Linear Response for Non-Equilibrium Steady States of Open Quantum Systems

Joint work with

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Summary

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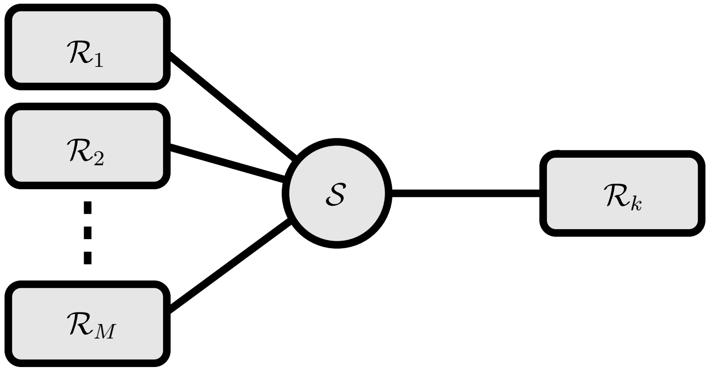
1. Thermally driven open quantum systems



Small system $\mathcal{S}$ — spatially confined, discrete spectrum
coupled to
ideal thermal reservoirs $\mathcal{R}_1, \ldots, \mathcal{R}_M$ — spatially extended ideal quantum gases
trough
junctions — interactions between $\mathcal{S}$ and $\mathcal{R}_k$.

Conserved extensive quantities A_k of $\mathcal{R}_k$ (e.g. energy $H_{\mathcal{R}_k}$, mass $M_{\mathcal{R}_k}$, charge $Q_{\mathcal{R}_k}$, ...) can cross the junction and flow through the system $\mathcal{S}$. The corresponding outgoing fluxes are

$$\Phi_{A_k} = -\left.\frac{d\,A_k}{dt}\right|_{t=0} = -\,i[H\,,A_k].$$

At joint thermal equilibrium

$$\langle \Phi_{A_k} \rangle_{\mathrm{eq}} = 0.$$

Under the joint dynamics initial state $\langle\,\cdot\,\rangle_0$ with inhomogeneous intensive thermodynamic parameters evolves towards steady state $\langle\,\cdot\,\rangle_+$ which may support non-trivial currents

$$\langle \Phi_{A_k} \rangle_+ \neq 0.$$

Calculating these currents is the main problem of Non-Equilibrium Statistical Mechanics of Open Quantum Systems.

2. NESS: Formal calculations of steady currents

A. Master equation techniques (Einstein 1917, Pauli 1928, van Hove 1962, ...).
Weak junctions $\longrightarrow$ Effective Markovian dynamics for the occupation numbers n_ω of the discrete energy levels ω of $\mathcal{S}$.

B. Landauer-Büttiker formula (Landauer 1957, Büttiker 1986).
Neglect interactions in the joint system $\longrightarrow$ One body problem. Steady charge currents given by the scattering matrix elements $S_{kl}(\omega)$ between $\mathcal{R}_l$ and $\mathcal{R}_k$

$$\langle \Phi_{Q_{\mathcal{R}_k}} \rangle_+ = \int \mathrm{tr}_{\mathcal{R}_k}(S(\omega) f(\omega) S(\omega)^* - f(\omega)) \frac{d\omega}{2\pi}.$$

C. Schwinger–Keldysh formalism (Schwinger 1961, Keldysh 1965).
Special form of perturbation theory. Book-keeping device to generate diagrammatic expansion of the steady state

$$\langle \cdot \rangle_+ = \lim_{t \to \infty} \frac{\mathrm{tr}(e^{-(\sum_k \beta_k H_{\mathcal{R}_k} + \beta_{\mathcal{S}} H_{\mathcal{S}})} e^{itH_{\mathrm{tot}}} (\cdot) e^{-itH_{\mathrm{tot}}})}{\mathrm{tr}\left(e^{-(\sum_k \beta_{\mathcal{R}_k} H_{\mathcal{R}_k} + \beta_{\mathcal{S}} H_{\mathcal{S}})}\right)}.$$

3. NESS: Mathematical constructions

Framework: Perturbation theory of C^*-dynamical systems.

