

# COHERENT and DISSIPATIVE TRANSPORT in APERIODIC SOLIDS

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# Main References

J. BELLISSARD, H. SCHULZ-BALDES, *A Kinetic Theory for Quantum Transport in Aperiodic Media*,  
J. Stat. Phys., **91**, 991-1026, (1998).

D. SPEHNER, J. BELLISSARD, *A Kinetic Model for Quantum Jumps*,  
J. Stat. Phys., **104**, 525-572, (2001).

J. BELLISSARD, R. REBOLLEDO, D. SPEHNER, W. VON WALDENFELS,  
*The Quantum Flow of Electronic transport I: The finite volume case*,  
in preparation.

# Content

1. Why Revisiting Transport ?
2. Dissipation: a Heuristic Approach
3. Aperiodic Solids
4. Kinetic Models
5. Coherent Transport

# 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.

# I.1)- Motivations

## Conceptual Difficulties

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,  $\sigma(\mathbf{T})$  increases as temperature decreases

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

2. For a thermally activated process

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

3. For weakly disordered systems

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

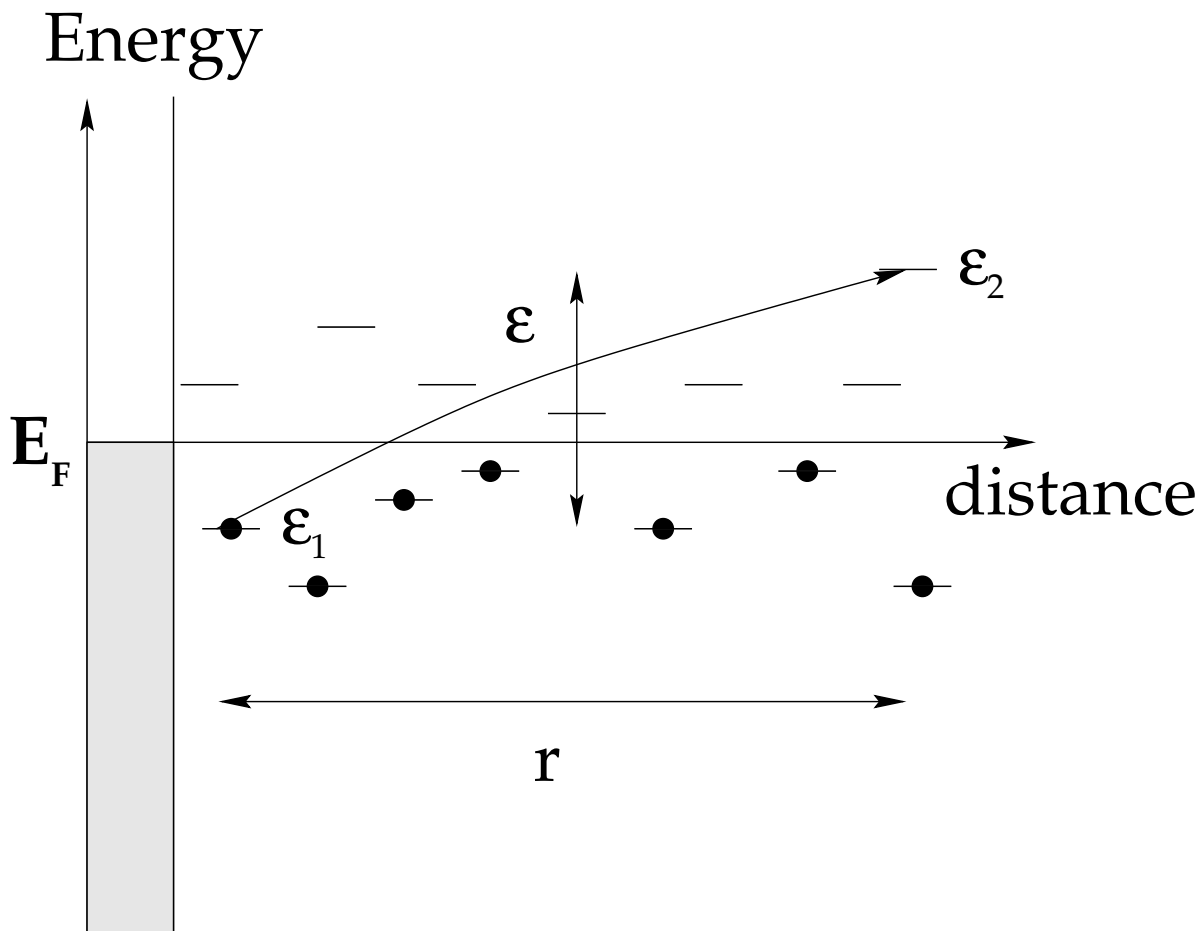
4. For strongly disordered systems in  $3D$

$$\sigma(\mathbf{T}) \stackrel{T \downarrow 0}{\sim} e^{-(\mathbf{T}_0/\mathbf{T})^{1/4}} \quad (\text{variable range hopping}).$$

