KUBO'S FORMULA

for

QUANTUM TRANSPORT

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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. Accuracy of plateaus in the Quantum Hall Effect: Mott variable range hopping.
5. Anomalous quantum diffusion in aperiodic media

Few Mechanisms

1. For metals, $\sigma(\mathbf{T})$ increases as temperature decreases

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

2. For a thermally activated process

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

3. For weakly disordered systems

$$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\rightarrow} \sigma(\mathbf{0}) > \mathbf{0} \ \ \big(\textit{residual conductivity}\big).$$

4. For strongly disordered systems in $3D$

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

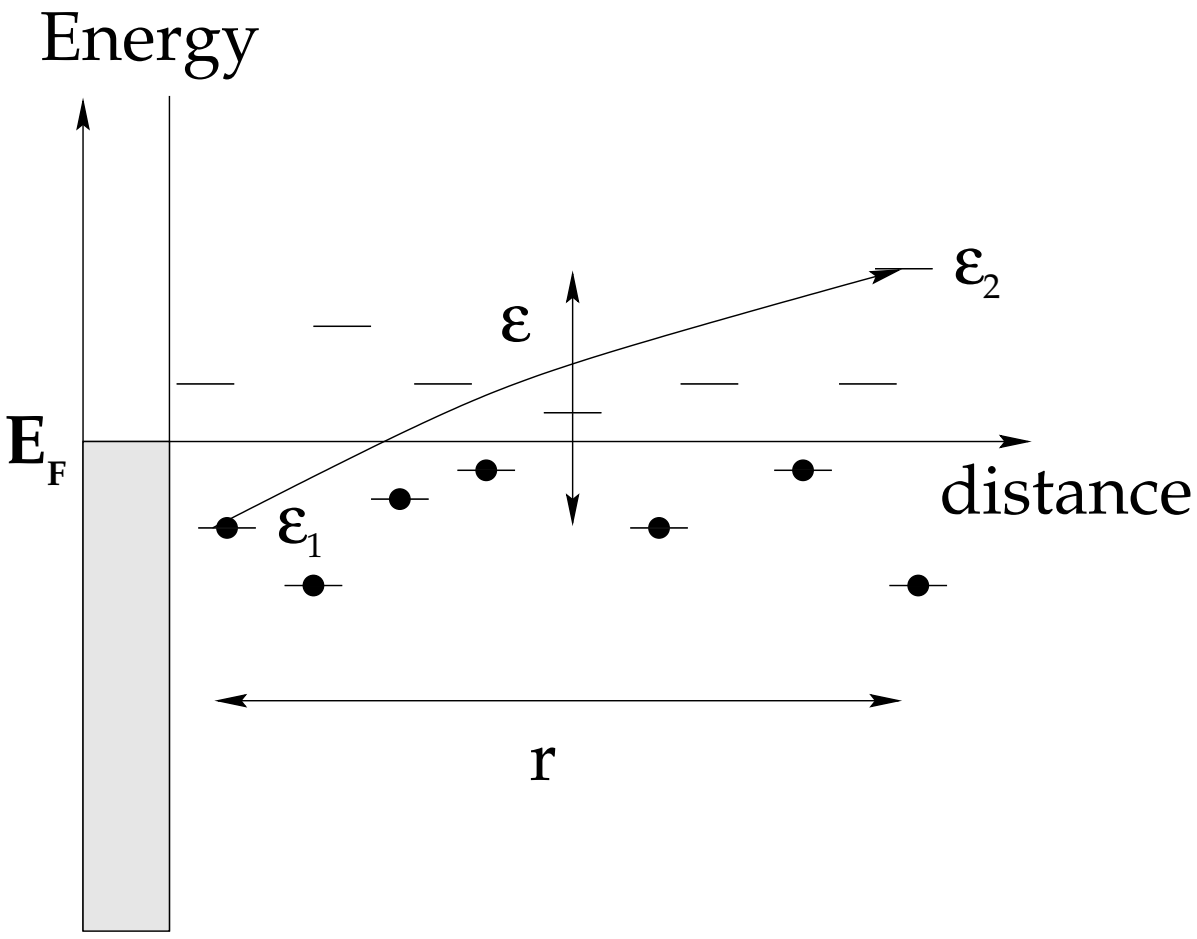
5. For quasicrystals

$$\sigma(\mathbf{T}) \sim \sigma_{\mathbf{0}} + \mathbf{aT}^{\gamma} \ \ \big(1 < \gamma < 1.5 \ \ a > 0\big).$$

Mott's variable range hopping

N. Mott, (1968).

B. Shklovskii, A. L. Efros, *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

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

- Tunneling 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

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

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

Questions

1. Is it possible to develop a rigorous mathematical theory of quantum transport valid also for aperiodic (ordered ou disordered) media ?
2. What are the important open problems ?
3. Can one give original contributions liable to be relevant in real physics ?

