# TOPICS

in

# DISSIPATIVE TRANSPORT THEORY

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# Motivations

1. To get a Kubo formula for transport cœfficients for electrons in *aperiodic solids* whenever there may be infinitely many scales of relaxation times.
2. Example of Mott's *variable range hopping* for Anderson insulators. Application to the *Quantum Hall effect*.
3. Transport in *quasicrystals*

## Assumptions

1. *Local equilibrium approximation* is valid.
2. Time and length scales:
   *microscopic* $\ll$ *mesoscopic* $\ll$ *macroscopic*
3. Beyond mesoscopic time scale
   *Markov approximation* is valid.

# Heuristics

1. A mesoscopic cell can be seen as an *infinite volume* compare to microscopic scale. But it is *infinitesimal* compare to macroscopic scale.

2. A mesoscopic cell is totally open to fluctuations of conserved quantities: the *biggest canonical ensemble* should be used.

3. After a mesoscopic time, a mesoscopic cell is at *thermal equilibrium*. The various thermodynamical quantities characterizing the equilibrium only *vary slowly in time & space* on macroscopic scale.

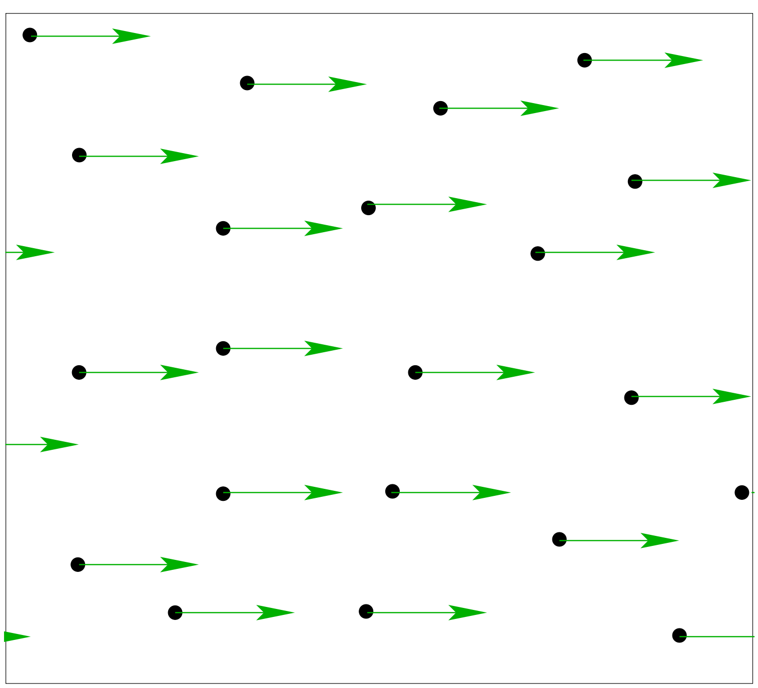
4. The dissipative dynamics in a mesoscopic cell is *Markovian*. It is described by a *Master Equation*

$$\frac{dA}{dt} = \mathfrak{L}(A) = \imath[\hat{H} - \mu\hat{N}, A] - \mathfrak{D}(A)$$

generating a *completely positive contractive semigroup*. The Hamiltonian part is called *Gibbs dynamics*.

# Aperiodicity

1. The atomic nuclei of an aperiodic solid are located on a *uniformly discrete* subset of $\mathcal{L} \subset \mathbb{R}^d$. In most cases $\mathcal{L}$ is also *relatively dense*, hence a *Delone* set.
2. The closure of the family of translated of $\mathcal{L}$ w.r.t. topology of convergence on compact subsets of $\mathbb{R}^d$ is a metrizable compact set $\Omega$ called the *Hull*.
3. Each element $\omega \in \Omega$ gives a uniformly discrete subset $\mathcal{L}_\omega$ which Delone if $\mathcal{L}$ is.



