$  is the *Lindbladian*.

- *Dual evolution*  $\Phi_t^\dagger(\rho) = \rho \circ \Phi_t$  giving rise to  $\mathfrak{L}^\dagger$ .



**Theorem 1 (Lindblad '76)** *If  $\mathcal{A}_S = \mathcal{B}(\mathcal{H})$  and if  $\|\Phi_t - \mathbf{1}\| \xrightarrow{t \downarrow 0} 0$ , there is a bounded selfadjoint operator  $H$  on  $\mathcal{H}$  and a countable family of operators  $L_i$  such that*

$$\mathfrak{L}(A) = i[H, A] + \sum_i \left( L_i^\dagger A L_i - \frac{1}{2} \{L_i^\dagger L_i, A\} \right)$$

The first term of  $\mathfrak{L}$  is the *coherent part* and corresponds to a usual Hamiltonian evolution.

The second one, denoted by  $\mathfrak{D}(A)$  is the *dissipative part* and produces damping.

- *Stationary* states correspond to solutions of  $\mathfrak{L}^\dagger \rho = 0$ .
- *Equilibrium* states are stationary states with maximum entropy. They are equivalent to *KMS* states with respect to the dynamics generated by  $H + \sum_{\alpha=2}^K F_\alpha \hat{X}_\alpha$ .

# Out of Equilibrium

1. The system is *out of equilibrium* when both the temperature and the chemical potential *vary slowly* in *time* and *space*.
2. The dynamics in a *mesoscopic cell* is then modified according to

$$\beta(\vec{x}; t) \simeq \beta + \vec{\nabla} \beta(t) \cdot \vec{x}$$

and similarly for the chemical potential.

3. The position  $\vec{x}$  multiplies some operators (particle number or energy) leading to *position operator contributions* in the perturbed Gibbs Hamiltonian and in the dissipative part.

**Ex.:**

$$\beta(\vec{x}; t)H \simeq \beta H + \vec{\nabla} \beta(t) \cdot \vec{x}H$$

The energy is localized at  $\vec{x}H = \vec{R}_u$  and ought to be *quantized* as well.

# Mesoscopic Currents

1. The charge position operator  $\vec{R}_e = (R_1, \dots, R_d)$  describes the position of charges in mesoscopic cells. It defines a *\*-derivation*  $\vec{\nabla}_e = i[\vec{R}_e, \cdot]$  on  $\mathfrak{A}$  generating a  $d$ -parameter group of \*-automorphisms.
2. The *mesoscopic electric current* is given by

$$\vec{J}_e = \frac{d\vec{R}_e}{dt} = \mathfrak{L}(\vec{R}_e) = \vec{\nabla}_e H - \mathfrak{D}(\vec{R}_e)$$

The first part corresponds to the *coherent part* the other to the *dissipative one*.

It defines a *\*-derivation* on  $\mathfrak{A}$ .

3. The electronic energy can also be localized through an energy position operator  $\vec{R}_u$ . Correspondingly the *mesoscopic energy current* is given by

$$\vec{J}_u = \frac{d\vec{R}_u}{dt} = \mathfrak{L}(\vec{R}_u) = \vec{\nabla}_u H - \mathfrak{D}(\vec{R}_u)$$

It also defines a *\*-derivation* on  $\mathfrak{A}$ .

# Derivation of Greene-Kubo Formulæ

(DC-conductivities)

1. At time  $t = 0$  the system is at equilibrium. At  $t > 0$  *forces* are switched on

$$\mathcal{E} = (\vec{\mathcal{E}}_e, \vec{\mathcal{E}}_u) \quad \vec{\mathcal{E}}_e = -\vec{\nabla}\mu \quad \vec{\mathcal{E}}_u = -\vec{\nabla}T$$

so that

$$\mathfrak{L}_{\mathcal{E}} = \mathfrak{L} + \sum_{\alpha,j} \mathcal{E}_{\alpha}^j \mathfrak{L}_{\alpha}^j + O(\mathcal{E}^2)$$

2. Hence the current becomes

$$J_{\alpha}^{\mathcal{E},i} = J_{\alpha}^i + \sum_{\alpha',j} \mathcal{E}_{\alpha'}^j \mathfrak{L}_{\alpha'}^j(R_{\alpha}^i) + O(\mathcal{E}^2)$$

3. Then, if the forces are constant in time

$$\begin{aligned} \vec{j}_{\alpha} &= \lim_{t \uparrow \infty} \int_0^t \frac{ds}{t} \rho_{eq.} \left( e^{s\mathfrak{L}_{\mathcal{E}}} \vec{j}_{\alpha}^{\mathcal{E}} \right) \\ &= \lim_{\epsilon \downarrow 0} \int_0^{\infty} \epsilon dt e^{-t\epsilon} \rho_{eq.} \left( e^{t\mathfrak{L}_{\mathcal{E}}} \vec{j}_{\alpha}^{\mathcal{E}} \right) \\ &= \lim_{\epsilon \downarrow 0} \rho_{eq.} \left( \frac{\epsilon}{\epsilon - \mathfrak{L}_{\mathcal{E}}} \vec{j}_{\alpha}^{\mathcal{E}} \right) \end{aligned}$$

4. Since  $\mathfrak{L}^\dagger \rho_{eq.} = 0$ ,

$$\rho_{eq.} \left( \frac{\epsilon}{\epsilon - \mathfrak{L}} \vec{J}_\alpha \right) = 0$$

5. Thus

$$\begin{aligned} \vec{j}_\alpha &= \lim_{\epsilon \downarrow 0} \rho_{eq.} \left( \frac{\epsilon}{\epsilon - \mathfrak{L}_\mathcal{E}} \vec{J}_\alpha^\mathcal{E} - \frac{\epsilon}{\epsilon - \mathfrak{L}} \vec{J}_\alpha \right) \\ &= \lim_{\epsilon \downarrow 0} \rho_{eq.} \left( \frac{\epsilon}{\epsilon - \mathfrak{L}} \sum_{\alpha'} \vec{\mathcal{E}}_{\alpha'} \cdot \vec{\mathfrak{L}}_{\alpha'} \frac{1}{\epsilon - \mathfrak{L}_\mathcal{E}} \vec{J}_\alpha \right) \\ &\quad + \lim_{\epsilon \downarrow 0} \rho_{eq.} \left( \frac{\epsilon}{\epsilon - \mathfrak{L}} \sum_{\alpha'} \vec{\mathcal{E}}_{\alpha'} \cdot \vec{\mathfrak{L}}_{\alpha'}(\vec{R}) \right) \\ &\quad + O(\mathcal{E}^2) \end{aligned}$$

6. Since  $\rho_{eq.} \circ \mathfrak{L} = 0$  this gives

$$\begin{aligned} \vec{j}_\alpha &= - \sum_{\alpha'} \vec{\mathcal{E}}_{\alpha'} \rho_{eq.} \left( \vec{\mathfrak{L}}_{\alpha'} \frac{1}{\mathfrak{L}} \vec{J}_\alpha + \vec{\mathfrak{L}}_{\alpha'}(\vec{R}) \right) \\ &\quad + O(\mathcal{E}^2) \end{aligned}$$

7. In particular

$$\vec{j}_\alpha^i = \sum_{\alpha', j} L_{\alpha, \alpha'}^{i, j} \mathcal{E}_{\alpha'}^j + O(\mathcal{E}^2)$$

where the *Onsager coefficients*  $L_{\alpha, \alpha'}^{i, j}$  are given by the *Greene-Kubo* formula

$$L_{\alpha, \alpha'}^{i, j} = -\rho_{eq.} \left( \mathfrak{L}_{\alpha'}^j \frac{1}{\mathfrak{L}} J_\alpha^i + \mathfrak{L}_{\alpha'}^j (R_\alpha^i) \right)$$

### Remark:

1. Each term containing  $\mathfrak{L}$  have a coherent and dissipative part. The equilibrium current vanishing, the previous formula contains *five terms* with distinct physical meaning.
2. AC-conductivity at frequency  $\omega$  can also be obtained using a Floquet type approach (*Schulz-Baldes, Bellissard '98*)

$$L_{\alpha, \alpha'}^{i, j}(\omega) = -\rho_{eq.} \left( \mathfrak{L}_{\alpha'}^j \frac{1}{\mathfrak{L} + i\hbar\omega} J_\alpha^i + \mathfrak{L}_{\alpha'}^j (R_\alpha^i) \right)$$

# Validity of Greene-Kubo Formulæ

The previous derivation is formal. Various conditions must be assumed.

- The explicit expressions for  $\mathfrak{L}$  and the  $\vec{\mathfrak{L}}_{\alpha'}$ 's are *model dependent*.
- It is necessary to prove that  $\mathfrak{L}_{\mathcal{E}}(\vec{R}) \in \mathcal{A}_S$ .
- The *inverse* of  $\mathfrak{L}$  is not *a priori* well defined.

However, the dissipative part  $\mathfrak{D}$  is usually responsible for the existence of the inverse. This is because

$$\text{Spec}(i[H, \cdot]) \subset i\mathbb{R}$$

while  $\mathfrak{D}$  gives a *non zero real part* to eigenvalues. In the *Relaxation Time Approximation*,

$$\mathfrak{D}(A) = A/\tau \quad \Rightarrow \quad \text{Spec}\left(i[H, \cdot] + \frac{\mathbf{1}}{\tau}\right) \subset i\mathbb{R} + \frac{1}{\tau}$$

where  $\tau$  is the *relaxation time*.

# V - Aperiodic Solids

J. BELLISSARD, D. HERMMANN, M. ZARROUATI,  
*Hull of Aperiodic Solids and Gap Labelling Theorems,*  
*in Directions in Mathematical Quasicrystals,*  
CRM Monograph Series, Volume **13**, (2000), 207-259,  
M. B. Baake & R. V. Moody Eds., AMS Providence.



# Aperiodic Materials

1. *Perfect crystals* in  $d$ -dimensions:  
translation and crystal symmetries.  
Translation group  $\mathcal{T} \simeq \mathbb{Z}^d$ .
2. *Crystals in a Uniform Magnetic Field*; magnetic oscillations, Shubnikov-de Haas, de Haas-van Alfen.  
The magnetic field breaks the translation invariance to give some quasiperiodicity.
3. *Quasicrystals*: no translation symmetry, but icosahedral symmetry. Ex.:
  - (a) **Al<sub>62.5</sub>Cu<sub>25</sub>Fe<sub>12.5</sub>**;
  - (b) **Al<sub>70</sub>Pd<sub>22</sub>Mn<sub>8</sub>**;
  - (c) **Al<sub>70</sub>Pd<sub>22</sub>Re<sub>8</sub>**;
4. *Disordered media*: random atomic positions
  - (a) Normal metals (with defects or impurities);
  - (b) Alloys
  - (c) Doped semiconductors (**Si**, **AsGa**, ...);

# 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 two points of  $\mathcal{L}$ .
4. A *Delone* set:  
 $\mathcal{L}$  is uniformly discrete and relatively dense.
5. A *Meyer* set:  
 $\mathcal{L}$  and  $\mathcal{L} - \mathcal{L}$  are Delone sets.

# 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.

# Point Measures

$\mathfrak{M}(\mathbb{R}^d)$  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  $\mathbb{R}^d$

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

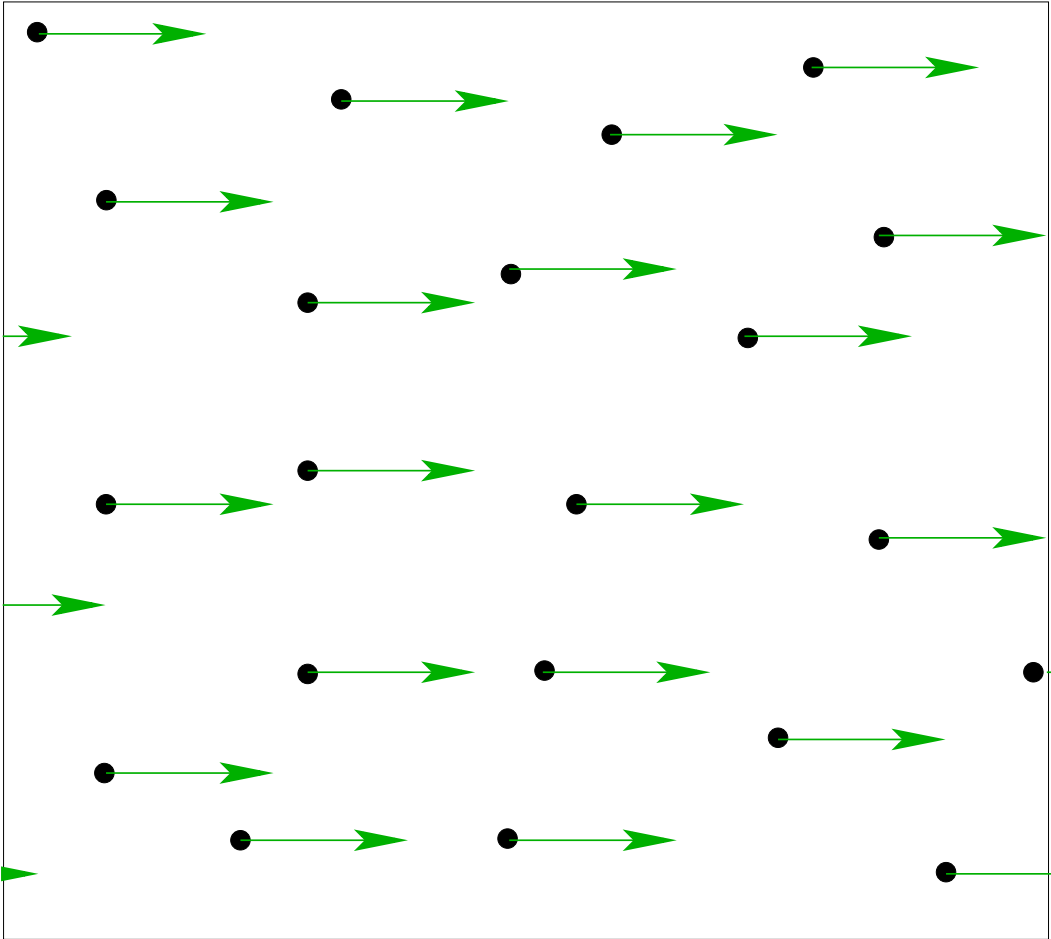
The *Hull* is the closure in  $\mathfrak{M}(\mathbb{R}^d)$