Decoupled system $(\mathcal{O}, \tau_0^t, \langle\,\cdot\,\rangle_0)$: $\mathcal{O}$ is a C^*-algebra, $\tau_0^t = e^{t\,\delta_0}$ a strongly continuous group of $*$-automorphisms of $\mathcal{O}$, $\langle\,\cdot\,\rangle_0$ a τ_0^t-invariant state.
Sub-algebras structure: $\mathcal{O}_\alpha \subset \mathcal{O}$, $\alpha = \mathcal{S}, \mathcal{R}_1, \ldots, \mathcal{R}_M$,

$$\mathcal{O}_\alpha \cap \mathcal{O}_{\alpha'} = \{I\} \text{ for } \alpha \neq \alpha',$$

$$\mathcal{O} = \mathcal{O}_\mathcal{S} \vee \mathcal{O}_\mathcal{R} = \mathcal{O}_\mathcal{S} \vee (\mathcal{O}_{\mathcal{R}_1} \vee \cdots \vee \mathcal{O}_{\mathcal{R}_M}),$$

$$\tau_0^t(\mathcal{O}_\alpha) = \mathcal{O}_\alpha.$$

Coupling:

$$V = \sum_{k=1}^{M} V_k, \quad V_k = V_k^* \in \mathcal{O}_\mathcal{S} \vee \mathcal{O}_{\mathcal{R}_k}.$$

Coupled system $(\mathcal{O}, \tau_\lambda^t)$: Locally perturbed dynamics

$$\tau_\lambda^t = e^{t\delta_\lambda}, \quad \delta_\lambda = \delta_0 + i\lambda[V,\ \cdot\ ],$$

with junction strength $\lambda \in \mathbb{R}$.

A. The van Hove limit.

- Rigorous derivation of master equation for $\mathcal{S}$ from microscopic dynamics of the joint system on time scale λ^{-2} (Davies 1974): For $A_{\mathcal{S}} \in \mathcal{O}_{\mathcal{S}}$,

$$\lim_{\lambda \to 0} \left\langle \tau_0^{-t/\lambda^2} \circ \tau_\lambda^{t/\lambda^2}(A_{\mathcal{S}}) \right\rangle_{\mathcal{R}\,0} = e^{t\mathcal{L}}(A_{\mathcal{S}}),$$

  defines a quantum Markov semi-group. NESS is obtained by solving $\mathcal{L}^* \rho = 0$.

- Thermodynamics of weakly coupled open systems, including linear response theory (Lebowitz-Spohn 1978).

- The van Hove limit gives exact results for the currents to second order in the junction strength λ.

- Extension of the convergence to the joint system (Derezinski–De Roeck 2006) connection with quantum stochastic differential equations.

B. Scattering approach (Ruelle 2000)

- If the Møller morphism

$$\mathcal{O}_{\mathcal{R}} \ni A \mapsto \eta_+(A) = \lim_{t\to\infty} \tau_\lambda^{-t} \circ \tau_0^t(A),$$

exist and is an isomorphism between $\mathcal{O}_{\mathcal{R}}$ and $\mathcal{O}$ (completeness of C^*-scattering) then

$$\langle A \rangle_+ = \lim_{t\to\infty} \left\langle \tau_0^{-t} \circ \tau_\lambda^t(A) \right\rangle_0 = \left\langle \eta_+^{-1}(A) \right\rangle_{\mathcal{R}\,0}.$$

- Fairly well understood perturbation theory (Botvich-Malyshev 1983) allows to handle locally interacting Fermions! (Fröhlich–Merkli–Ueltschi 2004).