- *Building the Hull* -

# Second Quantization

1. Tight-binding second quantized electrons are represented by *fermion creation annihilation operators* (with $\sigma, \tau \in \{\uparrow, \downarrow\}$)

$$f_{\omega,x,\sigma} f^{\dagger}_{\omega,y,\tau} + f^{\dagger}_{\omega,y,\tau} f_{\omega,x,\sigma} \;=\; \delta_{x,y}\delta_{\sigma,\tau}\,,$$
$$f_{\omega,x,\sigma} f_{\omega,y,\tau} + f_{\omega,y,\tau} f_{\omega,x,\sigma} \;=\; 0 \qquad (x, y \in \mathcal{L}_\omega)$$

2. For $\Lambda \subset \mathbb{R}^d$ bounded, $\mathfrak{A}_\omega(\Lambda)$ is the $C^*$-algebra generated by the $f_{\omega,x,\sigma}$'s for $x \in \mathcal{L}_\omega \cup \Lambda$. Then $\mathfrak{A}_\omega$ is the completion of $\bigcup_{\Lambda \uparrow \mathbb{R}^d} \mathfrak{A}_\omega(\Lambda)$ *(Haag, Kastler '64)*.

3. The field $(\mathfrak{A}_\omega)_{\omega \in \Omega}$ is *continuous* *(Tomiyama '62)* and *covariant*: $\exists$ a continuous family of $*$-isomorphisms

$$\eta_{\omega,a} : \mathfrak{A}_{\mathrm{T}^{-a}\omega} \mapsto \mathfrak{A}_\omega$$
$$\eta_{\omega,a} \circ \eta_{\mathrm{T}^{-a}\omega,b} = \eta_{\omega,a+b}$$

   defined by

$$\eta_{\omega,a}\left(f_{\mathrm{T}^{-a}\omega,x,\sigma}\right) = f_{\omega,x+a,\sigma}$$

# Existence Theorems

1. The generator of the dissipative evolution belongs to the class of operators of the form $\mathfrak{L} = \imath[\hat{H}, \cdot] - \mathfrak{D}$ with *covariant random operators* as follows

$$\hat{H}_\omega = \sum_{X \subset \mathcal{L}_\omega} H_{\omega,X} \qquad H_{\omega,X} = H^\dagger_{\omega,X} \in \mathfrak{A}_\omega(X)$$

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

$$L_{\omega,X} \in \mathfrak{A}_\omega(X)\,, c_\omega(X,Y) \in \mathbb{C} \quad \sum_{m,n} \overline{\lambda_m}\,\lambda_n\, c_\omega(X_m, X_m) \geq 0$$

2. *Covariance* means

$$\eta_{\omega,a}(A_{\omega,X}) = A_{\mathrm{T}^a\omega, X+a} \qquad c_{\mathrm{T}^a\omega}(X+a, Y+a) = c_\omega(X,Y)$$

3. If $r > 0$ set *(Bratteli, Robinson '76)*

$$|||\mathfrak{L}|||_r = \sup_\omega \sum_{0 \in X} e^{r|X|} \|H_X\| + \sum_{0 \in X,Y} e^{r(|X|+|Y|)} |c(X,Y)| \|L_X\| \|L_Y\|$$

**Theorem 1** *Let $\mathfrak{L}_\omega$ be defined as before. If for some $r > 0$, $|||\mathfrak{L}_\omega|||_r < \infty$, then $(exp(t\mathfrak{L}_\omega))_{t>0}$ defines a norm pointwise continuous completely positive semigroup on the $C^*$-algebra $\mathfrak{A}_\omega$. The corresponding field of such semigroups is covariant and continuous.*

**Remarks:** (i) if quasilocal algebras includes bosons, some of the $H_X$'s or the $L_X$'s may be unbounded. Using a modified norm for them leads to a similar result.

(ii) In most results found in the literature the semigroup is well defined but does not leaves $\mathfrak{A}$ invariant.

(iii) *Matsui ('93)* has weakened significantly the conditions for existence of the Markov semigroup.

# Phenomenology: Approximations

In general the dissipative evolution described by $\mathfrak{L}$ does not converge to an equilibrium state. However some simplification arises in practice

1. **Independent electrons approximation:** when the Fermi liquid theory applies, electrons can be considered as independent quasi particles. The existence of equilibrium state becomes elementary then (perfect Fermi gas).

2. **Adiabatic approximation:** the frequencies involved in the Gibbs dynamics are large compare with the one describing the dissipative part. The dissipative part may be replaced by its time average $\mathfrak{D}_0$ *w.r.t.* the Hamiltonian dynamics which commutes with the Hamiltonian part.