Difficulties

1. Dissipative transport theory requires playing with several scales of time, space, energy. Notion of *effective theory* valid at a given scale.
2. Illustration in this talk with Mott's *Variable Range Hopping model (VRH)*

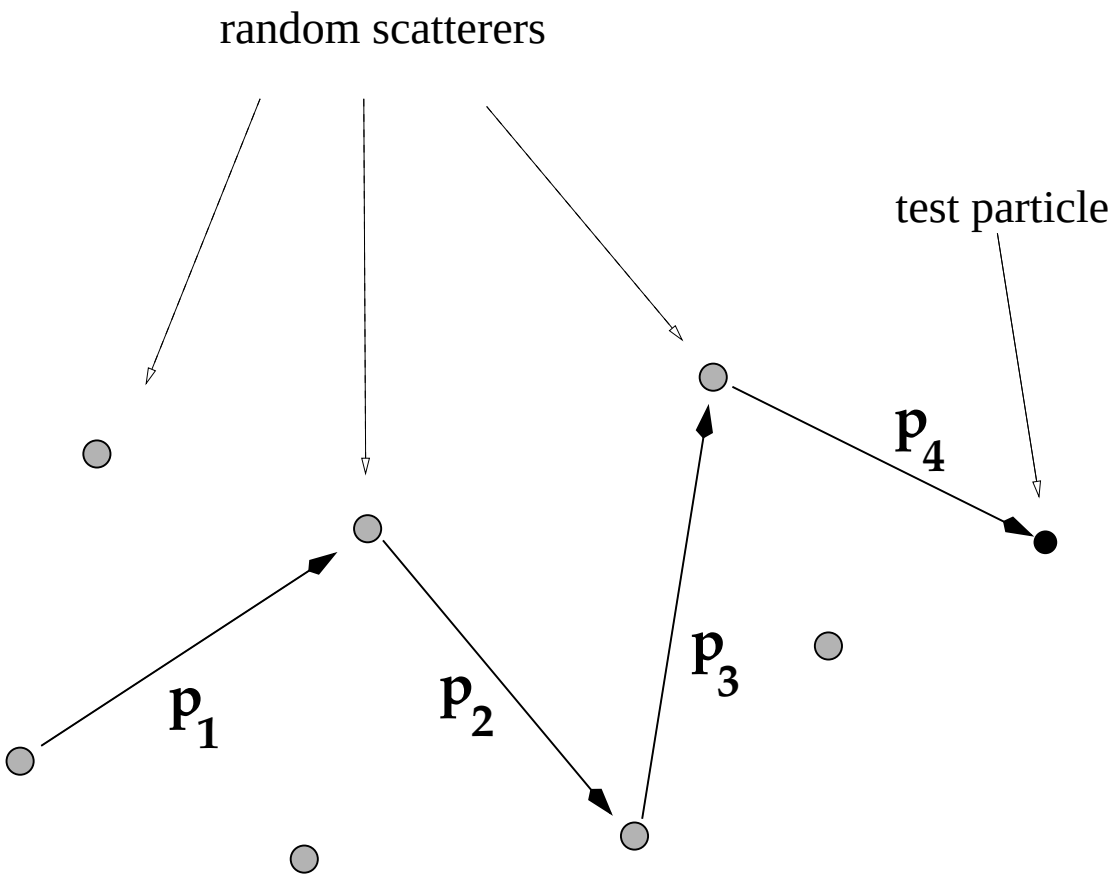
The Drude Model

Assumptions :

1. Electrons in a metal are free classical particles of mass m_* and charge q.
2. They experience collisions at random Poissonnian times $\cdots < t_n < t_{n+1} < \cdots$, with average relaxation time τ_{rel}.
3. If p_n is the electron momentum between times t_n and t_{n+1}, p_{n+1} is updated according to Maxwell's distribution at temperature T.