- In the special case of noninteracting fermions τ_0^t and τ_λ^t are groups of Bogoliubov automorphisms generated by one-particle Hamiltonians h_0 and h_λ. The formula

$$\langle a^*(f)a(g) \rangle_+ = \langle a^*(\Omega_-^* f)a(\Omega_-^* g) \rangle_{\mathcal{R}\,0},$$

together with Wick theorem completely describes the NESS. Landauer-Büttiker formula is an elementary consequence of it.

C. C-Liouvillean approach (Jakšić–P 2002)

$(\mathcal{H}, \pi, \Omega)$ GNS representation of $\mathcal{O}$ associated to $\langle \cdot \rangle_0$.

Assumption: $\langle \cdot \rangle_0$ is modular i.e.,

$$A\Omega = 0 \quad \Longrightarrow \quad A = 0,$$

for all $A \in \pi(\mathcal{O})''$ (true if each reservoir is in thermal equilibrium).

For sufficiently regular V one can construct the C-Liouvillean L s.t.

$$L_\lambda \Omega = 0, \quad e^{itL_\lambda}\pi(A)e^{-itL_\lambda} = \pi(\tau_\lambda^t(A)).$$

NESS is obtained as zero-resonance of L_λ^*: if

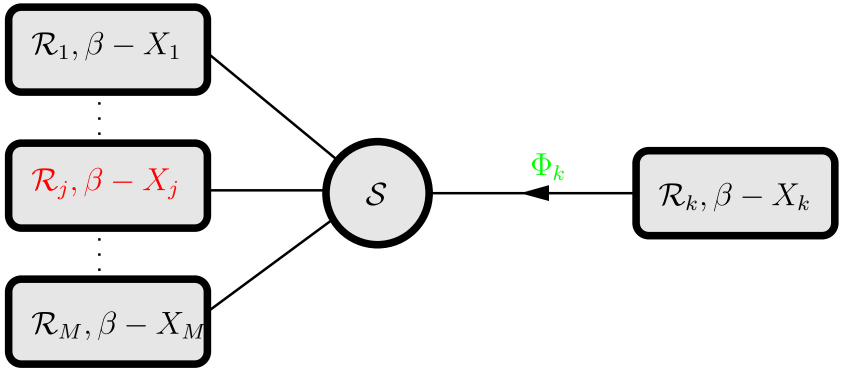
$$L_\lambda^* \Psi_\lambda = 0, \quad (\Psi_\lambda, \Omega) = 1,$$

then, for sufficiently regular $A \in \mathcal{O}$:

$$\langle A \rangle_+ = (\Psi_\lambda, \pi(A)\Omega).$$

The C-Liouvillean approach is well suited for perturbative analysis. In a way it can be considered as a rigorous implementation of Schwinger-Keldysh formalism.

3. Linear response to thermal drive — generalities



Thermodynamic force $X_k \longleftrightarrow$ Conjugated flux Φ_k

$\updownarrow$

Entropy production rate $\sigma = \sum_k X_k \Phi_k$

Transport coefficients:

$$L_{kj} = \partial_{X_j} \langle \Phi_k \rangle_+ \Big|_{X=0}.$$

Mean entropy production rate:

$$\langle \sigma \rangle_+ = \sum_k X_k \langle \Phi_k \rangle_+ = \sum_{kj} L_{kj} X_k X_j + O(|X|^2) \geqslant 0.$$

Kubo formula (Kubo 1957, Kubo–Yokota–Nakajima 1957, Luttinger 1964):

$$L_{kj} = \frac{1}{\beta}\int_0^\infty ds \int_0^\beta du \left\langle \tau^s(\Phi_k)\tau^{iu}(\Phi_j)\right\rangle_{\rm eq}.$$

Here and in the sequel $\tau = \tau_\lambda$ denotes the coupled dynamics.