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

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

## Facts:

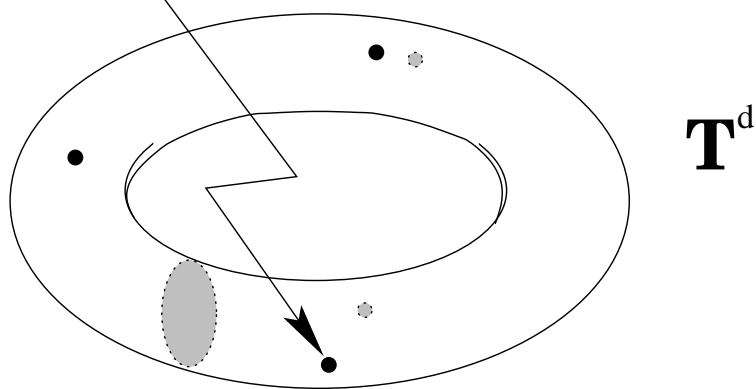
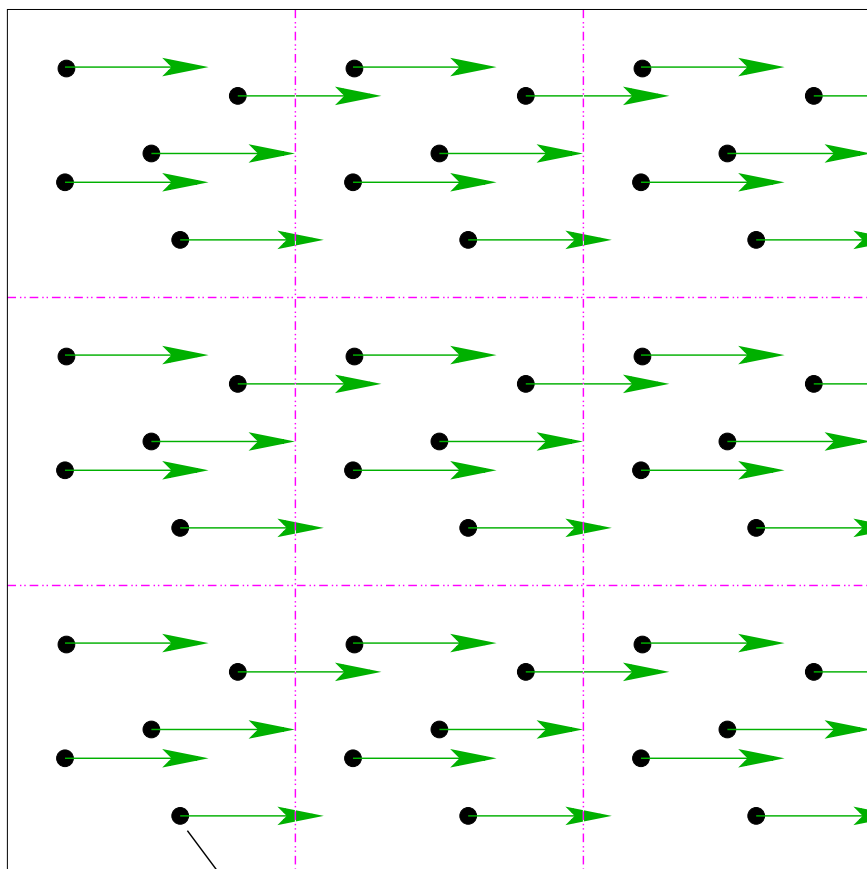
1.  $\Omega$  is compact and  $\mathbb{R}^d$  acts by homeomorphisms.
2. If  $\omega \in \Omega$ , there is a uniformly discrete point set  $\mathcal{L}_\omega$  in  $\mathbb{R}^d$  such that  $\omega$  coincides with  $\nu_\omega = \nu^{\mathcal{L}_\omega}$ .
3. If  $\mathcal{L}$  is *Delone* (resp. *Meyer*) so are the  $\mathcal{L}_\omega$ 's.



Building the Hull

# Examples of Hulls

1. *Crystals* :  $\Omega = \mathbb{R}^d / \mathcal{T} \simeq \mathbb{T}^d$  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  $\mathfrak{A}$  be a finite set (*alphabet*) indexing the types of impurities. One sets  $\Xi = \mathfrak{A}^{\mathcal{L}}$  with  $\mathbb{Z}^d$ -action given by shifts. Then  $\Omega$  is the mapping torus of  $\Xi$ .



The Hull of a Periodic Lattice  
and its transversal

# The Canonical Transversal

Definition

$$\Xi = \{\omega \in \Omega; 0 \in \mathcal{L}_\omega\}$$

It is a closed transversal. Then

$$\mathcal{L}_\omega = \text{Orb}(\omega) \cap \Xi,$$

if the orbit of  $\omega$  is identified with  $\mathbb{R}^d$ .

The *groupoid* of this transversal will be denoted by  $\Gamma_\Xi$   
Elements of  $\Gamma_\Xi$  are *arrows*

$$\gamma = (\omega, a) \in \Xi \times \mathbb{R}^d \quad \mathbb{T}^{-a}\omega \in \Xi$$

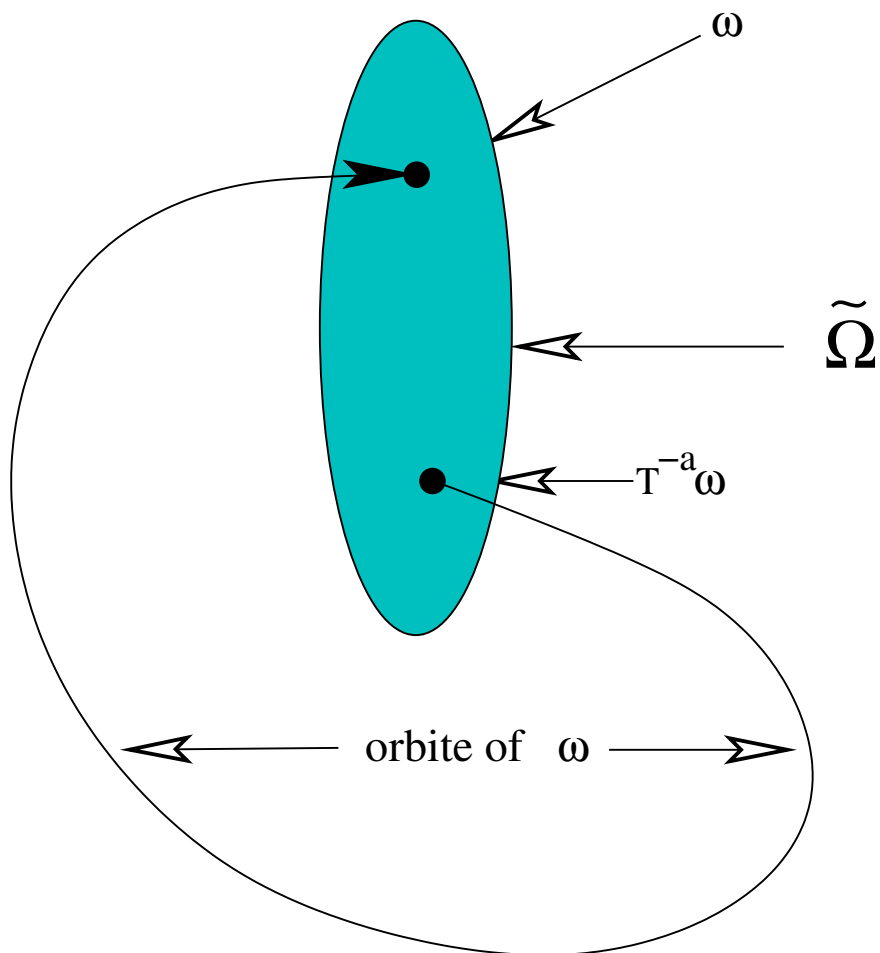
with *range* and the *source* are

$$r(\gamma) = \omega \in \Xi \quad s(\gamma) = \mathbb{T}^{-a}\omega \in \Xi$$

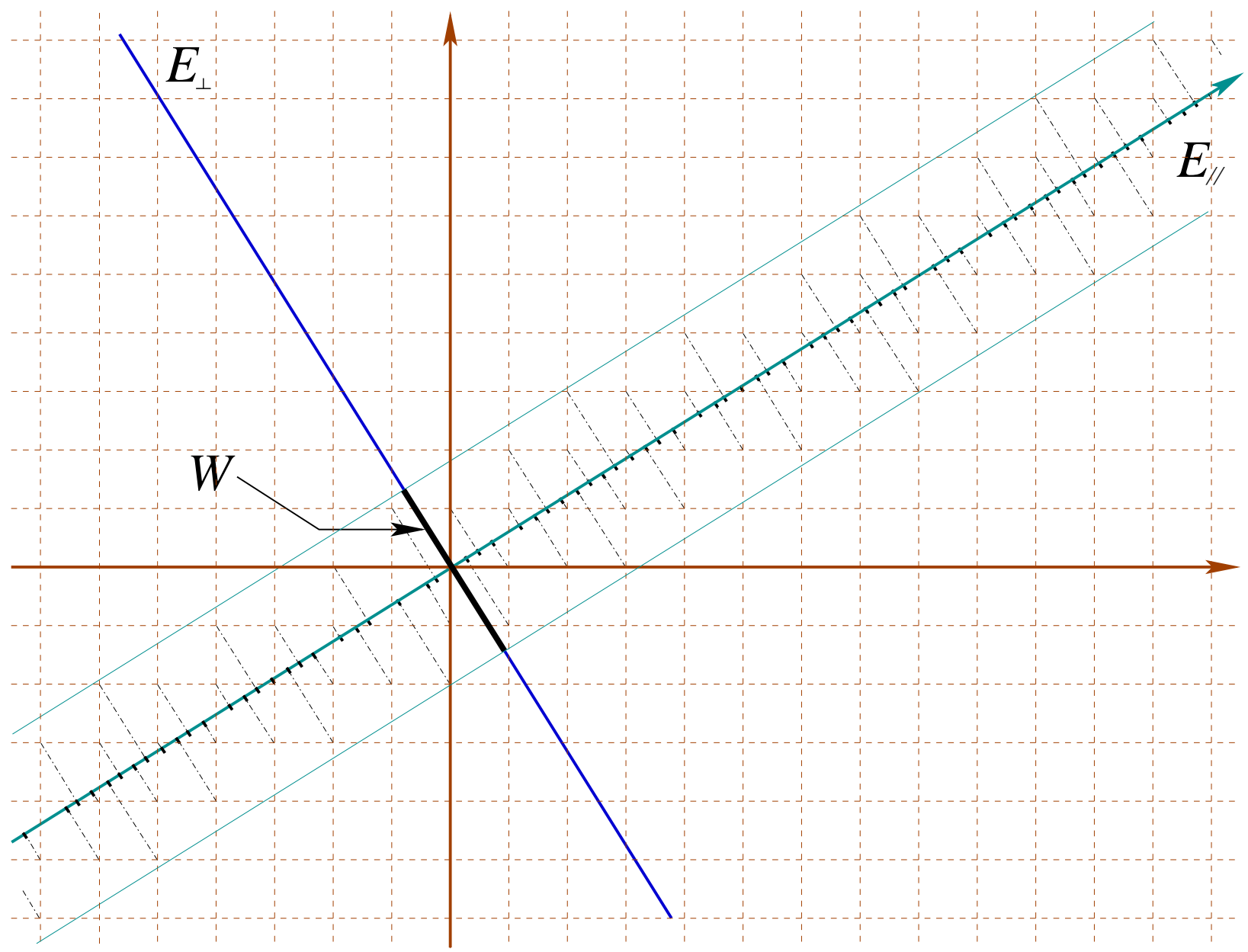
*composition* and *inverse*

$$(\omega, a) \circ (\mathbb{T}^{-a}\omega, b) = (\omega, a) \quad (\omega, a)^{-1} = (\mathbb{T}^{-a}\omega, -a)$$