## I.2)- 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  $\mathbf{r}$

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

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

- Optimal distance  $\mathbf{r}_{\text{opt}} \sim 1/T^{1/(d+1)} \gg \xi$



## I.3)- Transport in Quasicrystals

*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).

### Quasicrystalline alloys :

Metastable QC's:

**AlMn**

(Shechtman D., Blech I., Gratias D. & Cahn J., PRL **53**, 1951 (1984))

**AlMnSi**

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

Defective stable QC's: **AlLiCu** (*Sainfort-Dubost, (1986)*)

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

High quality QC's:

**AlCuT** ( $T = Fe, Ru, Os$ )

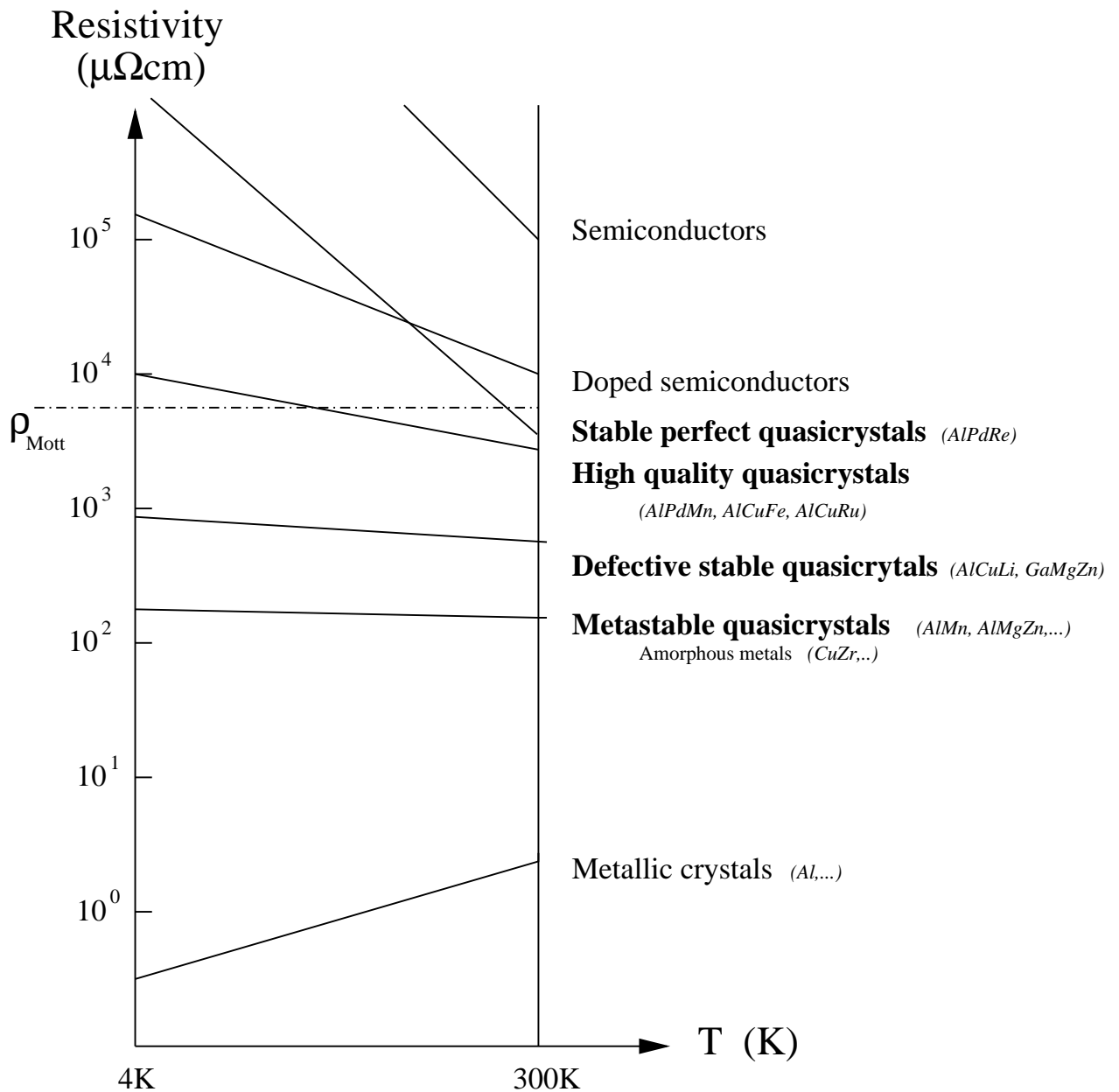
(*Hiraga, Zhang, Hirakoyashi, Inoue, (1988)*; *Gurnan et al., Inoue et al., (1989)*;