For TRI systems one has the equivalent nicer looking formula

$$L_{kj} = \frac{1}{2}\int_{-\infty}^\infty ds \langle \tau^s(\Phi_k)\Phi_j\rangle_{\rm eq},$$

and the Onsager reciprocity relations (Onsager 1931):

$$L_{kj} = L_{jk}.$$

More generally, for conserved extensive observables A_k of $\mathcal{R}_k$

$$\partial_{X_j}\langle \Phi_{A_k}\rangle_+\Big|_{X=0} = \frac{1}{\beta}\int_0^\infty ds \int_0^\beta du \left\langle \tau^s(\Phi_{A_k})\tau^{iu}(\Phi_j)\right\rangle_{\rm eq},$$

and for TRI system if A_k is even under time reversal

$$\partial_{X_j}\langle \Phi_{A_k}\rangle_+\Big|_{X=0} = \frac{1}{2}\int_{-\infty}^\infty ds \langle \tau^s(\Phi_{A_k})\Phi_j\rangle_{\rm eq}.$$

Proving Kubo formula ?

2 conceptually distinct cases:

- Mechanical drive: Perturbing the dynamics by external fields
  - $\longrightarrow$ Time dependent perturbation theory.
- Thermal drive: Perturbing the initial state. Formal derivations based on disputable
  - $\longrightarrow$ Local thermal equilibrium.
  - $\longrightarrow$ Entropy production argument.

We propose a mechanical treatment of thermal drive:

> After a finite time t the perturbation of initial state is equivalent to the action of some external field.
>
> (Zubarev, 1974; Tasaki–Matsui 2001).

4. Linear response — formal calculation

Open quantum system near equilibrium driven by temperature differentials (adaptation to other thermal forces is easy !).

- $H = H_{\mathcal{S}} + H_{\mathcal{R}} + \lambda V = H_{\mathcal{S}} + \sum_k H_{\mathcal{R}_k} + \lambda V = H^{(0)} + \lambda V.$
- Equilibrium state at inverse temperature β

$$\omega_{\mathrm{eq}} = \frac{1}{Z_{\mathrm{eq}}} e^{-\beta H}.$$

- Initial product state

$$\omega_X^{(0)} = \frac{1}{Z_X^{(0)}} e^{-(\beta H_{\mathcal{S}} + \sum_k (\beta - X_k) H_{\mathcal{R}_k})} = \frac{1}{Z_X^{(0)}} e^{-\beta H_X^{(0)}},$$

with thermodynamic forces $X = (X_1, \ldots, X_M)$ is Gibbs state for

$$H_X^{(0)} = H^{(0)} - \sum_{k=1}^{M} \frac{X_k}{\beta} H_{\mathcal{R}_k}.$$

- Heat fluxes

$$\Phi_k = -\frac{dH_{\mathcal{R}_k}}{dt} = -i[H, H_{\mathcal{R}_k}] = i\lambda[H_{\mathcal{R}_k}, V].$$

Step 0. Since the junction V is local the Gibbs state

$$\omega_X = \frac{1}{Z_X} e^{-\beta H_X}, \quad H_X = H_X^{(0)} + \lambda V = H - \sum_{k=1}^{M} \frac{X_k}{\beta} H_{\mathcal{R}_k},$$

is thermodynamically equivalent to $\omega_X^{(0)}$, $\omega_{X=0} = \omega_{\mathrm{eq}}$.

Step 1. ω_X is Gibbs state for $H_X \implies \omega_X \circ \tau^t$ is Gibbs state for

$$\tau^{-t}(H_X) = H_X - \sum_{k=1}^{M} \frac{X_k}{\beta} \int_0^t \tau^{-s}(\Phi_k)\, ds = H_X + P_X(t). \tag{1}$$