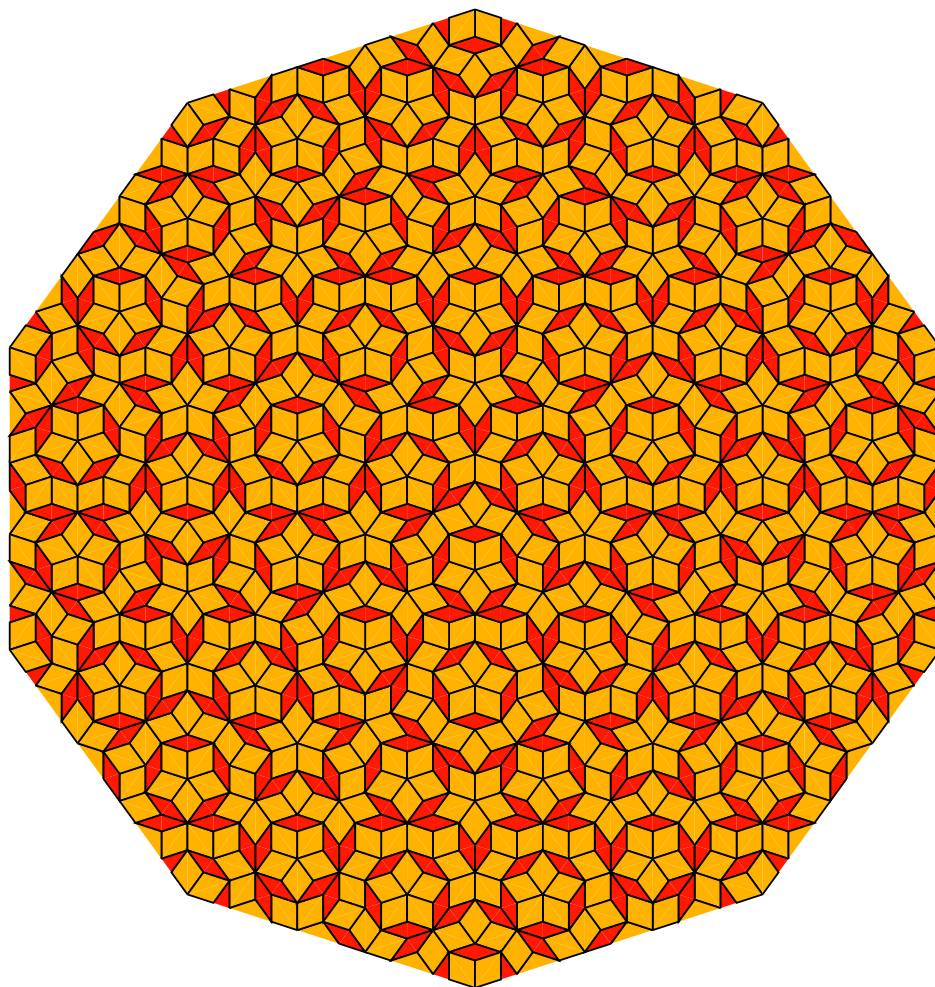




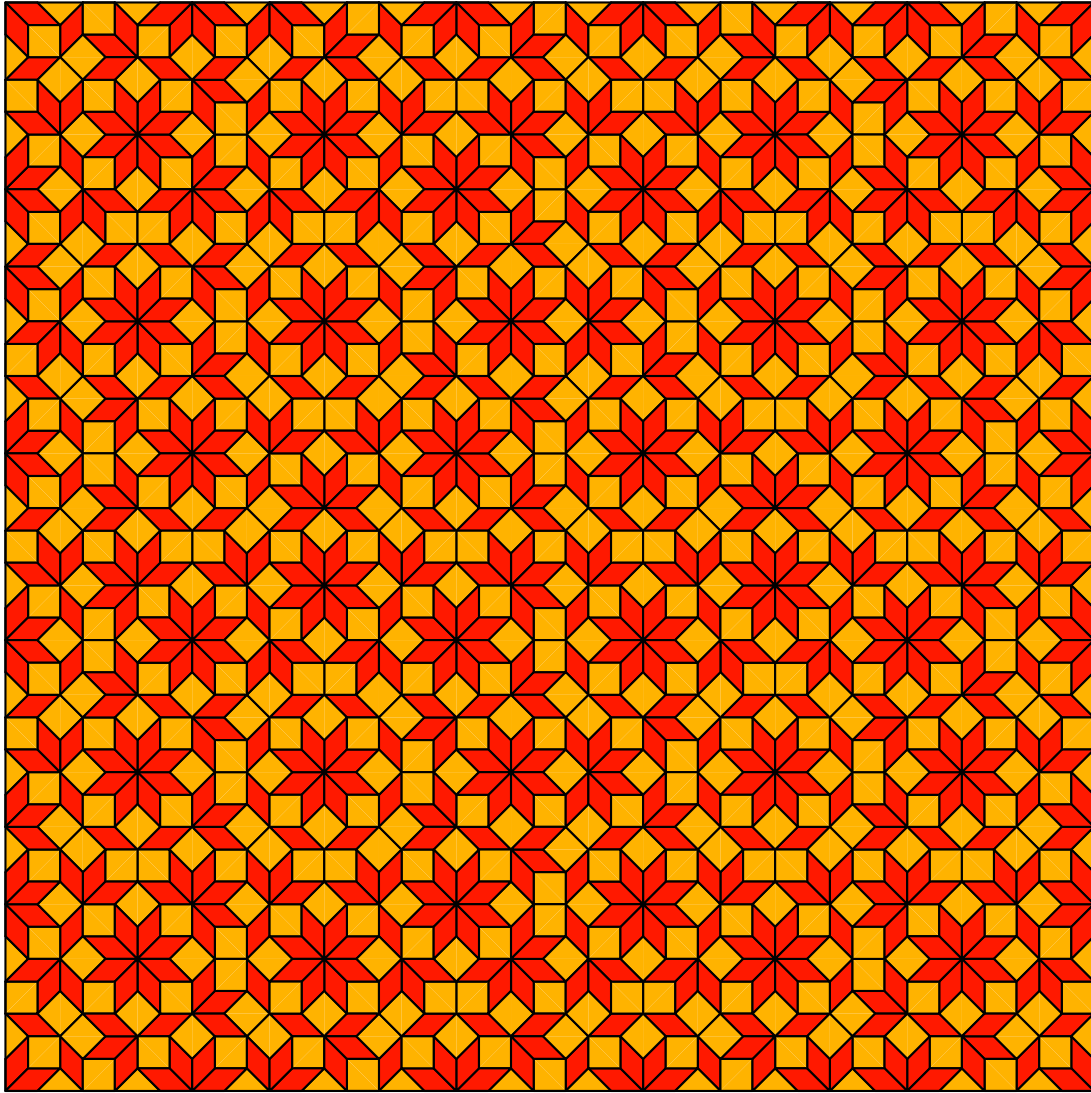
### Transversal and Groupoid Arrows



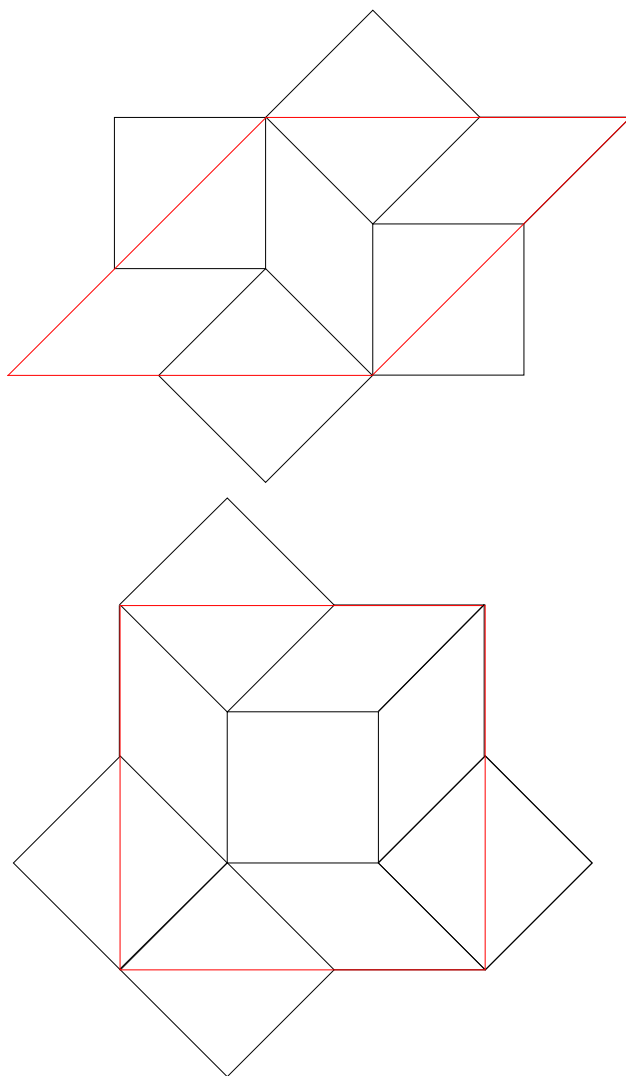
– The cut-and-project construction –



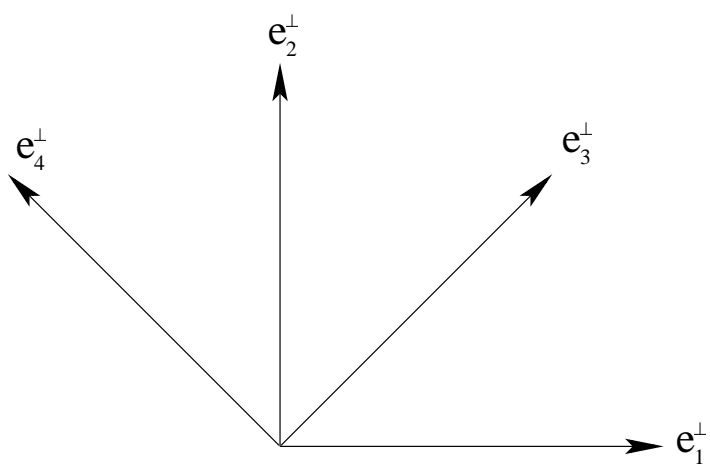
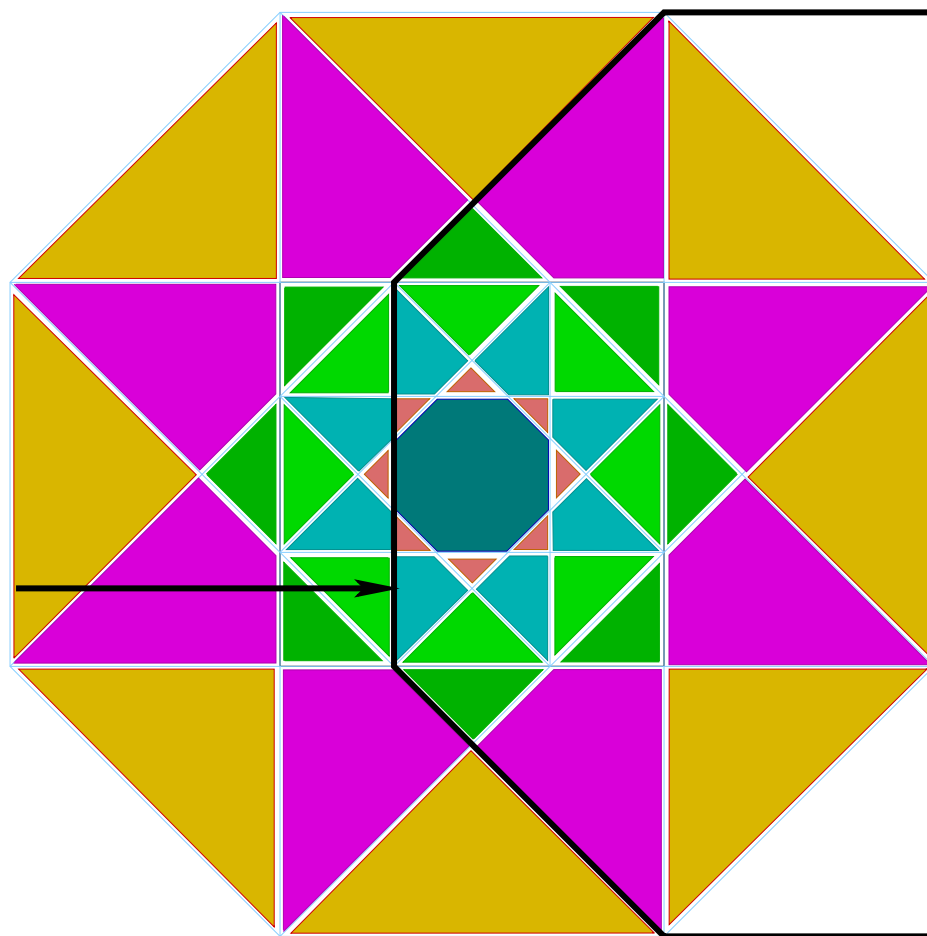
**The Penrose tiling**



The octagonal tiling



**Inflation rules for the octagonal tiling**



**The transversal of the Octagonal Tiling  
is completely disconnected**

# Diffraction

The diffraction intensity of a sample in box  $\Lambda$  is proportionnal to the diffraction measure :

$$I_{\Lambda}(k) = \frac{1}{|\Lambda|} \left| \sum_{x \in \Lambda \cap \mathcal{L}} e^{i\langle k|x \rangle} \right|^2$$

Its Fourier transform defines the *diffraction measure*

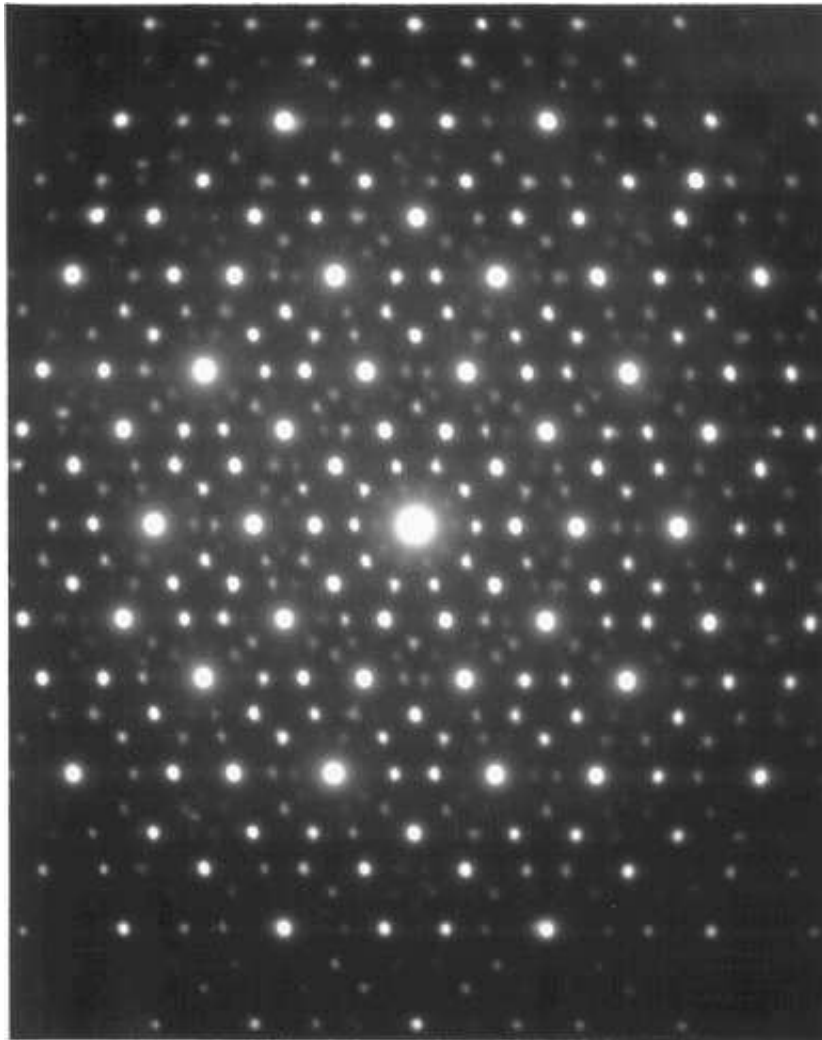
$$\rho_{\Lambda}(f) = \int d^d k I_{\Lambda}(k) \tilde{f}(k) = \frac{1}{|\Lambda|} \sum_{x, y \in \Lambda \cap \mathcal{L}} f(x - y)$$

## Facts:

1. For every probability measure  $\mathbb{P}$  on the hull, translation invariant and ergodic, there is a unique measure  $\rho$  on  $\mathbb{R}^d$  such that for  $\mathbb{P}$ -almost every  $\mathcal{L}$ 's (vaguely)

$$\rho_{\Lambda} \rightarrow \rho$$

2. Both  $\rho$  and its Fourier transform are positive measures on  $\mathbb{R}^d$ .



A typical T.E.M. diffraction picture  
for quasicrystals



# Bloch Theory (Periodic Lattices)

If  $\mathcal{L}$  is a point set, the *Voronoi cell* of  $x \in \mathcal{L}$  is the set of points closer to  $x$  than to any  $y \in \mathcal{L}$ .

If  $\mathcal{L}$  is *periodic*, with period group  $G$ , the Voronoi cell of any site is called the *Wigner-Seitz cell*.

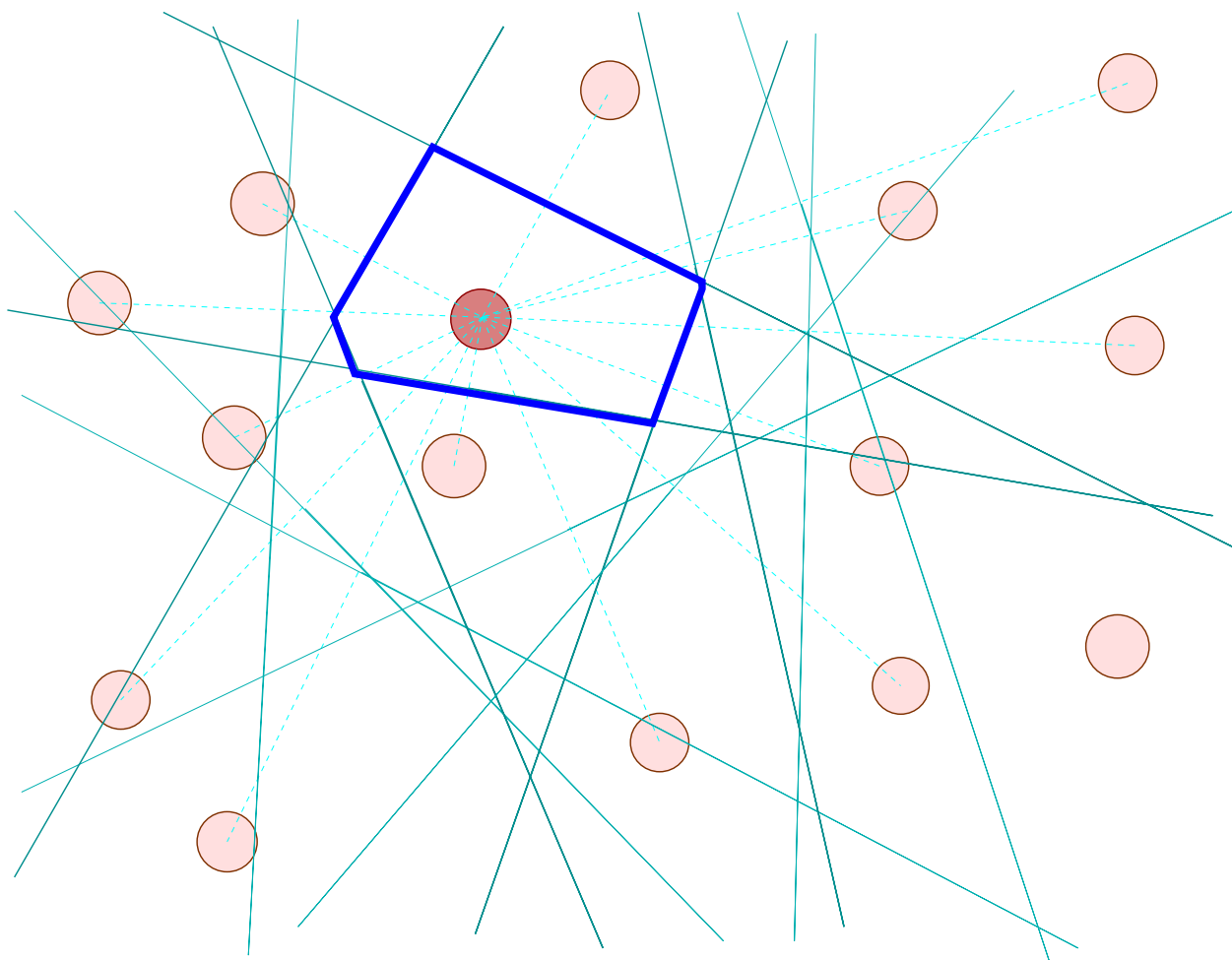
The *reciprocal lattice* is the orthogonal  $G^\perp$  of  $G$  in the momentum space  $\hat{\mathbb{R}}^d$ .