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

“Perfect” QC's:

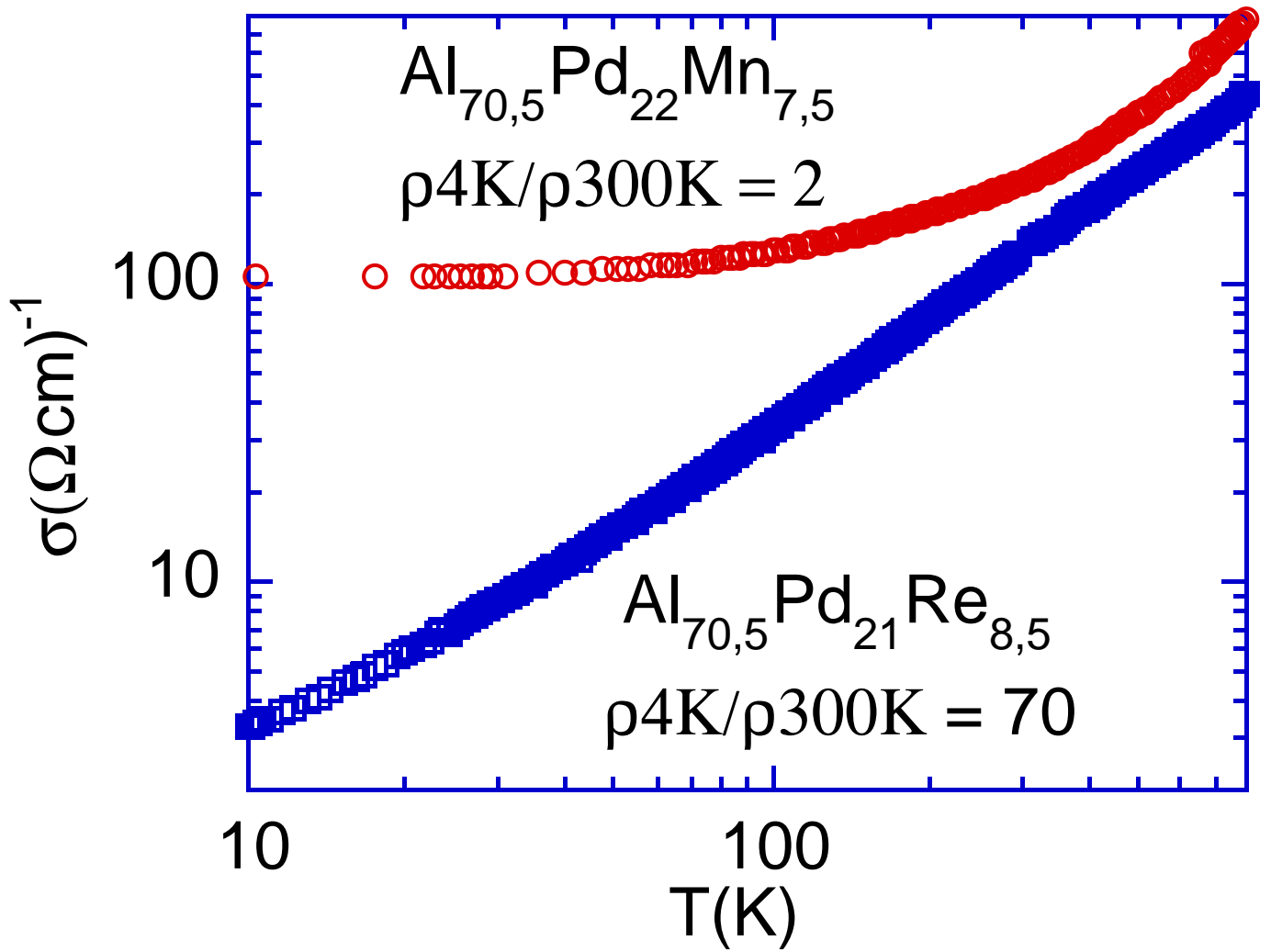
**AlPdMn**

**AlPdRe**



## Typical values of the resistivity

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



Comparison between conductivities of the two QC's

## For QC's

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

2. At high enough temperature

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

*There is a new mechanism here!*

3. At low temperature for  $\text{Al}_{70.5}\text{Pd}_{22}\text{Mn}_{7.5}$ ,

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

4. At low temperature for  $\text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5}$ ,

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

*Disorder may dominate in both alloys at very low temperature.*

## II - Dissipation: Heuristics

H. B. CALLEN, *Thermodynamics*, John Wiley & Sons, Inc., New-York, London, (1963).

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

- $\mathcal{S}$  is a system in a finite volume in  $\mathbb{R}^d$ .
- For simplicity it will be considered as classical.
- For a quantum one, the space of microstates is a Hilbert space  $\mathcal{H}$ . Probabilities are replaced by density matrices.

## II.1)- Gibbs States

- Space of microstates  $\mathcal{Q}$  (a large but finite set).
- Evolution and first integrals  $X_1, \dots, X_K$ .  
 $X_1 = U$  is the *energy*.
- $X$  is a fluctuating first integral if the system is partially open and exchange  $X$  with the outside.
- An ensemble is given by a subset  $\Phi \subset \{1, \dots, K\}$  indexing the fluctuating variables.
- The space  $\mathcal{Q}$  depends on  $\{X_\alpha; \alpha \notin \Phi\}$ .  