Step 2. By Duhamel formula

$$e^{-\beta(H_X + P_X(t))} = e^{-\beta H_X} - \int_0^\beta \sigma_X^{iu}(P_X(t))\, e^{-\beta H_X} du + O(P_X(t)^2),$$

where σ_X^t is the dynamics generated by H_X. It follows that

$$\begin{aligned} \omega_X(\tau^t(A)) &= \omega_X(A) \\ &+ \sum_{k=1}^{M} \frac{X_k}{\beta} \int_0^t ds \int_0^\beta du\, \omega_X(A \sigma_X^{iu}(\tau^{-s}(\Phi_k))) + O(|X|^2). \end{aligned}$$

Step 3. Observable A is centered if $\omega_X(A) = 0$ for all X near $X = 0$. Since $\omega_{X=0}$ is a Gibbs state for H we have $\omega_{X=0}(\tau^t(A)) = \omega_{X=0}(A) = 0$, hence

$$\begin{aligned}\omega_X(\tau^t(A)) - \omega_{X=0}(\tau^t(A)) &= \sum_{k=1}^{M} \frac{X_k}{\beta} \int_0^t ds \int_0^\beta du\, \omega_X(A\sigma_X^{iu}(\tau^{-s}(\Phi_k))) \\ &+ O(|X|^2).\end{aligned}$$

Step 4. Since $H_{X=0} = H$, $\omega_{X=0} = \omega_{\mathrm{eq}}$ and $\sigma_{X=0} = \tau$

$$\lim_{X \to 0} \omega_X(A\sigma_X^{iu}(\tau^{-s}(\Phi_k))) = \omega_{\mathrm{eq}}(A\tau^{-s+iu}(\Phi_k)) = \omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(\Phi_k)),$$

and we get

$$\partial_{X_k}\omega_X(\tau^t(A))\big|_{X=0} = \frac{1}{\beta} \int_0^t ds \int_0^\beta du\, \omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(\Phi_k)).$$

Step 5. Assume now that NESS

$$\lim_{t\to\infty} \omega_X(\tau^t(A)) = \omega_{X+}(A),$$

exists. Exchange of the $t\to\infty$ limit with ∂_{X_k} leads to Kubo formula

$$\partial_{X_k}\omega_{X+}(A)|_{X=0} = \frac{1}{\beta}\int_0^\infty ds \int_0^\beta du\, \omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(\Phi_k)).$$

Remark 1. 3 crucial points:

- Step 0: Choice of reference state ω_X.
- Step 3: Observable A must be centered !
- Step 5: Exchange of limits.

Remark 2. Taking $t\to\infty$ in (1) leads to Zubarev-MacLennan ensemble

$$\omega_{X+} = \frac{1}{Z} e^{-\beta H_X + \sum_k X_k \int_{-\infty}^0 \tau^s(\Phi_k)\, ds}.$$

4. Linear response — an axiomatic approach

4.1. Entropy balance and its consequences

Decoupled dynamics $(\mathcal{O}, \tau_0^t)$

$$\tau_{\mathcal{S}}^t = \tau_0^t|_{\mathcal{O}_{\mathcal{S}}}, \quad \tau_{\mathcal{R}_k}^t = \tau_0^t|_{\mathcal{O}_{\mathcal{R}_k}},$$

$$\tau_0^t = e^{t\delta_0}, \quad \tau_{\mathcal{S}}^t = e^{t\delta_{\mathcal{S}}}, \quad \tau_{\mathcal{R}_k}^t = e^{t\delta_{\mathcal{R}_k}}, \quad \delta_0 = \delta_{\mathcal{S}} + \sum_{k=1}^{M} \delta_{\mathcal{R}_k}.$$

A1. Initial state. For any

$$X = (X_1, \ldots, X_M) \in I_\epsilon =]-\epsilon, \epsilon[^M,$$

let $\omega_X^{(0)}$ be such that:

- $\omega_X^{(0)}\Big|_{\mathcal{O}_{\mathcal{R}_k}}$ is unique $(\tau_{\mathcal{R}_k}^t, \beta - X_k)$-KMS state.
- $\omega_X^{(0)}\Big|_{\mathcal{O}_{\mathcal{S}}}$ is unique $(\tau_{\mathcal{S}}^t, \beta)$-KMS state.