The Voronoi cell of  $0 \in G^\perp$  is the *Brillouin zone*. Using periodic boundary conditions, it is

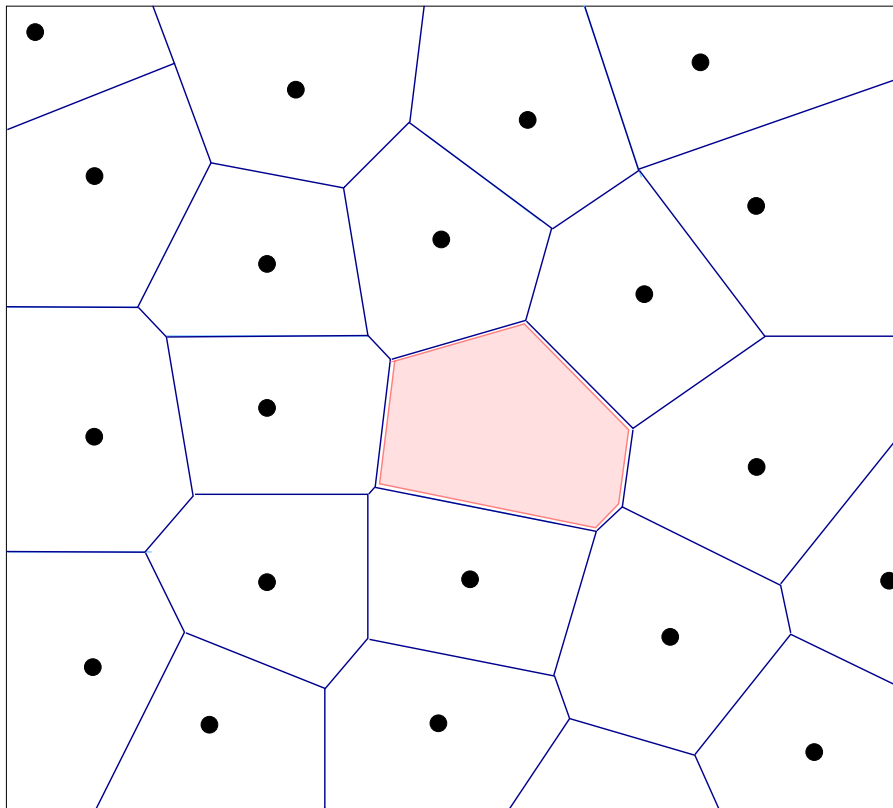
$$\mathbb{B} = \hat{\mathbb{R}}^d / G^\perp \simeq \mathbb{T}^d$$

$\mathbb{B}$  is a (smooth) manifold. Its topology can be reconstructed from  $\mathcal{C}(\mathbb{B})$ . Its differential structure from  $\mathcal{C}^\infty(\mathbb{B})$ .

$\mathcal{C}(\mathbb{B})$  is a *commutative  $C^*$ -algebra* .



**Construction of a Voronoi cell**



Voronoi's Cells of  $\mathcal{L}$

# The Noncommutative Brillouin Zone

## Question:

Is there a group of unitaries  $\{T(a); a \in \mathbb{R}^d\}$  such that

$$T(a) F T(a)^{-1} = F \circ T^{-a} \quad \forall F \in \mathcal{C}(\Omega) \quad ? \quad (1)$$

**Answer:** The *crossed product* is the smallest  $C^*$ -algebra generated by  $\mathcal{C}(\Omega)$  and by smooth functions  $\int_{\mathbb{R}^d} d^d a g(a) T(a)$  of  $T$  satisfying (1) and  $g \in L^1(\mathbb{R}^d)$ .

$$\mathcal{A} = \mathcal{C}(\Omega) \rtimes \mathbb{R}^d$$

## Facts:

1. For a perfect crystal  $\mathcal{A}$  is isomorphic to  $\mathcal{C}(\mathbb{B}) \otimes \mathcal{K}$ , where  $\mathcal{K}$  is the  $C^*$ -algebra generated by finite dimensional matrices.
2. If the solid is not periodic,  $\mathcal{A}$  is non commutative in a non trivial way (*it is type II*).

By analogy with perfect crystals, we propose:

**Definition 1** *The NC topological space associated with  $\mathcal{A} = \mathcal{C}(\Omega) \rtimes \mathbb{R}^d$  is called the Non Commutative Brillouin zone (NCBZ).* □

# Noncommutative Calculus

1.  $\mathcal{A}$  is generated by functions  $A(\omega, x)$  on  $\Omega \times \mathbb{R}^d$  continuous with compact support (the sub-algebra  $\mathcal{A}_0$ ):

2. *Product*

$$A \cdot B(\omega, x) = \int_{\mathbb{R}^d} d^d y A(\omega, y) B(\mathbb{T}^{-x}\omega, x - y)$$

3. *Adjoint*

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

4. *Derivative* with  $(x = (x_1, \dots, x_d) \in \mathbb{R}^d)$

$$(\partial_i A)(\omega, x) = ix_i A(\omega, x)$$

$$\Rightarrow \partial_i(AB) = (\partial_i A)B + A(\partial_i B)$$

5.  $\mathcal{A}_0$  acts on  $\mathcal{H} = L^2(\mathbb{R}^d)$  with matrix elements

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

(a)  $(A \cdot B)_\omega = A_\omega B_\omega$  and  $(A^*)_\omega = A_\omega^*$

(b) *Covariance*:

$$T(a)A_\omega T(a)^{-1} = A_{T^a\omega}$$

(c) *Strong continuity*:  $\omega \in \Omega \mapsto A_\omega \psi \in \mathcal{H}$  is continuous (if  $\psi \in \mathcal{H}$ ).

6. A  *$C^*$ -norm* is defined by:

$$\|A\| = \sup_{\omega \in \Omega} \|A_\omega\|$$

$\mathcal{A}$  is the completion of  $\mathcal{A}_0$  *w.r.t.* this norm.

7. If  $\vec{\nabla} = (\partial_1, \dots, \partial_d)$  and  $\vec{X} = (X_1, \dots, X_d)$  is the position operator acting on  $\mathcal{H}$  then:

$$(\vec{\nabla} A)_\omega = i[\vec{X}, A_\omega]$$

8. For any  $\mathbb{R}^d$ -invariant, ergodic probability measure  $\mathbb{P}$  on the Hull  $\Omega$ , integration over the Brillouin Zone is given by a *trace*  $\mathcal{T}_{\mathbb{P}}$  on  $\mathcal{A}_0$  given by

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

It is the *trace per unit volume*

$$\mathcal{T}_{\mathbb{P}}(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \int_{\Lambda} d^d x \operatorname{Tr} (A_\omega \upharpoonright_{\Lambda}) \quad \mathbb{P}\text{-a.e } \omega$$



# Schrödinger's Operator

The Hamiltonian describing the electronic motion in  $\mathcal{L}$ , is the Schrödinger operator (ignoring interactions)

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{y \in \mathcal{L}} v(\cdot - y) .$$

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

- $\mathcal{L}$  is the set of atomic positions,
- $v \in L^1(\mathbb{R}^d)$  is the effective potential for valence electrons near an atom.

By taking limit points of translated such operators, we get a covariant and strong resolvent continuous family  $H_\omega$  of self adjoint operators obtained by replacing  $\mathcal{L}$  by  $\mathcal{L}_\omega$ .

**Theorem 2** *The resolvent  $(z - H_\omega)^{-1} = \pi_\omega(R(z))$  is the representative of an element  $R(z) \in \mathcal{A}$ . For all  $\omega \in \Omega$  with dense orbit,  $H_\omega$  has same spectrum  $\Sigma$  (as a set) as  $H$ .*

# Density of States

1. The function (defined for  $\mathbb{P}$ -a.e.  $\omega$ ),

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

is called the *integrated density of states* (IDS).

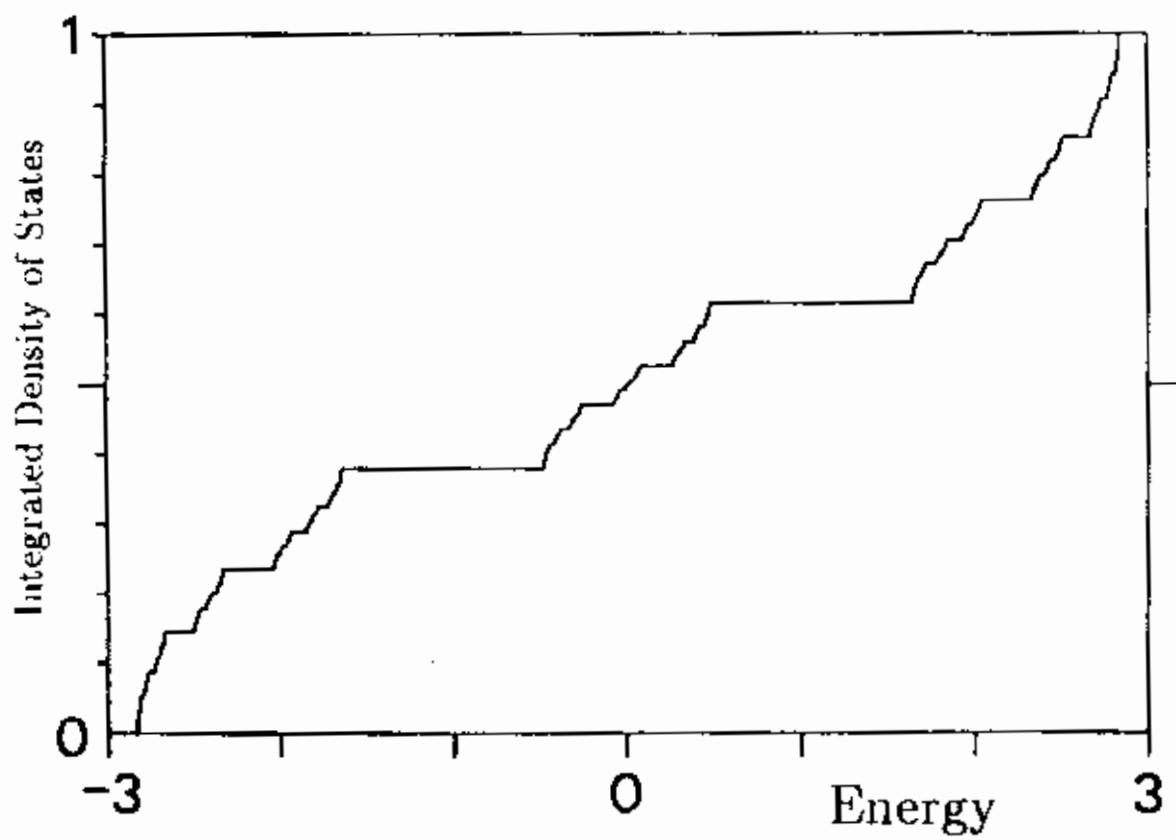
2. It is given by (*Shubin '76, JB '86 & '93*)

$$\mathcal{N}_{\mathbb{P}}(E) = \mathcal{T}_{\mathbb{P}} (\chi(H \leq E))$$

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

3.  $\mathcal{N}_{\mathbb{P}}$  is non decreasing, non negative and constant on gaps.  $\mathcal{N}_{\mathbb{P}}(E) = 0$  for  $E < \inf \Sigma$ . For  $E \rightarrow \infty$   $\mathcal{N}_{\mathbb{P}}(E) \sim \mathcal{N}_0(E)$  where  $\mathcal{N}_0$  is the IDS of the free case (namely  $V = 0$ ).

4.  $d\mathcal{N}_{\mathbb{P}}/dE = n_{\text{DOS}}$  defines a Stieljes measure called the *density of States* (DOS).



An example of IDS

# Current-Current Correlations

1. The coherent velocity operator nothing but  $d\vec{X}/dt = \imath[H, \vec{X}]/\hbar$ .

The electric current is just the velocity times the charge of the carriers

$$\vec{J} = \frac{-\imath e}{\hbar} [H, \vec{X}] = \frac{e}{\hbar} \vec{\nabla} H$$

2. If  $f, g \in \mathcal{C}_0(\mathbb{R})$  then there is a Borel measure  $m_2$  on  $\mathbb{R}^2$ , called the *current-current correlation* such that

$$\int_{\mathbb{R}^2} m_2(dE, dE') f(E) g(E') = \mathcal{T}_{\mathbb{P}} \left( f(H) \vec{\nabla} H g(H) \vec{\nabla} H \right)$$

3. If  $\mathcal{L}_H = \imath[H, \cdot]$  acting on the GNS-representation of  $\mathcal{T}_{\mathbb{P}}$ , then

$$\mathcal{T}_{\mathbb{P}} \left( \vec{\nabla} H e^{t\mathcal{L}_H} (\vec{\nabla} H) \right) = \int_{\mathbb{R}^2} m_2(dE, dE') e^{\imath t(E-E')}$$

4. What are the regularity properties of the current-current correlation ?

*Very few results are available. One result is*

**Theorem 3 (Hislop, J.B. '05)** *Let  $H$  be the Hamiltonian for the Anderson model on a lattice. If the on-site potential distribution is analytic, at high enough disorder the current-current correlation is absolutely continuous with analytic density in the complement of a small open neighbourhood of the diagonal  $\{(E, E') \in \mathbb{R}^2; E = E'\}$ .*

It is expected that in the localization regime,  $m_2$  vanishes near the diagonal like  $(E - E')^2 \ln^{d+1} |E - E'|$

*(A. KLEIN et al. '05)*

**Theorem 4 (J.B. '91 & 94)** *Let  $H$  be a selfadjoint element of the algebra  $C^*(\Gamma_{\Xi})$  where  $\Gamma_{\Xi}$  is the groupoid of the transversal of a uniformly discrete set. Then the localization length of states at energy  $E$  is an  $L^2$  function w.r.t. the DOS such that*

$$\int_{\Delta} \mathcal{N}(dE) \ell(E)^2 = \int_{\Delta \times \mathbb{R}} \frac{m_2(dE, dE')}{|E - E'|^2}$$

# Complements

1. *Phonons* and other degrees of freedom (*lacunæ, spins, etc.*) can be described using the Noncommutative Brillouin zone as well.
2. A natural choice of  $\mathbb{R}^d$ -invariant, ergodic probability measure  $\mathbb{P}$  on the Hull  $\Omega$ , is given by the *zero temperature limit* of the *Gibbs* measure describing the thermodynamical equilibrium of *atoms*.
3. It can be proved that, if the atoms interact through a 2-body potential, repulsive at short distance and attractive at large distance, such zero temperature Gibbs state is supported by Delone sets  
*(Radin & J.B. '06)*.
4. Using ergodicity of the zero temperature Gibbs state, it is possible to prove that with probability one the Hull of a configuration is the topological support of the Gibbs state  
*(Hermmann, Zarrouati & J.B. '00)*.