If  $\alpha \in \Phi$ ,  $X_\alpha$  becomes a function  $\hat{X}_\alpha(q)$ .
- The *state* of the system is a *probability* on  $\mathcal{Q}$ :

$$\mathbb{P}(q) \geq 0, \quad \forall q \in \mathcal{Q}, \quad \sum_{q \in \mathcal{Q}} \mathbb{P}(q) = 1.$$

- The *Shannon entropy* of the state is

$$s(\mathbb{P}) = (-1) \sum_{q \in \mathcal{Q}} \mathbb{P}(q) \ln \mathbb{P}(q).$$

It measures the *lack of information* contained in the state.

- The only information conserved under the evolution is the values of the first integrals  $X_1, \dots, X_K$ .
- For a fluctuating variable this value is

$$X_\alpha = \langle \hat{X}_\alpha \rangle = \sum_{q \in \mathcal{Q}} \mathbb{P}(q) \hat{X}_\alpha(q).$$

- 2nd Principle of Thermodynamics :  
*no information can be spontaneously created during the evolution.*
- A *Gibbs state* is an equilibrium state. Its entropy must be *maximal* among the states with given  $X_1, \dots, X_K$ 's. Using *Lagrange multipliers*,

$$\frac{\partial}{\partial \mathbb{P}(q)} \left( s(\mathbb{P}) - \lambda_0 \sum_{q \in \mathcal{Q}} \mathbb{P}(q) - \sum_{\alpha \in \Phi} \lambda_\alpha \langle \hat{X}_\alpha \rangle \right) = 0.$$

- The solution is

$$\mathbb{P}(q) = \frac{e^{-\sum_{\alpha \in \Phi} \lambda_\alpha \hat{X}_\alpha(q)}}{\mathcal{Z}}$$

$\mathcal{Z}$  is a normalization: the *partition function*

## II.2)- Thermodynamics

- Boltzmann's relation:

$$S = k_B s(\mathbb{P}) \quad k_B = 1.38 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$$

Where  $S$  is the *Clausius entropy*.

- Under an infinitesimal change of equilibrium:

$$T dS = dU + \sum_{\alpha=2}^K F_{\alpha} dX_{\alpha}$$

where  $F_{\alpha}$  are the *conjugate variables* and  $T$  is the *temperature*.