Then models for the *equilibrium dissipative dynamics* $\mathfrak{D}_0$ can be described *axiomatically.*

# Axioms

The *equilibrium dynamics* is defined by

$$\mathfrak{L} = \imath[H, \cdot] + \mathfrak{D} \qquad \text{“}H = H^*\text{”}$$

where the dissipative part $\mathfrak{D}$ satisfies

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

1. $\mathfrak{J}$ is a countable set *(or a continuum if the sum is replaced by integrals)*, the set of *jumps*,
   There is an involution $x \mapsto \overline{x}$, *(time reversal)*.
2. For each $x$, $L_x \in \mathfrak{A}$ and satisfies
   (a) *Jumps*: $\exists \epsilon_x \in \mathbb{R}$ such that $[H, L_x] = \epsilon_x L_x$,
   (b) *Detailed balance*: $L_{\overline{x}} = e^{\beta\epsilon_x/2} L_x^*$
3. *Convergence*: $|||\mathfrak{D}|||_r < \infty$
4. *Irreducibility*: The commutant of the $L_x$'s is trivial

# Comments

*(Frigerio '78)*

1. Axiom 1: describes the possible dissipative mechanisms including time reversal symmetry,

2. Axiom 2: the Gibbs state at temperature $\beta$ relative to $H$ is invariant by the dynamics.

   It is equivalent to saying that $\mathfrak{D}$ defines a positive operator in the GNS representation of the equilibrium state:

$$\rho_{eq}(A^*\mathfrak{D}(A))\rangle = \sum_{x\in\mathfrak{J}} \rho_{eq}(|[L_x, A]|^2) \geq 0$$

3. Axiom 3: the dynamics is well-defined,

4. Axiom 4 : the equilibrium state is *unique*.
   It also implies that $\mathfrak{L}$ is *invertible* when restricted to the subspace $\eta(\mathbf{1})^\perp$ of the GNS representation perpendicular to the cyclic vector.

# Ex.: Quantum Jump Models

The class of *Quantum Jump Models* provides many practical examples. In *finite volume* it goes as

1. The Gibbs dynamics is given as the *second quantized* of a 1-particle dynamics $H_1$ on the lattice. Then let $|i\rangle\,,\ 1 \leq i \leq N$ be a complete set of eigenvectors $H_1$ corresponding to energy $\epsilon_i$.
2. The set of jumps $\mathfrak{J}$ is given by pairs $(i,j) \in [1,N]^{\times 2}$ such that $i \neq j$.
3. Let $b_i^\dagger$ be the creation operator for a particle in state $|i\rangle$. Then $L_{ij} = \sqrt{\gamma_{ij}}\ b_j^\dagger b_i$
   Here $\gamma_{ij} \geq 0$ represents the probability of a *jump* from state $i$ to state $j$.
4. To account for the heat bath it is convenient to add $b_\infty^\dagger = \mathbf{1}$ with an energy $\epsilon_\infty = \mu$ *(chemical potential)*.

All axioms are satisfied with $\epsilon_{ij} = \epsilon_j - \epsilon_i$.

# Quantum Jump *vs.* $XY$ Models

*(JB '04)*

The dissipative part of the Quantum Jump model, expressed as a positive operator in the GNS representation of the equilibrium state is equivalent to an $XY$-model of the form:

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

where the $\vec{S}_i$'s and the $\vec{T}_i$'s are spin-1/2 operators on the sites $i$'s such that $T_i^3S_i^3 = S_i^3T_i^3 = 0$

UNEXPECTED !!

# 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.

# Mesoscopic Currents

1. The charge position operator $\vec{R}_e = (R_1, \cdots, R_d)$ is defined as $\vec{R}_e = -e \sum_{x \in \mathcal{L}_\omega} f^\dagger_{\omega,x,\sigma} f_{\omega,x,\sigma}\ \vec{x}$. More precisely it defines a *$*$-derivation* $\vec{\nabla}_e = \imath[\vec{R}_e, \ \cdot\ ]$ 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*.
   Again this is defined as a *$*$-derivation* on $\mathfrak{A}$.