## VI - Coherent Transport

J. BELLISSARD, *Coherent and dissipative transport in aperiodic solids*,  
in *Dynamics of Dissipation*, pp. 413-486, Lecture Notes in Physics, 597, Springer (2002).  
P. Garbaczewski, R. Olkiewicz (Eds.).

# What is Coherent Transport ?

Coherent transport corresponds to charge transport (*electrons* or *holes*) ignoring dissipation sources such as *electron-phonon* or *electron-electron* interactions.

1. The *independent electrons* approximation is justified.
2. One-particle Hamiltonian  $H$  is sufficient.
3. Measures associated with  $H$ :
  - (a) The *density of state* (DOS)
  - (b) Its *spectral measure* associated with a given state  $\psi$  in the Hilbert space.  
If  $\psi$  is localized in space, the spectral measure is called *local density of state* (LDOS)
  - (c) The *current-current correlation* (CCC) describes transport properties.



# Local Exponents

Given a positive measure  $\mu$  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  $\Delta$  a Borel subset of  $\mathbb{R}$ :

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

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

# Fractal Exponents

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

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

1.  $D_{\mu, \Delta}^{\pm}(q)$  is a non decreasing function of  $q$ .
2.  $D_{\mu, \Delta}^{\pm}(q)$  is **NOT** an invariant of the measure class, in general.
- 3.(a) If  $\mu$  is *ac* on  $\Delta$  then  $D_{\mu, \Delta}^{\pm}(q) = 1$ .  
 (b) If  $\mu$  is *pp* on  $\Delta$  then  $D_{\mu, \Delta}^{\pm}(q) = 0$ .

# 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  $H_\omega$  relative to a vector  $\varphi \in \mathcal{H}$ .
2. The corresponding local exponent is obtained after maximizing (+) or minimizing (-) over  $\varphi$ . It is denoted  $\alpha_{\text{LDOS}}^\pm$ . It is  $\mathbb{P} - a. s.$  independent of  $\omega$ .
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  $\alpha_{\text{DOS}}^\pm$ .
5. Inequality :  $\alpha_{\text{LDOS}}^\pm(\Delta) \leq \alpha_{\text{DOS}}^\pm(\Delta)$  .
6. The fractal exponents for the LDOS are defined in the same way, provided we consider the average over  $\omega$  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  $H_\omega$ . Set

$$\vec{X}_\omega(t) = e^{itH_\omega} \vec{X} e^{-itH_\omega}$$

2. The averaged spread of a typical wave packet with energy in  $\Delta$  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. The transport exponent is the *spectral exponent* of the Liouvillian  $\mathcal{L}_H$  localized around energies in  $\Delta$  near the eigenvalue 0 (diagonal of the current-current correlation).

## 6. *Heuristic*

(a)  $\beta = 0 \rightarrow$  absence of diffusion  
(*ex: localization*)

(b)  $\beta = 1 \rightarrow$  ballistic motion  
(*ex: in crystals*)

(c)  $\beta = 1/2 \rightarrow$  quantum diffusion  
(*ex: weak localization*)

(d)  $\beta < 1 \rightarrow$  subballistic regime

(e)  $\beta < 1/2 \rightarrow$  subdiffusive regime  
(*ex: in quasicrystals*)

# Inequalities

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

$$\beta_p^\pm(\Delta) \geq \frac{\alpha_{\text{LDOS}}^\pm(\Delta)}{d}$$

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

$$\beta_p^\pm(\Delta) \geq \frac{1}{d} D_{\text{LDOS},\Delta}^\pm\left(\frac{d}{d+p}\right)$$

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. Jacobi matrices (1D chains): position operator defined by spectral measure  $\Rightarrow$  transport exponents should be defined through the spectral ones.
2. For Jacobi matrices of a Julia set, with  $\mu$  the  $\sigma$ -balanced measure (*Barbaroux, Schulz-Baldes '99*)

$$\beta_p^+ \leq D_\mu(1-p) \quad \text{for all } 0 \leq p \leq 2$$

3. If  $H_1, \dots, H_d$  are Jacobi matrices,  $\eta_1, \dots, \eta_d$  are positive numbers and if

$$H^{(\eta)} = \sum_{j=1}^d \eta_j \mathbf{1} \otimes \dots \otimes H_j \otimes \dots \otimes \mathbf{1}$$

Then (*Schulz-Baldes, Bellissard '00*)

$$\beta_p^+(H^{(\eta)}) = \max_j \beta_p^+(H_j)$$

$$\alpha_{\text{LDOS}}(H^{(\eta)}) = \min\left\{1, \sum_j \alpha_{\text{LDOS}}(H_j)\right\}$$

for a.e.  $\eta$ . 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 matrix  $H_0$  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.*  $\eta$ .

*(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)*



## VII - Relaxation Time Approximation

J. BELLISSARD, *Coherent and dissipative transport in aperiodic solids*,  
in *Dynamics of Dissipation*, pp. 413-486, Lecture Notes in Physics, 597, Springer (2002).  
P. Garbaczewski, R. Olkiewicz (Eds.).

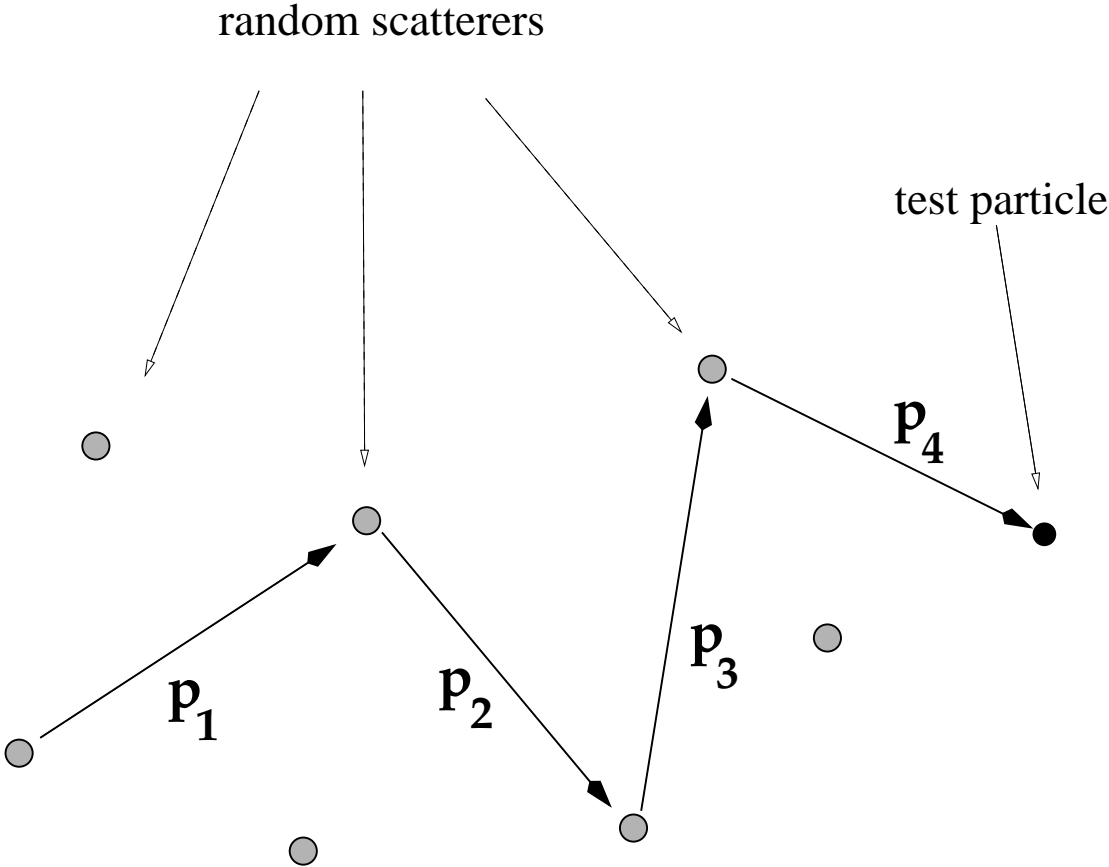
# The Drude Model (1900)

Hypothesis :

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

# Main Assumptions

1. Use the *Independent Electrons Approximation*
2. The one-particle Hamiltonian  $h$  for charge carriers is sufficient. For an aperiodic solid with Hull  $\Omega$ ,  $h = (h_\omega)_{\omega \in \Omega}$  is represented on  $\mathcal{H} = L^2(\mathbb{R}^d)$
3. The  $N$ -body Hilbert space is the Fermion Fock space built on the one-particle Hilbert space. The  $N$ -body Hamiltonian is the family  $H = (H_\omega)_{\omega \in \Omega}$  given by the second quantized

$$H_\omega = \sum_{i,j} \langle i | h_\omega | j \rangle f_i^* f_j$$

where  $\{|i\rangle; i \in I\}$  is an orthonormal basis of  $\mathcal{H}$  and the  $f_i, f_i^*$ 's are Fermion annihilation-creation operators

$$f_i f_j^* + f_j^* f_i = 2 \delta_{ij}$$

4. The equilibrium state is a *perfect Fermi gas* at inverse temperature  $\beta$  and chemical potential  $\mu$ . The  $n$ -point correlations  $\langle f_{i_1}^{\epsilon_1} \cdots f_{i_n}^{\epsilon_n} \rangle$  are given by the 2-point one through *Wick's theorem* and

$$\langle f_i^* f_j \rangle = \langle i | \frac{1}{\mathbf{1} + e^{\beta(h_\omega - \mu \mathbf{1})}} | j \rangle$$

5. *Ex.:* the charge carrier density is

$$\begin{aligned} n_{el} &= \lim_{\Lambda \uparrow \mathbb{R}^d} \frac{1}{|\Lambda|} \sum_{i,j} \langle f_i^* f_j \rangle \langle i | \chi_\Lambda | j \rangle \\ &= \mathcal{T}_{\mathbb{P}} \left\{ \frac{1}{\mathbf{1} + e^{\beta(h - \mu \mathbf{1})}} \right\} \end{aligned}$$

because the resolvent of  $h$  belongs to the *NCBZ*  $\mathcal{A}$  so that every continuous bounded function of  $h$  vanishing at infinity belongs to  $\mathcal{A}$ . Since  $h$  is bounded from below, the previous expression makes sense.

6. If  $\beta$  is fixed, *this expression defines*  $\mu$

# Kubo's formula (RTA)

1. Use the Drude model, but 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*  $\tau_{rel}$ . By a similar calculation the electric conductivity is then given by Kubo's formula:

$$\sigma_{i,j} = \frac{q^2}{\hbar} \mathcal{T}_{\mathbb{P}} \left( \partial_j \left( \frac{1}{1 + e^{\beta(\hbar - \mu)}} \right) \frac{1}{1/\tau_{rel} - \mathcal{L}_h} \partial_i \hbar \right)$$

- (a)  $q$  is the charge of the carriers,
- (b)  $\beta = 1/(k_B T)$  and  $\tau_{rel} \uparrow \infty$  as  $T \downarrow 0$ .
- (c)  $\mu$  is the chemical potential
- (d)  $\mathcal{L}_h = \iota/\hbar [h, \cdot]$  is the 1-particle *Liouville operator*

4. Using the current-current correlation the Kubo formula can be written as

$$\sum_{i=1}^d \sigma_{ii} = q^2 \int_{\mathbb{R}^2} \frac{m_2(dE, dE')}{\hbar/\tau_{rel} - i(E - E')} \frac{f_{\beta,\mu}(E) - f_{\beta,\mu}(E')}{E' - E}$$

where

$$f_{\beta,\mu}(E) = \frac{1}{1 + e^{\beta(E-\mu)}}$$

5. In the limit of zero temperature (where  $\beta, \tau_{rel} \uparrow \infty$ ), if  $m_2$  is absolutely continuous with density  $\tilde{\rho}$  then

$$\lim_{T \downarrow 0} \sum_{i=1}^d \sigma_{ii} = \text{const. } \tilde{\rho}(E_F, E_F)$$

where  $E_F$  is the *Fermi level*.

*Proving the existence and continuity of  $\tilde{\rho}$  with  $\tilde{\rho}(E_F, E_F) > 0$  is necessary and sufficient for the existence of a delocalized phase in the Anderson model.*

# Anomalous Drude formula (RTA)

1. The trace per unit volume  $\mathcal{T}_{\mathbb{P}}$  defines on  $\mathcal{A}$  a Hilbert-Schmidt inner product by

$$\langle A|B \rangle = \mathcal{T}_{\mathbb{P}}(A^*B) \quad A, B \in \mathcal{A}$$

The corresponding Hilbert space is called  $L^2(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$

2.  $\mathcal{L}_h$  is an *anti-selfadjoint* operator on  $L^2(\mathcal{A}, \mathcal{T}_{\mathbb{P}})$ .  $\Rightarrow (1/\tau_{rel} + \mathcal{L}_h)^{-1}$  is well-defined for  $\tau_{rel} > 0$ .
3. The *transport exponent*  $\beta_2$  for  $h$  becomes the *spectral exponent* for  $\mathcal{L}_h$  at eigenvalue 0.
4. as  $T \downarrow 0$ , the resolvent of  $\mathcal{L}_h$  is evaluated closer to the spectrum near 0. Then

(Mayou '92, Sire '93, Bellissard & Schulz-Baldes '95)

$$\sigma \stackrel{T \downarrow 0}{\sim} \tau_{rel}^{2\beta_F - 1} \quad \text{anomalous Drude formula}$$

where  $\beta_F$  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 might be incorrect however at low temperature.
4. If  $\beta_F = 1/2$  (*quantum diffusion*),  $\sigma \sim const.$ : residual conductivity at low temperature.  
*Ex.:* Random Matrix theory, Wegner  $n$ -orbital model  
(*P. Neu, R. Speicher '95, Bellissard & Schulz-Baldes '98*)
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*.

# Conductivity in Quasicrystals

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

1. LMTO *ab initio* computations for  $i - AlCuCo$  give  $\beta_F = 0,375$
2. If only electron-phonon collisions are considered, *Bloch's law* leads to :  $\tau \stackrel{T \downarrow 0}{\sim} T^{-5}$ .
3. Hence

$$\sigma(T) \stackrel{T \downarrow 0}{\sim} T^{1.25}$$

*compatible with experimental results !*

4. Why a *residual conductivity* in certain cases ?

# A Possible Mechanism: Quantum Chaos

1. Numerical simulations performed for the octagonal lattice exhibit level repulsion and Wigner-Dyson's distribution (*Zhong et al. 1998*).
2. For a sample of size  $L$  :  
 Mean level spacing  $\Delta \sim L^{-D}$ .  
 Thus Heisenberg time  $\tau_H \sim L^D$ .
3. Thouless time for anomalous diffusion  $L \sim t_{Th}^\beta$ .  
 Heisenberg's length  $L_H \sim L^{D\beta}$ .
4. Thus :
  - (a) if  $\beta > 1/d$  level repulsion dominates implying
    - quantum diffusion  $\langle x^2 \rangle \sim t$
    - (random matrix theory)
    - *residual conductivity*
    - *absolutely continuous spectrum* at Fermi level;
  - (b) if  $\beta < 1/d$  level repulsion can be ignored and
    - anomalous diffusion dominates  $\langle x^2 \rangle \sim t^{2\beta}$
    - insulating behaviour with scaling law
    - *singular continuous spectrum* near Fermi level.

