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

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2. Dissipation: a Heuristic Approach
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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.

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

$$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{T^{-2}}, \left(\textit{Fermi liquid theory}\right).$$

2. For a thermally activated process

$$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{e^{-\Delta/T}} \left(\textit{If a gap holds at Fermi level}\right).$$

3. For weakly disordered systems

$$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\longrightarrow} \sigma(\mathbf{0}) > \mathbf{0} \quad \left(\textit{residual conductivity}\right).$$

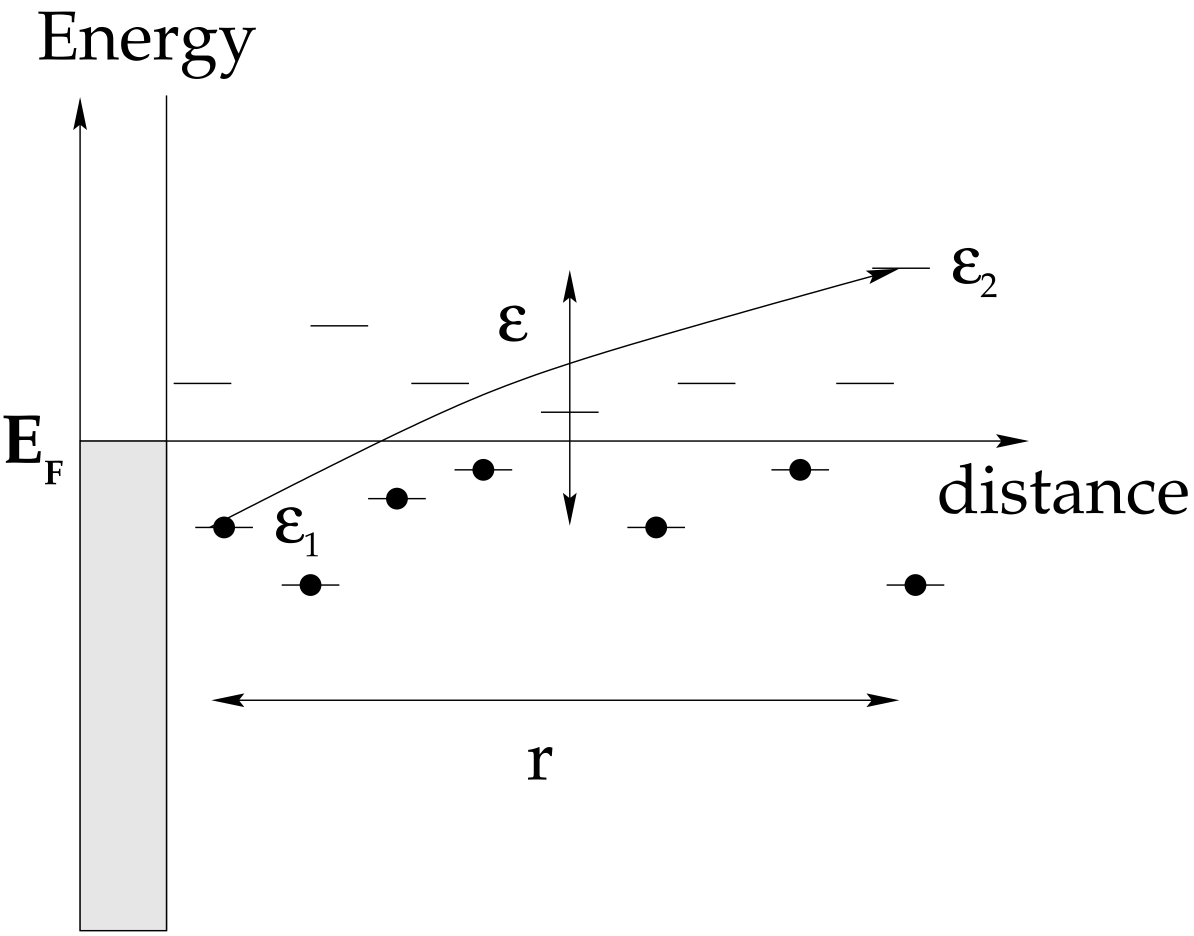
4. For strongly disordered systems in $3D$

$$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{e^{-(T_0/T)^{1/4}}} \quad \left(\textit{variable range hopping}\right).$$

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 ε

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

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

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

- Density of state at Fermi level n_F,

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

- Optimizing, the conductivity satisfies

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

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

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)*)