To define heat fluxes we also need to assume

A2. Regularity of junction. $V \in \mathrm{Dom}(\delta_{\mathcal{R}_k})$ for $k = 1, \ldots, M$.

The heat flux out of $\mathcal{R}_k$ is given by

$$\Phi_k = \delta_{\mathcal{R}_k}(V).$$

Denote $\sigma_X^{(0)t}$ and σ_X^t the dynamics generated by

$$\delta_X^{(0)} = \delta_0 - \sum_{k=1}^{M} \frac{X_k}{\beta} \delta_{\mathcal{R}_k}, \quad \delta_X = \delta_X^{(0)} + i\lambda[V, \cdot\,].$$

$\omega_X^{(0)}$ is unique $(\sigma_X^{(0)}, \beta)$-KMS state (modular dynamics).

By Araki perturbation theory there is a unique (σ_X, β)-KMS state ω_X which is normal w.r.t. $\omega_X^{(0)}$ and thus has the same thermodynamics.

$\sigma_{X=0} = \tau \implies \omega_{X=0} = \omega_{\mathrm{eq}}$ is unique (τ, β)-KMS state.

Proposition 1. *(A1)&(A2) imply the entropy balance equation*

$$\mathrm{Ent}(\omega_X \circ \sigma_Y^t \,|\omega_X) = -\sum_{k=1}^{M} (X_k - Y_k) \int_0^t \omega_X \circ \sigma_Y^s(\Phi_k)\, ds.$$

Since $\sigma_{X=0} = \tau$, setting $Y = 0$ and $t \to \infty$ in this formula implies

$$\sum_{k=1}^{M} X_k \omega_{X+}(\Phi_k) \geqslant 0, \qquad (2^{\mathrm{nd}}\, \text{law of TD}).$$

Another important consequence of Proposition 1 is

Proposition 2. *(A1)&(A2) imply that the fluxes Φ_k are centered:*

$$\omega_X(\Phi_k) = 0,$$

hold for $k = 1, \ldots, M$ and all $X \in I_\epsilon$.

Proof. By the entropy balance equation

$$0 \leqslant -\lim_{t \to 0} \frac{\mathrm{Ent}(\omega_X \circ \sigma_Y^t | \omega_X)}{t} = \sum_{k=1}^{M} (X_k - Y_k) \omega_X(\Phi_k),$$

holds for any $X, Y \in I_\epsilon$.$\square$

4.2. Finite time Kubo formula

Proposition 3. *(A1)&(A2) imply that for any centered observable $A \in \mathcal{O}$ and all $t \in \mathbb{R}$ the function*

$$X \mapsto \omega_X(\tau^t(A)),$$

is differentiable at $X = 0$ and

$$\partial_{X_k} \omega_X(\tau^t(A))\big|_{X=0} = \frac{1}{\beta} \int_0^t ds \int_0^\beta du \, \omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(\Phi_k)).$$

Sketch of proof. Follow the formal calculation!
Step 1. Let

$$\Gamma_t = I + \sum_{n \geqslant 1} (i\lambda)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \; \tau_0^{t_n}(V) \cdots \tau_0^{t_1}(V),$$

be the unitary cocycle

$$\begin{aligned} \tau^t(A) &= \Gamma_t \tau_0^t(A) \Gamma_t^*, \\ \partial_t \Gamma_t &= i \Gamma_t \tau_0^t(V), \\ \partial_t \Gamma_t^* &= -i \tau_0^t(V) \Gamma_t^*. \end{aligned}$$