# VIII - Multiparticle Models

# Motivation

1. The RTA is no longer valid at low temperature when several dissipative mechanism compete. It does not explain the Mott hopping transport.
2. The Fermion statistics produces correlations requiring second quantizations.
3. The Bloch equation for interaction between an atom and photons and Jaynes-Cumming model used in Quantum Optics gives a guideline to built multiparticle model for describing dissipative mechanisms for electronic transport in solids.

# Quantum Jumps for 2-level Atoms

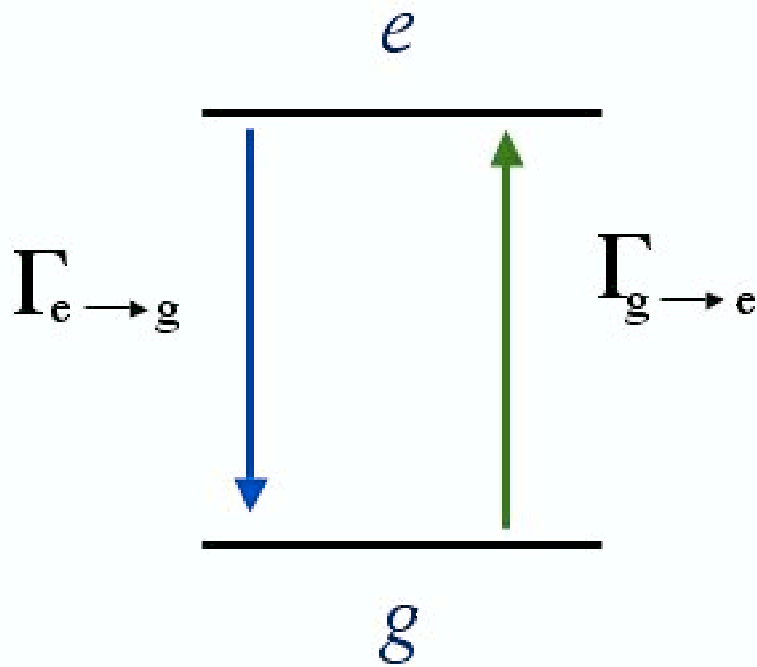
F. BLOCH, *Phys. Rev.*, 70 (1946), 460-474.

1. A 2-level atom interact with a thermal photon bath. Then  $\mathfrak{A} = M_2(\mathbb{C})$  the Hamiltonian is (using Pauli matrices)

$$h = E \sigma_+ \sigma_- = \begin{bmatrix} E & 0 \\ 0 & 0 \end{bmatrix}$$

2. The probability amplitudes that a photon of frequency  $\omega = E/\hbar$  in the thermal bath produces a transition between the groundstate  $g$  and the excited state  $e$  and vice-versa are  $\Gamma_{g \rightarrow e}$  and  $\Gamma_{e \rightarrow g}$ .
3. At *equilibrium*, at inverse temperature  $\beta$ , they are related by the *detailed balance* condition

$$\frac{\Gamma_{g \rightarrow e}}{\Gamma_{e \rightarrow g}} = e^{-\beta \hbar \omega}$$



### Quantum Jumps for the Bloch Equations

# Bloch Equations

1. The operators  $L_{g \rightarrow e}$  describes the jump from the groundstate to the excited state

$$L_{g \rightarrow e} = \sqrt{\Gamma_{g \rightarrow e}} \sigma_+ = \begin{bmatrix} 0 & \sqrt{\Gamma_{g \rightarrow e}} \\ 0 & 0 \end{bmatrix}$$

2. The operators  $L_{e \rightarrow g} = \sqrt{\Gamma_{g \rightarrow e}} \sigma_-$  describes the decay from the excited state to the groundstate

3. The corresponding Lindblad operator  $\mathfrak{L}^\dagger$  describes the dissipative dynamics for the states

*(here a density matrix  $\rho$ )*

$$\mathfrak{L}^\dagger(\rho) = -i[H, \rho] + \sum_i \left( L_i \rho L_i^\dagger - \frac{1}{2} \{L_i^\dagger L_i, \rho\} \right)$$

$$\mathfrak{L}^\dagger(\rho) = -i[h, \rho] - \mathfrak{D}^\dagger(\rho)$$

$$\begin{aligned} \mathfrak{D}^\dagger(\rho) = & \Gamma_{g \rightarrow e} \left( \frac{1}{2} \{ \sigma_- \sigma_+, \rho \} - \sigma_+ \rho \sigma_- \right) \\ & + \Gamma_{e \rightarrow g} \left( \frac{1}{2} \{ \sigma_+ \sigma_-, \rho \} - \sigma_- \rho \sigma_+ \right) \end{aligned}$$



4. Solving the evolution equation  $\frac{d\rho}{dt} = \mathfrak{L}^\dagger(\rho)$  gives  
(since  $\mathcal{L}_h$  commutes with  $\mathfrak{D}^\dagger$ )

$$\rho(t) = e^{-ith} e^{-t\mathfrak{D}^\dagger}(\rho) e^{+ith} = \rho_{eq.} + O(e^{-at})$$

(for some  $a > 0$ ) with

$$\rho_{st.} = \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix} \quad p = \frac{\Gamma_{g \rightarrow e}}{\Gamma_{e \rightarrow g} + \Gamma_{g \rightarrow e}}$$

If the detailed balance condition hold

$$\rho_{st.} = \rho_{eq.} = \frac{1}{1 + e^{-\beta E}} \begin{bmatrix} e^{-\beta E} & 0 \\ 0 & 1 \end{bmatrix}$$

# The Jaynes-Cummings Model

E.T. JAYNES, F.W. CUMMINGS, *Proc. IEEE* (1963).

1. Coupling between a single photon mode to a family of two-level atoms. The observable algebra is

$$\mathcal{K} = \varinjlim (M_n(\mathbb{C})) \text{ (compact operators)}$$

2. The free-photon Hamiltonian is

$$H_0 = \hbar\omega a^\dagger a \quad a^\dagger = a^* \quad [a, a^\dagger] = \mathbf{1}$$

3. Jumps are described by the *unbounded* creation annihilation operators  $a^\dagger, a$  with jumps probabilities  $\Gamma_\pm$  such that (*detailed balance*)

$$\frac{\Gamma_+}{\Gamma_-} = e^{-\beta\hbar\omega}$$

4. The dissipative part of the Lindblad operator is then

$$\mathfrak{D}^\dagger(\rho) = \Gamma_+ \left( \frac{1}{2} \{aa^\dagger, \rho\} - a^\dagger \rho a \right) + \Gamma_- \left( \frac{1}{2} \{a^\dagger a, \rho\} - a \rho a^\dagger \right)$$

# Quantum Jump Models for Fermions

J. BELLISSARD, R. REBOLLEDO, D. SPEHNER, W. VON WALDENFELS,  
*The Quantum Flow of Electronic transport I: The finite volume case,*  
 mp-arc 02-212, (2002)

1. A *perfect Fermi gas* with  $N$  particles. The 1-particle Hamiltonian is (*here  $i$  labels the energy levels !*)

$$h = \sum_{i=1}^N \epsilon_i |i\rangle\langle i|$$

2. Second quantization requires creation-annihilation Fermion operators (*CAR algebra*)

$$f_i^\dagger = f_i^* \quad f_i f_j^\dagger + f_j^\dagger f_i = 2\delta_{ij} \mathbf{1}$$

3. The Gibbs dynamic in mesoscopic cells is given by the second-quantized *free energy* Hamiltonian

$$F = H - \mu N = \sum_{i=1}^N (\epsilon_i - \mu) f_i^\dagger f_i$$

where  $N$  is the *number of particle*.

4. Jumps operators have the form  $\sqrt{\Gamma_{i \rightarrow j}} f_j^\dagger f_i$ :  
*the state  $i$  is emptied then the state  $j$  is filled,*  
 giving the dissipative part of the Lindblad operator

$$\mathfrak{D}_{gas}^\dagger(\rho) = \sum_{i,j=1}^N \Gamma_{i \rightarrow j} \left( \frac{1}{2} \{f_j^\dagger f_i f_i^\dagger f_j, \rho\} - f_i^\dagger f_j \rho f_j^\dagger f_i \right)$$

5. The Fermi gas is coupled to a *reservoir* keeping the average number of particle and the temperature (average energy) fixed. This is described by

- (a) *introduction of a particle from the reservoir in the state  $i$*  with jump operators  $\sqrt{\Gamma_{\cdot \rightarrow i}} f_i^\dagger$   
 (b) *absorption of a particle in state  $i$  by the reservoir* with jump operator  $\sqrt{\Gamma_{i \rightarrow \cdot}} f_i$

$$\begin{aligned} \mathfrak{D}_{res}^\dagger(\rho) &= \sum_{i=1}^N \Gamma_{i \rightarrow \cdot} \left( \frac{1}{2} \{f_i^\dagger f_i, \rho\} - f_i \rho f_i^\dagger \right) \\ &+ \sum_{i=1}^N \Gamma_{\cdot \rightarrow i} \left( \frac{1}{2} \{f_i f_i^\dagger, \rho\} - f_i^\dagger \rho f_i \right) \end{aligned}$$

6. At equilibrium the detailed balance condition will be

$$\frac{\Gamma_{i \rightarrow j}}{\Gamma_{j \rightarrow i}} = e^{-\beta(\epsilon_j - \epsilon_i)} \quad \frac{\Gamma_{i \rightarrow \cdot}}{\Gamma_{\cdot \rightarrow i}} = e^{-\beta(\mu - \epsilon_i)}$$

where  $\mu$  is the *chemical potential*.

**Theorem 5** *If the detailed balance condition holds, the Lindblad operator*

$$\mathfrak{L}^\dagger = -i[H - \mu N, \cdot] - \mathfrak{D}_{\text{gas}}^\dagger - \mathfrak{D}_{\text{res}}^\dagger$$

*induces a dynamics for which the density matrix converges to the equilibrium state*

$$\rho_{\text{eq.}} = \frac{e^{-\beta(H - \mu N)}}{\text{Tr} \left( e^{-\beta(H - \mu N)} \right)}$$

*Thus  $\rho_{\text{eq.}} \left( f_i^\dagger f_i / n \right) = (1 + e^{\beta(\epsilon_i - \mu)})^{-1}$  (Fermi-Dirac).*

**Remark :** *in this model, the observable algebra is finite dimensional.*

# Finite Systems: Axiomatic Approach

For dissipative models with *finite dimensional observable algebra*  $\mathfrak{A}$  an axiomatic approach will be useful

## 1)- Equilibrium GNS-Representation

1. The Gibbs dynamic is described by a selfadjoint operator  $F \in \mathfrak{A}$  with spectral representation

$$F = \sum_{n \geq 0} E_n p_n \quad E_0 \leq E_1 \leq \dots \quad p_n = p_n^2 = p_n^*$$

2. The thermal equilibrium is given by the Gibbs state with density matrix

$$\rho_{eq.} = \frac{e^{-\beta F}}{\text{Tr} (e^{-\beta F})}$$

3. Let  $\mathcal{H}_{eq.}$  be the Hilbert space of the corresponding *GNS representation* of  $\mathfrak{A}$ : as a vector space  $\mathcal{H}_{eq.} = \mathfrak{A}$ , with inner product

$$\langle A|B \rangle_{eq.} = \text{Tr} (\rho_{eq.} A^* B)$$

4. *Gibbs dynamics*: if  $\mathcal{L}_F = [F, \cdot]$

$$\alpha_t(A) = e^{itF} A e^{-itF} = e^{it\mathcal{L}_F}(A)$$

defines a unitary operator on  $\mathcal{H}_{eq.}$ .

5. *KMS-condition*:

$$\langle B^*|A^* \rangle_{eq.} = \langle A|\alpha_{i\beta}(B) \rangle_{eq.}$$

The Tomita operator is  $SA = A^*$  and the modular operator  $\Delta = S^*S = \exp(-\beta\mathcal{L}_F)$ .

## 2)- Jump Operators

1. There is a discrete set  $\mathcal{J}$  of indices called *jumps* endowed with a one-to-one involutive bijection  $x \in \mathcal{J} \mapsto \bar{x} \in \mathcal{J}$  (*time reversal*).

2. With each  $x \in \mathcal{J}$  is associated a *jump operator*  $L_x \in \mathfrak{A}$  and a *jump energy*  $\epsilon_x \in \mathbb{R}$  such that

- $[F, L_x] = \epsilon_x L_x$
- *detailed balance*  $L_x^* = e^{-\beta\epsilon_x/2} L_{\bar{x}}$

Both conditions imply  $\epsilon_{\bar{x}} = -\epsilon_x$

3. If  $\mathcal{J}$  is not a finite set then

$$\|\mathfrak{D}^\dagger\|_r = \sum_{x \in \mathcal{J}} \|L_x\|_{\mathfrak{A}}^2 e^{2r|\epsilon_x|} < \infty$$

4. The family  $\{L_x; x \in \mathcal{J}\}$  will be called *irreducible* if its commutant is trivial.



### 3)- Dissipative Dynamics

1. The Lindblad operator defining the dissipative dynamic is defined by  $\mathfrak{L}^\dagger = -i\mathcal{L}_F - \mathfrak{D}^\dagger$  on density matrices, with

$$\mathfrak{D}^\dagger(\rho) = \sum_{x \in \mathcal{J}} \left( \frac{1}{2} \{L_x^* L_x, \rho\} - L_x \rho L_x^* \right)$$

The first part  $\mathcal{L}_F$  is the *Liouvillian* and represents the coherent part of the evolution. The other part  $\mathfrak{D}^\dagger$  is the *dissipative* contribution to the evolution.