3. The electronic energy can also be localized through $\vec{R}_u = \sum_{x,y \in \mathbb{Z}^d} h_\omega(x,y) f^\dagger_{\omega,x,\sigma}\ f_{\omega,y,\sigma}\ (\vec{x} + \vec{y})/2$ if $h_\omega(x,y)$ are the matrix elements of the 1-particle Hamiltonian. Correspondingly the *mesoscopic energy current* is given by

$$\vec{J}_u \;=\; \frac{d\vec{R}_u}{dt} \;=\; \mathfrak{L}(\vec{R}_u)$$

# 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

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

2. Hence the current becomes

$$J^{\mathcal{E},i}_\alpha \;=\; J^i_\alpha + \sum_{\alpha',j} \mathcal{E}^j_{\alpha'} \mathfrak{L}^j_{\alpha'}(R^i_\alpha) + O(\mathcal{E}^2)$$

3. Then, if the forces are constant in time

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

4. A first order expansion in $\mathcal{E}$ gives the following formula
$$\vec{j}^{\,i}_{\alpha} = \sum_{\alpha',j} L^{i,j}_{\alpha,\alpha'} \mathcal{E}^{j}_{\alpha'} + O(\mathcal{E}^2)$$
where the *Onsager cœfficients* $L^{i,j}_{\alpha,\alpha'}$ are given by the *Greene-Kubo* formula

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

**Remark:**

1. The Greene-Kubo formula is valid because Axiom 4 insures that $\mathfrak{L}$ can be inverted.
   The coherent part is *anti-selfadjoint* while the dissipative part is *positive*.
2. 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.
3. AC-conductivity can also be obtained using a Floquet type approach *(Schulz-Baldes, Bellissard '98)*

# Invertibility of $\mathfrak{L}$

1. The Laplace transform gives $-\mathfrak{L}^{-1} = \int_0^\infty ds\, e^{s\mathfrak{L}}$. Hence the inverse can be estimated in terms of convergence of the dynamics at long time.
2. Finite volume models might suffice here if estimates are uniform in the volume.
3. The relative entropy of two density matrices $\rho, \rho_0$ is given by $H(\rho|\rho_0) = \mathrm{Tr}\,(\rho(\ln \rho - \ln \rho_0))$ Extension to $C^*$-algebras has also been defined *(Araki)*.
4. The relative entropy $H(\rho_t|\rho_{eq})$ is *non increasing* in time. Moreover, if Axiom 4 holds $\rho_t$ converges to $\rho_{eq}$. *(Lindblad '76)*.
5. There is a metric (the *Wasserstein distance* $d_W$) on the set of states, defining the weak topology, such that $d_W(\rho_t, \rho_{eq}) \leq H(\rho_t|\rho_{eq})$.
   *(Talagrand '96, Voiculescu-Biane '01)*
6. Consequently one may expect to get an estimate of the conductivity in terms of the *convergence of the relative entropy to zero*.

# Information Inequalities

1. For the case of the Boltzmann equation, the relative entropy can be estimated in terms of the Fisher information and a log-Sobolev inequality permits to estimate the Fisher information in terms of the relative entropy. Hence one gets the rate of decay of the relative entropy *(Carlen '91, Carlen-Carvalho '92)*.
2. These inequalities are now used to get convergence results in PDE's such as the Fokker-Planck, porous media, Fokker-Planck-Landau or various versions of the Boltzmann equations *(Villani-Desvillette '01)*.
3. Some of these inequalities have been extended to Fermion systems at infinite temperature *(Carlen-Lieb '93)*.
4. There are reasons to expect that these techniques extend to Quantum Jump Models *(JB, Carlen, Loss in progress)*.

# Conclusions

1. Nonequilibrium Thermodynamics in the *linear response theory* applies to the electron gas in a solid, periodic or not.
2. Various approximations leads to *Quantum Jump Models* as a paradigm for the mesoscopic description of local dissipative dynamics.
3. A *Kubo formula* for transport cœfficients has been derived and it validity is controlled by the invertibility of the equilibrium Lindblad operator.
4. Control of this inverse might eventually be obtained through *information inequalities* in a way similar to the classical Boltzmann equation.
5. An unexpected relation between the dissipative part of the Lindblad operator and a class of $XY$*-models* has been found, raising the question of whether information estimates could be used in Quantum Spin models to study the *low lying spectrum*.