- It then follows

$$\Rightarrow \lambda_{\alpha} = F_{\alpha}/k_B T \quad \alpha \in \Phi$$

- The energy conjugate variable is  $F_1 = 1$ .
- The *thermodynamic potential* is

$$A_{\Phi} = -k_B T \ln \mathcal{Z} = \sum_{\alpha \in \Phi} F_{\alpha} X_{\alpha} - T S$$

$$dA_{\Phi} = \sum_{\alpha \in \Phi} dF_{\alpha} X_{\alpha} - \sum_{\alpha \notin \Phi} F_{\alpha} dX_{\alpha} - S dT$$



<i>Name of X</i>	<i>Notation <math>\hat{X}</math></i>	<i>Average</i>	<i>Conj. Var. F</i>	<i>Name of F</i>
Energy	$\hat{E}(q)$	$U$	1	$T =$ temperature
Local momentum	$\hat{p}_i(q)$ $i = x, y, z$	$\vec{p} = (p_x, p_y, p_z)$	$-\vec{v}$	$\vec{v} =$ local velocity
Angular momentum	$\hat{L}_i(q)$ $i = x, y, z$	$\vec{L} = (L_x, L_y, L_z)$	$-\vec{\omega}$	local $\vec{\omega} =$ angular velocity
Volume	$\hat{V}(q)$	$V$	$P$	$P =$ pressure
Number of particles of species $a$	$\hat{N}_a(q)$	$N_a$	$-\mu_a$	chemical $\mu_a =$ potential of species $a$
Magneti- zation	$\hat{M}_i(q)$ $i = x, y, z$	$\vec{M} = (M_x, M_y, M_z)$	$-\vec{B}$	$\vec{B} =$ magnetic field
Electric charge	$\hat{Q}(q)$	$Q$	$-\mathcal{V}$	$\mathcal{V} =$ Electric potential
Deformation tensor ( <i>in solids</i> )	$\hat{\Sigma}_{i,j}(q)$ $i, j \in \{x, y, z\}$	$\Sigma_{i,j}$	$\Pi_{i,j}$	$\Pi =$ stress tensor

## First Integrals and their Conjugate Variables in 3D

## II.3)- 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 partitionned into *mesoscopic cells*  
 the time is partitionned into *mesoscopic intervals*.
- Mesoscopic cells are *completely open* systems  
 After a time  $O(\delta t)$  they return to *equilibrium*.

- 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  $T(\vec{x},t)$ ,  $F_{\alpha}(\vec{x},t)$ 's are the conjugate variables attached to each cell and time interval.
- The average values of the first integrals are

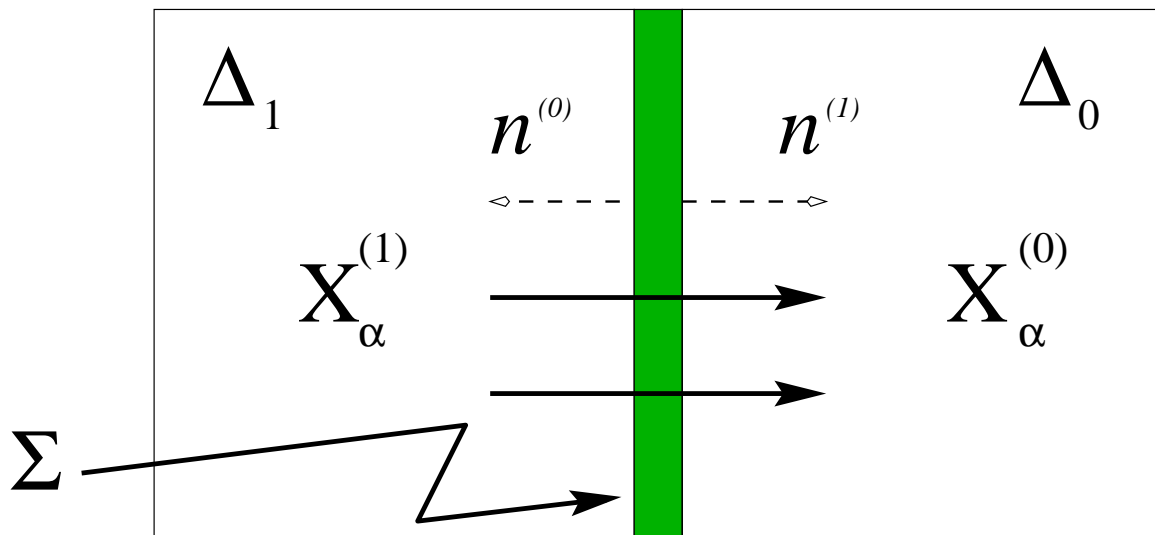
$$\delta X_{\alpha}(\vec{x},t) = \sum_{q \in \mathcal{Q}(\vec{x},t)} \mathbb{P}_{(\vec{x},t)}(q) \hat{X}_{\alpha}(q).$$

- 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

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

is the *local density* of  $X_{\alpha}$

## II.4)- 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  $X_\alpha$ .

- 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 Principle.

## II.5)- 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 Principle, 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

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

## II.5)- 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:** 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.