2. The dual operator  $\mathfrak{L} = +i\mathcal{L}_F - \mathfrak{D}$  acts on  $\mathfrak{A}$  as

$$\mathfrak{D}(A) = \sum_{x \in \mathcal{J}} \left( \frac{1}{2} \{L_x^* L_x, A\} - L_x^* A L_x \right)$$

**Theorem 6** *The family  $\{\Phi_t = \exp(t\mathfrak{L}); t \in \mathbb{R}_+\}$  defines a Markov semigroup on  $\mathfrak{A}$ .*

#### 4)- Entropy

1. Since  $\mathfrak{A}$  is finite dimensional any state  $\rho$  is represented by a density matrix in  $\mathfrak{A}$ . Its *von Neumann entropy* and its *Clausius entropy* are

$$s(\rho) = -\text{Tr}(\rho \ln \rho) \quad S(\rho) = k_B s(\rho)$$

2. Given two states  $\rho$  and  $\rho_0$  their *relative entropy* (also called *Kullback-Leibler distance*) is

$$D(\rho|\rho_0) = \text{Tr}(\rho(\ln \rho - \ln \rho_0)) \geq 0$$

3. If  $\beta = 1/(k_B T)$  then the relative entropy gives the difference of the *grand potential*  $J = U - \mu N - TS$

$$k_B T D(\rho|\rho_{eq.}) = F(\rho) - F_{eq.} - T(S(\rho) - S_{eq.})$$

$$F(\rho) = \rho(F) \quad \rho(H) = U(\rho) \quad \rho(N) = N(\rho)$$

*Thus  $J$  is minimum at equilibrium.*

## 5)- Results

G. LINDBLAD, *CMP*, 40, 147-151 (1975)

G. LINDBLAD, *CMP*, 48, 119-130 (1976)

**Theorem 7** *Let  $\rho_t = \Phi_t^\dagger(\rho)$  be the state evolution under the dissipative dynamic. Then*

*(i) the relative entropy  $D(\rho_t|\rho_{eq.})$  is non increasing in time,*

*(ii) any time invariant state has the form  $\rho(A) = \rho_{eq.}(AM)$  for some  $M$  in the commutant of the jump operators and of the Gibbs Hamiltonian,*

**Theorem 8** *If, in addition, the family of jump operators is irreducible then*

*(i)  $\rho_{eq.}$  is the only invariant state,*

*(ii)  $\rho_t$  converges to  $\rho_{eq.}$ .*

*(iii)  $\mathfrak{L}$  defines an invertible operator on the subspace of the GNS-representation  $\mathcal{H}_{eq.}$  orthogonal to  $\mathbf{1}$ .*

*(iv) the Kubo formula makes sense.*

# Equivalence with Quantum Spin Models

J. BELLISSARD, *unpublished*.

There are operators  $\vec{S}_i$ 's and the  $\vec{T}_i$ 's in the algebra  $\mathfrak{A}$  obeying the commutation rules for spin-1/2 at each site  $i$  and satisfying  $T_i^3 S_i^3 = S_i^3 T_i^3 = 0$  such that the dissipative part of the *Quantum Jump model*, becomes the following *XY*-model

$$\begin{aligned} \mathfrak{D} &= \sum_{ij; i \neq j} 4\gamma_{ij} \cosh(\beta(\epsilon_j - \epsilon_i)/2) \left( \frac{1}{4} - T_i^3 T_j^3 - S_i^3 S_j^3 \right) \\ &- \sum_{ij; i \neq j} 2\gamma_{ij} (S_i^+ S_j^- + S_i^- S_j^+) - \sum_{i=1}^N h_i(\beta) S_i^3 \\ &+ \sum_{i=1}^N 4\gamma_i \left\{ \frac{\cosh(\beta\epsilon_i/2)}{2} + \sinh(\beta\epsilon_i/2) S_i^3 - (-\mathbf{1})^{\hat{N}-N} S_i^1 \right\}, \end{aligned}$$

UNEXPECTED !!

# IX - The Infinite Volume Limit

O. BRATTELI, D. W. ROBINSON,  
*Operator Algebras and Quantum Statistical Mechanics,*  
Vol. 1 (1979) & Vol. 2 (1997) Springer.

# Quasilocal Observable Algebra

**Question:** *How to extend the formalism to electrons (or holes) on a Delone set  $\mathcal{L}$  ?*

1. Let  $\mathcal{L}$  be the set of atomic position with Hull  $\Omega$  and transversal  $\Xi$ . If  $\omega \in \Xi$  let  $\mathcal{L}_\omega$  be the corresponding atomic set. At each site  $x \in \mathcal{L}_\omega$  let  $f_{\omega,x;\sigma}^\dagger$  and  $f_{\omega,x;\sigma}$  be the creation-annihilation for a *fermion* of type  $\sigma$ .

**Remark:**  $\sigma$  labels various possible degrees of freedom at each site such as *spin, orbital quantum number*

2. If  $\Lambda$  is a box in  $\mathbb{R}^d$  let  $\mathfrak{A}_\omega(\Lambda)$  be the  $C^*$ -algebra generated by the  $f_{\omega,x;\sigma}$ 's for  $x \in \mathcal{L}_\omega \cap \Lambda$ .  
For  $\Lambda \subset \Lambda'$ , let  $i_{\Lambda,\Lambda'} : \mathfrak{A}_\omega(\Lambda) \hookrightarrow \mathfrak{A}_\omega(\Lambda')$  be the canonical injection.
3. Let  $\mathfrak{A}_\omega = \varinjlim (\mathfrak{A}_\omega(\Lambda), i_{\Lambda,\Lambda'})$  be the *quasilocal algebra*.

4. An arrow in the *groupoid*  $\Gamma_{\Xi}$  of the transversal is a pair  $\gamma = (\omega, a) \in \Xi \times \mathbb{R}^d$  such that  $T^{-a}\omega \in \Xi$ . Equivalently,  $a \in \mathcal{L}_{\omega}$ .  
With each  $\gamma = (\omega, a) \in \Gamma_{\Xi}$  is associated the canonical  $*$ -isomorphism

$$\eta_{(\omega, a)} : \mathfrak{A}_{T^{-a}\omega} \mapsto \mathfrak{A}_{\omega}$$

defined by

$$\eta_{(\omega, a)}(f_{T^{-a}\omega, x-a; \sigma}) = f_{\omega, x; \sigma}$$

**Theorem 9 (Spehner '00)** *The field of  $C^*$ -algebras  $\mathfrak{A} = (\mathfrak{A}_{\omega})_{\omega \in \Xi}$  is continuous. The family  $(\eta_{\gamma})_{\gamma \in \Gamma_{\Xi}}$  defines a continuous functor from  $\Gamma_{\Xi}$  into the category of  $C^*$ -algebras that makes the field  $\mathfrak{A}$  covariant.*

# Gibbs Dynamics

1. A Gibbs Hamiltonian  $F$  is given in finite volume by

$$F_{\omega,\Lambda} = \sum_{X \subset \mathcal{L}_\omega; X \cap \Lambda \neq \emptyset} \hat{F}_{\omega,X} \quad \hat{F}_{\omega,X}^* = \hat{F}_{\omega,X} \in \mathfrak{A}_\omega(X)$$

with  $X$  finite and with *covariance* property

$$\eta_{(\omega,a)} \left( \hat{F}_{\mathbb{T}^{-a}\omega, X-a} \right) = \hat{F}_{\omega,X}$$

and some notion of *continuity* w.r.t.  $\omega \in \Xi$

2. Convergence can be obtained through (for  $r > 0$ )

$$\|F\|_r = \sup_{\omega \in \Xi} \sum_{0 \in X \subset \mathcal{L}_\omega} e^{r|X|} \|\hat{F}_{\omega,X}\|_{\mathfrak{A}_\omega(X)}$$



3. Then the evolution is defined by (*Bratteli-Robinson*)

$$\theta_\omega^t(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} e^{itF_{\omega,\Lambda}} A e^{-itF_{\omega,\Lambda}}$$

for  $A \in \mathfrak{A}_\omega^0 = \bigcup_\Lambda \mathfrak{A}_\omega(\Lambda)$

**Theorem 10 (Spehner '00)** (i) For each  $\omega \in \Xi$  the family  $\theta_\omega = (\theta_\omega^t)_{t \in \mathbb{R}}$  defines a norm pointwise continuous group of  $*$ -automorphisms of  $\mathfrak{A}_\omega$ .

(ii) The family  $\theta = (\theta_\omega)_{\omega \in \Xi}$  is continuous.

(iii) The family  $\theta = (\theta_\omega)_{\omega \in \Xi}$  is covariant, namely

$$\eta_{(\omega,a)} \circ \theta_{\mathbb{T}^{-a}\omega}^t = \theta_\omega^t \circ \eta_{(\omega,a)}$$

for all  $t \in \mathbb{R}$  and  $(\omega, a) \in \Gamma_\Xi$ .

**Remark:** The generator of the group  $\theta_\omega$  is given by the *Liouvillian*  $\mathcal{L}_{F_\omega} = i[F_\omega, \cdot]$  acting on  $\mathfrak{A}_\omega$  as a  $*$ -derivation.

# Thermal Equilibrium

1. A *KMS-state* at inverse temperature  $\beta$  is a family  $\Psi = (\Psi_\omega)_{\omega \in \Xi}$  of states on  $\mathfrak{A}$  such that
  - $\forall \omega \in \Xi$  the state  $\Psi_\omega$  is  $\theta_\omega$ -invariant
  - The family  $\Psi$  is *continuous* in  $\omega$  and *covariant*, namely  $\Psi_\omega \circ \eta_{(\omega, a)} = \Psi_{\tau^{-a}\omega}$
  - For  $A, B \in \mathfrak{A}_\omega$ , analytic with respect to  $\theta_\omega$  then

$$\Psi_\omega(AB) = \Psi_\omega(B \theta_\omega^{i\beta}(A))$$

Such a state always exists *see (BRATTELI-ROBINSON)*

2. The *GNS-representation* of  $\Psi$  provides a *continuous, covariant* field of Hilbert spaces

$$\mathcal{H} = (\mathcal{H}_\omega)_{\omega \in \Xi}$$

(also called a *representation of the groupoid*  $\Gamma_\Xi$ )  
with each a cyclic unit vector  $\xi_\omega \in \mathcal{H}_\omega$ .

# Dissipative Dynamics

1. Jump operators are elements  $L_{\omega, X} \in \mathfrak{A}_{\omega}(X)$  for  $X$  a finite subset of  $\mathcal{L}_{\omega}$ . *Covariance* and *continuity* are required.
2. The dissipative part of the evolution is defined in a finite volume by

$$\mathfrak{D}_{\omega, \Lambda}(A) = \sum_{X, Y \subset \Lambda \cap \mathcal{L}_{\omega}} c_{\omega}(X, Y) \cdot \left( \frac{1}{2} \{L_{\omega, X}^* L_{\omega, Y}, A\} - L_{\omega, X}^* A L_{\omega, Y} \right)$$

where  $c_{\omega}(X, Y) \in \mathbb{C}$  is continuous in  $\omega$ , covariant  $c_{T-a\omega}(X-a, Y-a) = c_{\omega}(X, Y)$  with positive type

$$\sum_{l, m=1}^n \bar{\lambda}_l \lambda_m c_{\omega}(X_l, X_m) \geq 0$$

$\forall (\lambda_1, \dots, \lambda_n) \in \mathbb{C}^n$  and finite subsets  $X_i$  of  $\mathcal{L}_{\omega}$ .

3. Convergence is provided by (for  $r > 0$ )

$$\begin{aligned} \|\mathfrak{D}\|_r &= \sup_{\omega \in \Xi} \sum_{0 \in X \cup Y \subset \mathcal{L}_\omega} e^{r(|X|+|Y|)} c_\omega(X, Y) \cdots \\ &\quad \cdots \|L_{\omega, X}\|_{\mathfrak{A}_\omega(X)} \|L_{\omega, Y}\|_{\mathfrak{A}_\omega(Y)} \end{aligned}$$

4. The dissipative dynamics is defined by

$$\Phi_\omega^t(A) = \lim_{\Lambda \uparrow \mathbb{R}^d} e^{t(\mathcal{L}_{F_{\omega, \Lambda}} - \mathfrak{D}_{\omega, \Lambda})} (A) \quad A \in \mathfrak{A}_\omega^0$$

Then the dissipative dynamics satisfies

(J. BELLISSARD-R. REBOLLEDO '04, unpublished  
see also BRATTELI-ROBINSON or MATSUI '93)

**Theorem 11** (i) *The limit above exists and for each  $\omega \in \Xi$  the family  $\Phi_\omega = (\Phi_\omega^t)_{t \geq 0}$  defines a norm pointwise continuous Markov semigroup on  $\mathfrak{A}_\omega$ .*

(ii) *The family  $\Phi = (\Phi_\omega)_{\omega \in \Xi}$  is continuous.*

(iii) *The family  $\Phi = (\Phi_\omega)_{\omega \in \Xi}$  is covariant, namely*

$$\eta_{(\omega, a)} \circ \Phi_{T^{-a}\omega}^t = \Phi_\omega^t \circ \eta_{(\omega, a)}$$

for all  $t \geq 0$  and  $(\omega, a) \in \Gamma_\Xi$ .

# Open Questions

1. The quasilocal algebra does not provide a good representation for the spectral decomposition of the Gibbs Hamiltonian in general. How then is it possible to express the *detailed balance* condition globally ?
2. What conditions must be satisfied by the local jump operators to imply (for  $A, B \in \mathfrak{A}_\omega$ )

$$\begin{aligned} \Psi_\omega(A^* \mathfrak{D}_\omega(B)) &= \sum_{X, Y \subset \mathcal{L}_\omega} c_\omega(X, Y) \cdots \\ &\cdots \Psi_\omega([L_{\omega, X}, A]^* [L_{\omega, Y}, B]) \end{aligned}$$

3. What is the infinite volume limit of the quantum jump model ? (for which the coherent dynamics is given by independent electrons).

# X - Markov Semigroups

# Motivations

1. Markov semigroups occurs in any dissipative system at time scale long enough for the local equilibrium approximation to be valid. Surprisingly very few is known beyond the two classical results: the *Levy-Khintchine* and the *Lindblad* theorems.
2. There is a need to characterize generators of Markov semigroups that are *not uniformly continuous*. Partial results are known on *Von Neumann Algebras* especially the *hyperfinite* ones.
3. Very little is known for  $C^*$ -algebras. In Quantum Statistical Mechanics, *UHF algebras* are essential. In Solid State Physics for aperiodic systems, *crossed product algebras* are involved.
4. Information theory seems to play a role in *non-hyperfinite type II factors*, (*Voiculescu et al.*). The  $L^2$  cohomology (*Connes-Shlyakhtenko '04*) provides invariants that may produce obstructions to extensions of the Lindblad or Levy-Khintchine theorems.

# Complete Positivity

1. A linear map  $\Phi : \mathfrak{A} \mapsto \mathfrak{B}$  between two  $C^*$ -algebras is *positive* if the image of any positive element in  $\mathfrak{A}$  is positive in  $\mathfrak{B}$ .

In addition it is *normalized* if both  $\mathfrak{A}, \mathfrak{B}$  are *unital* and  $\Phi(\mathbf{1}) = \mathbf{1}$ .

2. A linear map  $\Phi : \mathfrak{A} \mapsto \mathfrak{B}$  between two  $C^*$ -algebras is *completely positive* if for any  $n \in \mathbb{N}$  the induced map  $\Phi \otimes \text{id}_n : \mathfrak{A} \otimes M_n(\mathbb{C}) \mapsto \mathfrak{B} \otimes M_n(\mathbb{C})$  is positive.

Equivalently given any matrix  $S = (S_{ik})_{1 \leq i, k \leq n}$  with  $S_{ik} \in \mathfrak{A}$  there is a matrix  $T = (T_{ik})_{1 \leq i, k \leq n}$  with  $T_{ik} \in \mathfrak{B}$  such that

$$\sum_{k=1}^n \Phi(S_{ik} S_{jk}^*) = \sum_{k=1}^n T_{ik} T_{jk}^*$$



### 3. Examples of CP-maps are:

- $*$ -homomorphisms
- conditional expectations
- maps of the form  $a \in \mathfrak{A} \mapsto sas^* \in \mathfrak{A}$  for  $s \in \mathfrak{A}$
- Convex combinations of CP-maps
- Any weakly pointwise limit of a sequence of CP-maps

Hence a map of the form  $a \in \mathfrak{A} \mapsto \mathbb{E}(\pi(a)) \in \mathfrak{B}$  where  $\pi : \mathfrak{A} \mapsto \mathfrak{C}$  is a  *$*$ -homomorphism* and  $\mathbb{E} : \mathfrak{C} \mapsto \mathfrak{B}$  is a *conditional expectation*, is CP. The *Stinespring theorem* is a kind of converse.