Then the conductivity is given by the *Drude formula*

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



The Drude Kinetic Model

The Kubo Formula (*Relaxation time approximation*)

(*Bellissard, Schulz-Baldes '95*)

1. Replace the classical dynamics by the quantum one electron dynamic in the aperiodic solid.
2. At each collision, force the density matrix to come back to equilibrium. (*Relaxation time Approximation* or RTA).
3. Stochastic dynamics:
   (a) initial density matrix $\rho_{eq.}$ is the equilibrium one:

$$\rho_{eq.} = \frac{1}{1+e^{\beta(H-\mu)}},$$

   where $\beta = 1/k_B T$, μ is the chemical potential, H the one particle Hamiltonian.
   (b) For $t_n \leq t < t_{n+1}$

$$\rho(t) = e^{-(t-t_n)\mathcal{L}_H}\rho_n, \qquad \mathcal{L}_H = \frac{\imath}{\hbar}[H,\cdot]$$

   (c) At each collision n update the state to $\rho_{n+1} = \rho(t_{n+1}+0) = \rho_{eq.}$
   (d) Compute the averaged thermodynamical current as a function of the electric field $\vec{\mathcal{E}}$, average it over the random collisions and compute the term linear in $\vec{\mathcal{E}}$.

4. There is only one *relaxation time* τ_{rel}. The electric conductivity is then given by Kubo's formula:

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

$q =$ charge of carriers,

$\beta = 1/k_B T\,,$ $\qquad\qquad$ $\mu =$ chemical potential

$\mathcal{L}_H = \imath/\hbar\,[H,.]$

$\partial_j A = \imath[X_j, A]$

$\mathcal{T}_{\mathbb{P}} =$ trace per unit volume.

5. For the Hilbert-Schmidt inner product defined by $\mathcal{T}_{\mathbb{P}}$, $\mathcal{L}_H$ is *anti-selfadjoint*. Thus as $\tau_{rel} \uparrow \infty$, the resolvent of $\mathcal{L}_H$ is evaluated closer to the spectrum near 0.

Transport Exponents (*coherent transport*)

1. For $\Delta \subset \mathbb{R}$ Borel, let $P_{\Delta,\omega}$ be the corresponding spectral projection of H_ω. Set:

$$\vec{X}_\omega(t) \;=\; e^{\imath t H_\omega}\, \vec{X}\, e^{-\imath t H_\omega}$$

2. The averaged spread of a typical wave packet with energy in Δ is measured by:

$$L^{(p)}_\Delta(t) \;=\; \left(\int_0^t \frac{ds}{t} \int_\Omega d\mathbb{P}\, \langle x | P_{\Delta,\omega} | \vec{X}_\omega(t) - \vec{X} |^p P_{\Delta,\omega} | x \rangle \right)^{1/p}$$

3. Define $\beta = \beta^\pm_p(\Delta)$ so that $L^{(p)}_\Delta(t) \sim t^\beta$
   (take the relevant lim sup *or* lim inf *for* $\pm$ *resp.)*

4. $\beta^-_p(\Delta) \leq \beta^+_p(\Delta)$. $\beta^\pm_p(\Delta)$ is non decreasing in p.

5. *Heuristic*
   $\beta = 0 \rightarrow$ absence of diffusion (*ex: localization*),
   $\beta = 1 \rightarrow$ ballistic motion (*ex: in crystals*),
   $\beta = 1/2 \rightarrow$ quantum diffusion (*ex: weak localization*).
   $\beta < 1 \rightarrow$ subballistic regime,
   $\beta < 1/2 \rightarrow$ subdiffusive regime (*ex: in quasicrystals*).

The Anomalous Drude Formula

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

$$\sigma \overset{\tau_{rel} \uparrow \infty}{\sim} \tau_{rel}^{2\beta_F - 1}$$

where β_F is the transport exponent $\beta_2(E_F)$ evaluated at Fermi level.