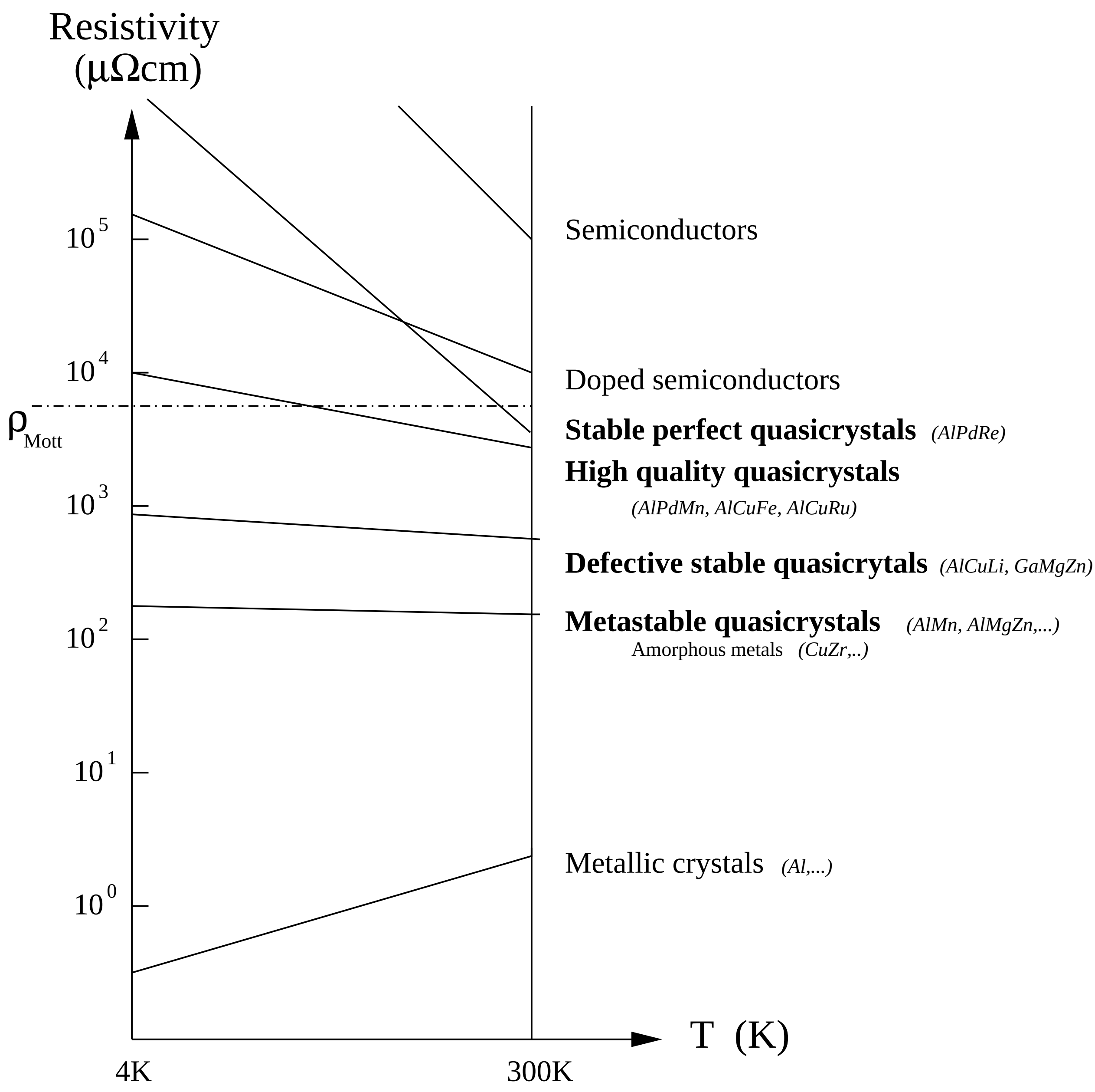
AlMnSi
AlMgT $(T = Ag, Cu, Zn)$

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)*)