### 4. A *conditional expectation* $\mathbb{E} : \mathfrak{C} \mapsto \mathfrak{B}$ is a projection of norm one from $\mathfrak{C}$ *onto* a subalgebra $\mathfrak{B}$

**TOMIYAMA '58**

A *partial trace* is a conditional expectation. Any way of averaging over a subset of degrees of freedom is also a conditional expectation.

# The Stinespring Theorem

W.F STINESPRING, *Proc. Am. Math. Soc.*, **6**, 211-216 (1955)

**Theorem 12** *Let  $\Phi : \mathfrak{A} \mapsto \mathcal{B}(\mathcal{H})$  be a CP-map. Then there is a Hilbert space  $\mathcal{K}$ , a linear map  $V : \mathcal{H} \mapsto \mathcal{K}$  and a representation  $\pi$  of  $\mathfrak{A}$  into  $\mathcal{K}$  such that*

$$\Phi(a) = V^* \pi(a) V$$

*If  $\Phi$  is normalized then  $V$  is a partial isometry:  $V^*V = \mathbf{1}_{\mathcal{H}}$ . In particular  $VV^*$  is a projection in  $\mathcal{K}$  onto a closed subspace isomorphic to  $\mathcal{H}$ .*

The triple  $(\mathcal{K}, \pi, V)$  is called a *Stinespring representation* of  $\Phi$ . Then the closed subspace  $\mathcal{K}_1 \subset \mathcal{K}$  generated by  $\{\pi(a)Vx; a \in \mathfrak{A}, x \in \mathcal{H}\}$  is *invariant* by  $\pi$ .  $(\mathcal{K}, \pi, V)$  is *minimal* if  $\mathcal{K}_1 = \mathcal{K}$ .

**Theorem 13** *If  $(\mathcal{K}_i, \pi_i, V_i)$   $i = 1, 2$  are two minimal Stinespring representations of  $\Phi$ , there is a unitary operator  $U : \mathcal{K}_1 \mapsto \mathcal{K}_2$  such that  $V_2 = UV_1$  and  $\pi_2(a) = U\pi_1(a)U^*$  for  $a \in \mathfrak{A}$ .*

# The Størmer-Schwarz Inequality

E. STØRMER, *Lecture Notes Phys.*, **29**, 85-106 (1974)

As a consequence of the Stinespring theorem, Størmer's version of the Cauchy-Schwarz inequality follows

**Theorem 14 (Størmer '74)** *Let  $\Phi : \mathfrak{A} \mapsto \mathfrak{A}$  be a normalized CP-map. Then*

$$\Phi(a^*)\Phi(a) \leq \Phi(a^*a) \quad \forall a \in \mathfrak{A}$$

# The Kraus Theorem

K. KRAUS, *Ann. Phys.*, **64**, 311-335 (1970)

**Theorem 15 (Kraus '70)** *If  $\mathfrak{A} = M_n(\mathbb{C})$  and if  $\Phi : \mathfrak{A} \mapsto \mathcal{B}(\mathcal{H})$  is a CP-map, there is a family  $\{v_s; s \in S\}$  of finite rank operators  $v_s : \mathcal{H} \mapsto \mathbb{C}^n$  such that (where the sums converge weakly*

$$\sum_{s \in S} v_s^* v_s = \Phi(\mathbf{1}_n) \quad \Phi(a) = \sum_{s \in S} v_s^* a v_s$$

This theorem occurs in the proof of *Lindblad's* theorem as an important step.

It became very popular in the '90s because of the measurement aspects of *Quantum Computing*.

# Markov Semigroups

If  $\mathfrak{A}$  is a *unital*  $C^*$ -algebra, a *Markov semigroup* is a one-parameter family  $\Phi = (\Phi_t)_{t \geq 0}$  of linear maps from  $\mathfrak{A}$  into itself such that

1. *Complete Positivity:*

for each  $t \geq 0$  the map  $\Phi_t$  is CP

2. *Normalization:*  $\Phi_t(\mathbf{1}) = \mathbf{1}$  for all  $t \geq 0$

3. *Norm Pointwise Continuity:* for each  $a \in \mathfrak{A}$  the map  $t \in [0, \infty) \mapsto \Phi_t(a) \in \mathfrak{A}$  is norm continuous

4. *Initial Condition:*  $\Phi_0 = id_{\mathfrak{A}}$

5. *Markov Property:* if  $s, t \geq 0$  then

$$\Phi_{s+t} = \Phi_s \circ \Phi_t$$

# Example: Markov Processes

1. If  $\mathfrak{A} = \mathcal{C}(K)$  for  $K$  a metrizable compact space a Markov semigroup is given by a family  $\mu_t(x|dy)$  of Borel probability measures on  $K$  (*transition probability*) such that

$$\Phi_t(f)(x) = \int_K \mu_t(x|dy) f(y)$$

2. Markov's property is equivalent to the *Chappman-Kolmogorov* equations

$$\int_{y' \in K} \mu_s(x|dy') \mu_t(y'|dy) = \mu_{s+t}(x|dy)$$

3. It defines a Markov Process, a family of  $K$ -valued random variables  $(X_t)_{t \geq 0}$  such that

$$\text{Prob}\{X_{t_i} \in B_i\} = \int_{B_1 \times \cdots \times B_n} \mu_{t_1}(x|dx_1) \mu_{t_2-t_1}(x_1|dx_2) \cdots \mu_{t_n-t_{n-1}}(x_{n-1}|dx_n)$$

# Levy-Khintchine Theorem on the Torus

If  $K = \mathbb{T}^d$ , the torus acts on itself by translation. Let then ( $d$ -parameter group of  $*$ -automorphisms)

$$\tau_k f(k') = f(k' - k) \quad f \in \mathcal{C}(\mathbb{T}^d) = \mathfrak{A}$$

A Markov semigroup on  $\mathbb{T}^d$  is a Levy process if

$$\tau_k \circ \Phi_t = \Phi_t \circ \tau_k \quad t \geq 0, k \in \mathbb{T}^d$$

Let  $u^m$  be the function  $u^m(k) = e^{ik \cdot m}$  if  $m \in \mathbb{Z}^d$ .

**Theorem 16 (Levy-Khintchine)** *If  $\Phi$  is a Levy process on  $\mathbb{T}^d$  then  $\Phi_t(u^m) = e^{t\psi_m} u^m$  where*

$$\psi_m = -\frac{1}{2} \langle m | A m \rangle + ia \cdot m + \int_{\mathbb{T}^d} (e^{ik \cdot m} - 1 - ik \cdot m \chi_{[0,1]}(|k|)) \nu(dk)$$

where (i)  $A$  is a  $d \times d$  real positive matrix, (ii)  $a \in \mathbb{R}^d$ , (iii)  $\nu$  is a positive Borel measure on  $\mathbb{T}^d$  such that  $\nu(\{0\}) = 0$  and  $\int_{\mathbb{T}^d} \min(k^2, \epsilon) \nu(dk) < \infty$  for  $\epsilon$  small enough, (iv)  $\chi_I$  is the characteristic function of  $I$ .

# Extensions of the LK Theorem

1. The Levy-Khintchine formula was initially proved on  $\mathcal{C}_0(\mathbb{R}^d)$ . It has been extended to all locally compact group.

(see HEYER, *Probability Measures on Locally Compact Groups*, Springer, (1977) )

2. The simplest example of Levy process on  $\mathbb{R}^d$  is the *Brownian motion* for which  $\Phi_t(f) = e^{t\Delta}(f)$  if  $f \in \mathcal{C}_0(\mathbb{R}^d)$  and  $\Delta$  denotes the  $d$ -dimensional Laplacian.

3. The LK theorem on the torus can be extended with the same proof to the *Noncommutative Tori*, that is the  $C^*$ -algebra generated by unitaries  $u_1, \dots, u_d$  such that  $u_i u_j = e^{\theta_{ij}} u_j u_i$  for some real valued antisymmetric matrix  $\theta_{i,j}$ . (J. B., unpublished)

4. The LK-theorem can also be generalized to Markov semigroups on the crossed product algebra  $\mathfrak{A} \rtimes \mathbb{Z}^d$  invariant by the dual action of  $\mathbb{T}^d$ . (J. B., unpublished)



# The Lindblad Theorem

G. LINDBLAD, *Comm. Math. Phys.*, **48**, 119-130 (1976)

The Lindblad theorem is the noncommutative analog of the Lévy-Khintchine theorem for Markov semigroups on  $M_n(\mathbb{C})$ .

Since probability are involved, *Von Neumann algebras* are more appropriate. This case coincide with *type I factors*.

**Theorem 17 (Lindblad '76)** *Let  $\mathcal{H}$  be a Hilbert space and let  $\Phi$  be a Markov semigroup on  $\mathcal{B}(\mathcal{H})$ . It will be assumed that  $\Phi$  is ultraweakly continuous instead of norm pointwise continuous. Then there is a family  $(v_i)_{i \in I}$  of bounded operators on  $\mathcal{H}$  such that  $\sum_{i \in I} v_i^* v_i < \infty$  and there is  $h = h^* \in \mathcal{B}(\mathcal{H})$  such that the generator  $L = d\Phi/dt|_{t=0}$  of  $\Phi$  is given by*

$$L(a) = \sum_{i \in I} \left( v_i^* a v_i - \frac{1}{2} \{v_i^* v_i, a\} \right) + i[h, a] \quad a \in \mathcal{B}(\mathcal{H})$$

It follows that  $L$  is bounded so that  $\Phi$  is uniformly continuous, namely  $\|\Phi_t - id\| \rightarrow 0$  as  $t \rightarrow 0$ .

# Comments on Levy-Khintchine Theorems

1. The main result in Levy-Khintchine's formula is that the *generator*  $L = d\Phi/dt|_{t=0}$  is a pseudodifferential operator of *degree at most 2*.
2. The simplest example is the Laplacian  $L = \Delta$  which satisfies

$$\Delta(fg) - f\Delta(g) - \Delta(f)g = 2\nabla f \cdot \nabla g \quad f, g \in \mathcal{C}^2$$

3. In the Lindblad theorem the generator satisfies also

$$L(a^*b) - a^*L(b) - L(a^*)b = \sum_{i \in I} [v_i, a]^* [v_i, b]$$

Since the maps  $\partial_i a \mapsto [v_i, a]$  are derivations, it follows that  $L$  a noncommutative analog of a Laplacian as well.

4. The inequality  $L(a^*a) - a^*L(a) - L(a^*)a \geq 0$  follows directly from the Størmer inequality.

# Hilbert- $C^*$ modules

Let  $\mathfrak{A}$  be a  $C^*$ -algebra. A complex vector space  $\mathcal{E}$  is a *Hilbert- $C^*$  right  $\mathfrak{A}$ -module* if it is endowed with a structure of right  $\mathfrak{A}$ -module together with a sesquilinear map  $(\xi, \eta) \in \mathcal{E} \times \mathcal{E} \mapsto \langle \xi | \eta \rangle_{\mathcal{E}} \in \mathfrak{A}$  (the  $\mathfrak{A}$ -inner product) such that

- $\langle \xi | \eta \rangle_{\mathcal{E}}^* = \langle \eta | \xi \rangle_{\mathcal{E}}$
- For  $a, b \in \mathfrak{A}$ ,  $\langle \xi a | \eta b \rangle_{\mathcal{E}} = a^* \langle \xi | \eta \rangle_{\mathcal{E}} b$
- $\langle \xi | \xi \rangle_{\mathcal{E}} > 0$  if  $0 \neq \xi \in \mathcal{E}$
- $\mathcal{E}$  becomes a Banach space with the norm
 
$$\|\xi\|_{\mathcal{E}} = \|\langle \xi | \xi \rangle_{\mathcal{E}}\|_{\mathfrak{A}}^{1/2}$$

An *endomorphism* of  $\mathcal{E}$  is a bounded linear map  $T : \mathcal{E} \mapsto \mathcal{E}$  such that  $T(\xi a) = T(\xi)a$  (that is  $T$  is a module map) and such that there is another module map  $T^*$  with  $\langle T\xi | \eta \rangle_{\mathcal{E}} = \langle \xi | T^*\eta \rangle_{\mathcal{E}}$  (namely  $T$  has an adjoint).

# The Stinespring and Lindblad Theorems

**Theorem 18** *Let  $\mathfrak{A}, \mathfrak{B}$  be unital  $C^*$ -algebras and let  $\Phi : \mathfrak{A} \mapsto \mathfrak{B}$  be a CP-map. Then there is a Hilbert- $C^*$  right  $\mathfrak{B}$ -module  $\mathcal{E}$ , an element  $\xi \in \mathcal{E}$  and a  $*$ -homomorphism (representation)  $\pi : \mathfrak{A} \mapsto \text{End}(\mathcal{E})$  such that, for any  $a \in \mathfrak{A}$*

$$\Phi(a) = \langle \xi | \pi(a) \xi \rangle_{\mathcal{E}}$$

**Theorem 19** *Let  $\mathfrak{A}$  be a unital  $C^*$ -algebra and  $\Phi$  a Markov semigroup on  $\mathfrak{A}$ . Let  $\mathcal{A}$  be a dense subalgebra contained in the domain of the generator  $L$  of  $\Phi$ . Then there is a Hilbert  $C^*$  right  $\mathfrak{A}$ -module  $\mathcal{E}$ , a representation  $\pi : \mathfrak{A} \mapsto \text{End}(\mathcal{E})$  and a linear map  $\eta : \mathcal{A} \mapsto \mathcal{E}$  such that*

$$\langle \eta(a) | \eta(b) \rangle_{\mathcal{E}} = L(a^*b) - a^*L(b) - L(a^*)b$$

where  $\eta$  is a  $\pi$ -derivation, namely

$$\eta(ab) = \eta(a)b + \pi(a)\eta(b) \quad a, b \in \mathcal{A}$$

**Remark:** Arveson (ARVESON '02) characterized the maximal  $*$ -subalgebra contained in the domain of  $L$ . There is a Markov semigroup with generator having no dense  $*$ -subalgebra in its domain. (FAGNOLA '00)

# Dissipative Part of the Lindbladian

Let  $\mathfrak{A}$  be a unital  $C^*$ -algebra and let  $\Phi$  be a Markov semigroup on  $\mathfrak{A}$ . If  $\rho$  is a  $\Phi$ -invariant state then

$$\rho(L(a)) = 0 \quad a \in \mathcal{D}(L)$$

The Theorem 19 show that

$$\rho(a^*L(a)) + \rho(L(a^*)a) \leq 0 \quad a \in \mathcal{D}(L)$$

Hence in the *GNS representation of  $\rho$* ,  $L$  induces a densely defined operator with *negative real part*.

# To Conclude

1. Is there a way of characterizing the *domain of the generator* of a Markov semigroup ?  
If NO, what about Markov semigroups of Quantum Statistical Physics ?  
(In this latter case, the observable algebra is *UHF*)
2. Is there an axiomatic way to describe the *detailed balance condition* on the generator of a Markov semigroup ?
3. Can one extend the entropy inequalities to Markov semigroups ? (the relative entropy between two states on a  $C^*$ -algebra exists (ARAKI))
4. What can be proved in general about the *speed of return to equilibrium* ? (see CARLEN, CARLEN-LIEB)
5. Since the dissipative part  $\mathfrak{D}$  of the Lindbladian is a Laplacian, or a Dirichlet form, is there a *Dirac operator* with square  $\mathfrak{D}$  ? (the notion of entropy-metric is floating around in many works)