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. For $1/2 < \beta_F \leq 1$, $\sigma \uparrow \infty$ as $T \downarrow 0$: the system behaves as a conductor.
4. If $\beta_F = 1/2$ (*quantum diffusion*), $\sigma \sim const.$: residual conductivity at low temperature.
5. For $0 \leq \beta_F < 1/2$, $\sigma \downarrow 0$ as $T \downarrow 0$: the system behaves as an insulator.

Comments

1. The anomalous Drude formula seems to be observed in several experiments *(relevance for practical purposes)*.

2. If $\beta_F < 1/2$ the *longest relaxation time dominate*. Hence the Bloch law $\tau_{rel} \sim T^{-5}$ due to electron-phonon coupling, becomes more important than the Fermi liquid prediction $\tau_{rel} \sim T^{-2}$.

3. In the strong localization regime, $\beta_F = 0$ and Mott's argument shows that there is an *infinite family of relaxation times*.

4. Need for a more sophisticated tool of calculation to treat these problems. Need for more systematic theory to account for the physics out of equilibrium.

A Variable Range Hopping model

(*Bellissard, Rebolledo, Spehner, v. Waldenfels '99-04*)

1. One-electron Hamiltonian given by the *Anderson model at strong disorder* on $\mathbb{Z}^d$.
   Energy within $O(k_B T)$ from the Fermi level.
   Thanks to *SULE* eigenstate ϕ_i localized at x_i with energy ϵ_i (*Klein et al.*)

2. Phonon absorption induces jumps from states $i \longrightarrow j$ at Poissonian times with parameter (*Mott assumptions*)

$$\Gamma_{i\to j} = \Gamma_0 e^{-\beta(\epsilon_j - \epsilon_i)_+ - |x_i - x_j|/\xi}$$

   ξ = *localization length* (tunneling distance).

3. Use second quantization to take fermion statistics into account: *jumps operators* are given by

$$W_{i\to j} = b_j^\dagger b_i$$

   $b_i^\dagger$, b_i = *creation, annihilation operators* of a fermion in state i.

4. The solid acts as a *thermal bath* represented by fictitional state $i = \infty$ with energy $\mu =$ *chemical potential* (keeping the electron density fixed) and $b_\infty = b_\infty^\dagger = \mathbf{1}$ and

$$\Gamma_{i\to\infty} = \Gamma_0 e^{-\beta(\mu-\epsilon_i)_+}\,,\ \Gamma_{\infty\to i} = \Gamma_0 e^{-\beta(\epsilon_i-\mu)_+}$$

In particular an electron in the state i can be created at out of the bath or can be annihilated in the bath. This is because the *system* is made only of electrons within a given energy interval, the rest being *in the bath*.

Variable Range Hopping : Dynamics

The dissipative dynamical evolution of the state of the previous *Variable Range Hopping Model (VRHM)* model is described by a *master equation*

$$\frac{d\rho}{dt} \;=\; \mathfrak{L}^{\dagger}\rho\,, \qquad\qquad \mathfrak{L} \;=\; \imath[\hat{H}-\mu\hat{N},\cdot]+\mathfrak{D}\,.$$

where $\mathfrak{L}$ acts on the *quasilocal observable algebra* $\mathfrak{A}$, (generated by the b_i's), ρ is the state of the system, $\hat{H}$ is the second quantization of the one-particle Hamiltonian, $\hat{N}$ is the particle number and the *dissipative part* $\mathfrak{D}$ is given by

$$\mathfrak{D}(A) \;=\; \sum_{i\neq j}\Gamma_{i\to j}\left(W^{\dagger}_{i\to j}AW_{i\to j}-\frac{1}{2}\{W^{\dagger}_{i\to j}W_{i\to j},A\}\right)$$

for $A\in\mathfrak{A}$.

Remark: since $\hat{H}$ is random, the b_i , $b_i^{\dagger}$'s and the $\Gamma_{i\to j}$ are random too, so are $\mathfrak{D}$ and $\mathfrak{L}$ and satisfy a *covariance condition*: if T is the automorphism group of $\mathfrak{A}$ implementing the translation group

$$\mathrm{T}^{a}\circ\mathfrak{L}_{\omega}\circ\mathrm{T}^{-a} \;=\; \mathfrak{L}_{\mathrm{T}^{a}\omega}\,, \qquad\qquad a\in\mathbb{Z}^{d}$$

Existence Theorems

1. The observable algebras $\mathfrak{A}$ is the completion of the union $\cup_{\Lambda\uparrow\mathbb{Z}^d}\,\mathfrak{A}_\Lambda$ where $\mathfrak{A}_\Lambda$ is the C^*-algebra generated by the b's corresponding to states supported in the *finite set* Λ *(Haag, Kastler '64)*.