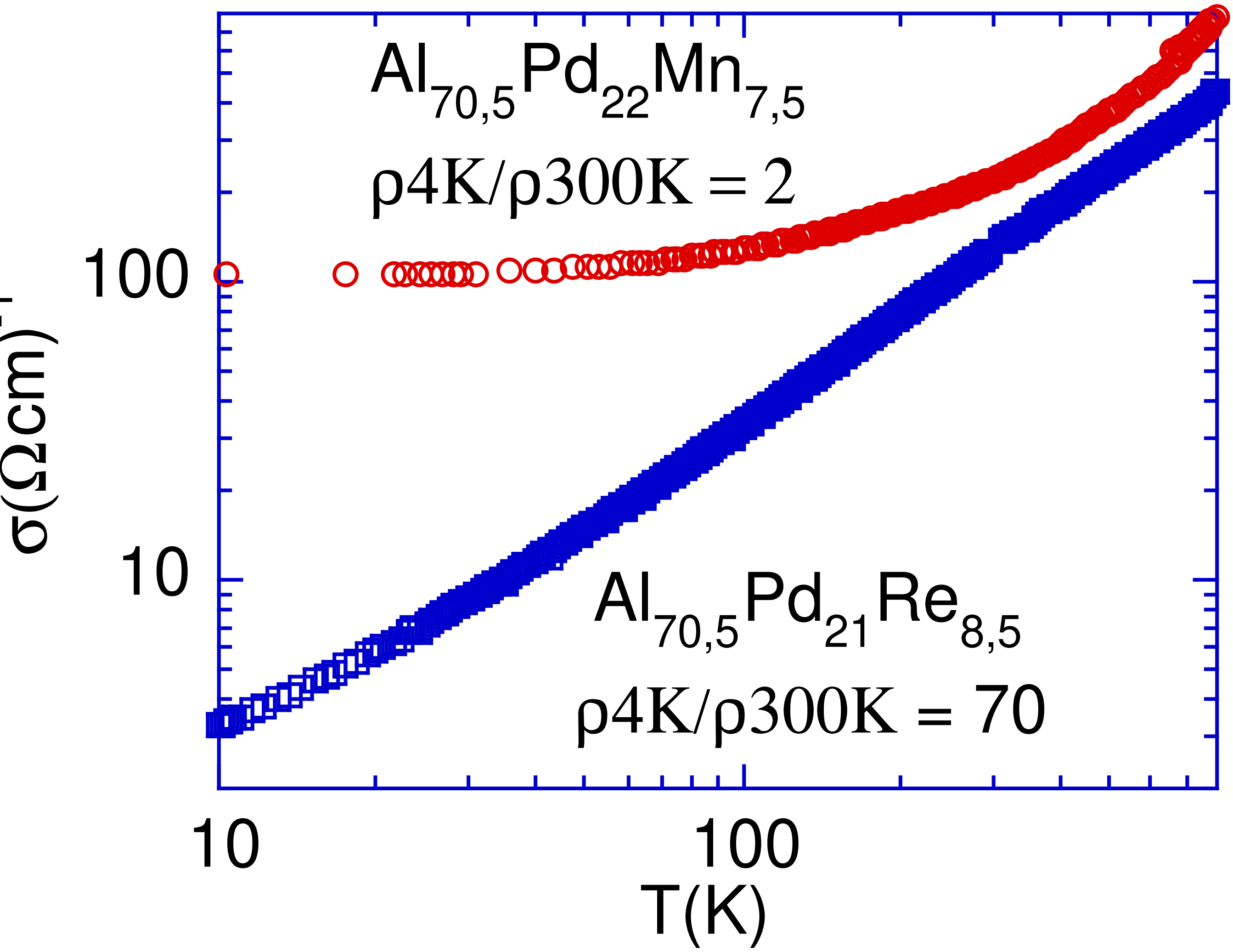
"Perfect" QC's: **AlPdMn**

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

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

   There is a new mechanism here!

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

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

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

$$\sigma \propto \mathbf{e}^{-(\mathbf{T_0}/\mathbf{T})^{\mathbf{1/4}}}$$ C. Berger *et al.* (1998)

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 $X_1, \cdots, X_K$.
  $X_1 = U$ 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 $\Phi \subset \{1, \cdots, K\}$ indexing the fluctuating variables.
- The space $\mathcal{Q}$ depends on $\{X_\alpha\,;\,\alpha \notin \Phi\}$.
  If $\alpha \in \Phi$, X_α becomes a function $\hat{X}_\alpha(q)$.
- The *state* of the system is a *probability* on $\mathcal{Q}$:

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

- 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 $X_1, \cdots, X_K$.
- 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 $X_1, \cdots, X_K$'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:

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

  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_α are the *conjugate variables*
  and T is the *temperature*.