2. 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

$$\hat{H}_\omega \;=\; \sum_{X\subset\mathbb{Z}^d} H_{\omega,X} \qquad\qquad H_{\omega,X} = H^\dagger_{\omega,X} \in \mathfrak{A}_X$$

$$\mathfrak{D}(A) \;=\; \sum_{X,Y\subset\mathbb{Z}^d} c_\omega(X,Y)\left(L^\dagger_{\omega,X}AL_{\omega,Y} - \frac{1}{2}\{L^\dagger_{\omega,X}L_{\omega,Y},A\}\right)$$

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

3. *Covariance* means

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

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

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

The following is true *(Bellissard, Rebolledo '04)*

Theorem 1 *Let $\mathfrak{L}$ be defined as before. If there is $r > 0$ such that $|||\mathfrak{L}|||_r < \infty$, then $(exp(t\mathfrak{L}))_{t>0}$ defines a norm pointwise continuous completely positive semigroup on the C^*-algebra $\mathfrak{A}$.*

Remarks: (i) the previous result includes quasilocal algebras with bosons where the H_X's or the L_X's may be unbounded.

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

Theorem 2 *Let $\mathfrak{L}$ be the generator of the VRHM. Under this evolution, every initial state converges to the Gibbs state associated with the Anderson Hamiltonian with temperature β and chemical potential μ.*

Derivation of Greene-Kubo Formulæ

1. The charge position operator $\vec{R}_e = (R_1, \cdots, R_d)$ is formally defined as $\vec{R}_e = -e \sum_{x \in \mathbb{Z}^d} b_x^\dagger b_x \, \vec{x}$. 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 $\vec{R}_u = \sum_{x,y \in \mathbb{Z}^d} h_\omega(x,y) b_x^\dagger b_y \ (\vec{x} + \vec{y})/2$ if $h_\omega(x,y)$ are the matrix elements of the one-particle Hamiltonian. Correspondingly the *mesoscopic energy current* is given by

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

4. 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

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

5. Hence the current becomes

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

6. Then, if the forces are constant in time

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

7. 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 provided $\mathfrak{L}$ can be inverted. By analogy with the RTA, the coherent part is *anti-selfadjoint* while the dissipative part is *hopefully* positive and should allow invertibility in general.
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.

The VRH Model

1. At very low temperature, the dissipative part is likely to be small. Ignoring it leads to use the *one-particle current-current correlation function* defined by

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

   for f, g continuous functions with compact support.

2. Since the coherent part of the VRHM is Anderson's model at high disorder the $L^{(2)}$-localization length is finite *(Bellissard, van Elst, Schulz-Baldes '94)*

$$L^{(2)}_{\Delta} = \lim_{t\to\infty} L^{(2)}_{\Delta}(t) = \int_{\Delta\times\mathbb{R}^2} \frac{dm(E,E')}{|E-E'|^2} < \infty$$

3. Consequently the Onsager cœfficients *vanishes at zero dissipation*. In particular the lowest order contribution to the conductivity is given by the first order expansion in $\mathfrak{D}$.

   (study under progress : Schulz-Baldes & Spehner, Bellissard & Hislop)

Conclusion

1. The VHRM gives a good illustration of the difficulties in dealing with dissipative transport and linear response theory.
2. A more systematic way to present the foundation of linear response theory is available:
   (a) local equilibrium approximation: time & length scales
   (b) mesoscopic currents and continuity equations: conservation laws
   (c) linear response theory: Onsager's cœfficients, reciprocity relations, positivity
3. Microscopic theory requires completely positive evolution: Markov approximation valid beyond mesoscopic scale
   $\Rightarrow$ Markov semigroup.
4. Lindblad's theorem characterizes such semigroups on $\mathcal{B}(\mathcal{H})$. Extension to C^*-algebras needed.
5. Problem: criterion for the invertibility of the Lindbladian
6. Study the regularity properties of the current-current correlation functions to get behaviour of transport cœfficient in terms of external parameters.