- It then follows

$$\Rightarrow \quad \lambda_\alpha \;=\; F_\alpha / k_B T \qquad\qquad \alpha \in \Phi$$

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

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

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

Name of X	*Notation* $\hat{X}$	*Average*	*Conj. Var. F*	*Name of F*
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	$\hat{L}_i(q)$ $i = x, y, z$	$\vec{L} = (L_x, L_y, L_z)$	$-\vec{\omega}$	$\vec{\omega}$ = local angular velocity
Volume	$\hat{V}(q)$	V	P	P = pressure
Number of particles of species a	$\hat{N}_a(q)$	N_a	$-\mu_a$	μ_a = chemical 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 *(in solids)*	$\hat{\Sigma}_{i,j}(q)$ $i, j \in \{x, y, z\}$	$\Sigma_{i,j}$	$\Pi_{i,j}$	Π = stress tensor

First Integrals and their Conjugate Variables in 3D

II.3)- Local Equilibrium Approximation

- **Length Scales:**

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

ℓ is a typical *microscopic* length scale
L the typical *macroscopic* length scale.
Then δL is called *mesoscopic*.

- **Time Scales:**

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

τ_{rel} is a typical *microscopic* time scale
t the typical *macroscopic* time scale.
Then δt 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

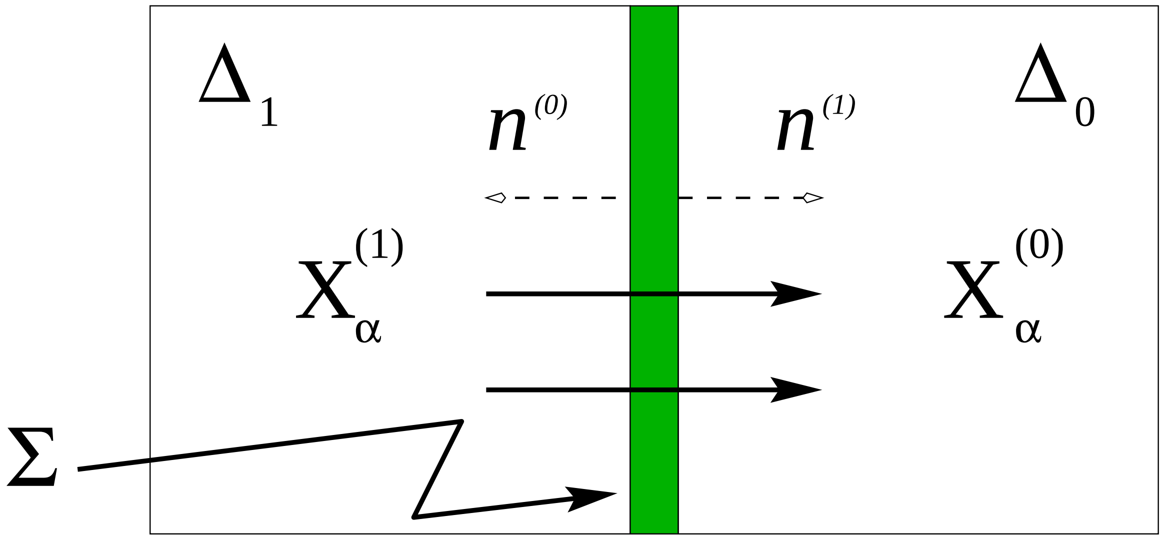
$$\delta X_\alpha(\vec{x},t) \;=\; \sum_{q \in \mathcal{Q}(\vec{x},t)} \mathbb{P}_{(\vec{x},t)}(q)\;\hat{X}_\alpha(q)\,.$$

- 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_α

II.4)- Fluxes, Currents



- Transfer of X_α from cell $\Delta^{(1)}$ to cell $\Delta^{(0)}$ across area $\delta\Sigma$ during time δt 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_α.

- Since X_α 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

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

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

II.5)- Linear Response

- A variation of the F_α/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 cœfficients*.
  - The gradient of F_α/T is an *affinity*. It plays a role similar to *forces*.

- By 2nd Principle, the positivity of entropy production rate implies

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

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

$$L_{\beta,\alpha}(\textit{parameters}) = \varepsilon_\alpha \, \varepsilon_\beta \, L^t_{\alpha,\beta}(\textit{TR-parameters}) \, .$$

II.5)- Dissipative & Nondissipative Response

- **Dissipation = Loss of Information**
  Dissipation contributes to entropy production.
  Hence
  $$\mathbb{L}^{(diss)} = \frac{1}{2}\left(\mathbb{L} + \mathbb{L}^t\right)$$

- The *nondissipative* part
  $$\mathbb{L}^{(nondis)} = \frac{1}{2}\left(\mathbb{L} - \mathbb{L}^t\right)$$
  contains quantities exhibiting *quantization* at very low temperature !
  - The *Hall conductivity* is nondissipative. It is quantized a $T = 0$.
  - 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.