Using (A2) one sees that $\Gamma_t \in \mathrm{Dom}(\delta_{\mathcal{R}_k})$, that $t \mapsto \delta_{\mathcal{R}_k}(\Gamma_t)$ is differentiable and that

$$\partial_t \delta_{\mathcal{R}_k}(\Gamma_t) = \delta_{\mathcal{R}_k}(\partial_t \Gamma_t) = \delta_{\mathcal{R}_k}(i\Gamma_t \tau_0^t(V)) = i\delta_{\mathcal{R}_k}(\Gamma_t)\tau_0^t(V) + i\Gamma_t \tau_0^t(\Phi_k).$$

It follows that

$$\partial_t(\delta_{\mathcal{R}_k}(\Gamma_t)\Gamma_t^*) = i\tau^t(\Phi_k),$$

and hence

$$\delta_{\mathcal{R}_k}(\Gamma_t)\Gamma_t^* = i\int_0^t \tau^s(\Phi_k)\,ds.$$

Computing

$$\delta_{\mathcal{R}_k}(\tau^t(A)) = \delta_{\mathcal{R}_k}(\Gamma_t \tau_0^t(A)\Gamma_t^*),$$

one immediately get

$$\delta_{\mathcal{R}_k}(\tau^t(A)) - \tau^t(\delta_{\mathcal{R}_k}(A)) = \int_0^t i[\tau^s(\Phi_k), \tau^t(A)]\,ds. \tag{2}$$

Set

$$P_X(t) = -\sum_{k=1}^{M} \frac{X_k}{\beta} \int_0^t \tau^{-s}(\Phi_k)\,ds,$$

and denote by $\alpha_{X,t}^u$ the dynamics generated by

$$\delta_{X,t} = \delta_X + i[P_X(t),\ \cdot\ ].$$

Using (2) one checks that

$$\partial_u(\sigma_X^u \circ \tau^t(A)) = \sigma_X^u \circ \tau^t(\delta_{X,t}(A)),$$

which shows that $\tau^{-t} \circ \sigma_X^u \circ \tau^t = \alpha_{X,t}^u$, and hence that $\omega_X \circ \tau^t$ is $(\alpha_{X,t}, \beta)$-KMS state.

Step 2. A simple application of Araki perturbation theory of KMS states yields

$$\begin{aligned}\omega_X(\tau^t(A)) &= \omega_X(A)\left(1 - \sum_k X_k \int_0^t \omega_X(\tau^{-s}(\Phi_k))ds\right) \\ &+ \sum_k \frac{X_k}{\beta} \int_0^t ds \int_0^\beta du\ \omega_X(A\sigma_X^{iu}(\tau^{-s}(\Phi_k))) \\ &+ O(|tX|^2).\end{aligned}$$

Step 3. If A is centered it follows that

$$\omega_X(\tau^t(A)) - \omega_{X=0}(\tau^t(A)) = \sum_k \frac{X_k}{\beta} \int_0^t ds \int_0^\beta du \omega_X(A\sigma_X^{iu}(\tau^{-s}(\Phi_k))) + O(|tX|^2).$$

Step 4. Using the $(\sigma_X,\ \beta)$-KMS condition and approximation by σ_X-analytic elements one shows that

$$\lim_{X\to 0} \omega_X(A\sigma_X^{iu}(B)) = \omega_{\mathrm{eq}}(A\tau^{iu}(B)),$$

holds for all $A, B \in \mathcal{O}$ and $0 \leqslant u \leqslant \beta$.□

4.3. The limit $t \to \infty$.

A3. NESS. For any $X \in I_\epsilon$ there exists a state ω_{X+} such that

$$\lim_{t\to\infty} \omega_X(\tau^t(A)) = \omega_{X+}(A),$$

for all $A \in \mathcal{O}$.

On physical grounds one expects that thermodynamically equivalent initial states lead to the same NESS i.e.,

$$\lim_{t\to\infty} \eta(\tau^t(A)) = \omega_{X+}(A),$$

for any ω_X-normal state η and in particular for the product state $\eta = \omega_X^{(0)}$.

We shall hide the main difficulty of a general proof of Kubo formula into

Definition 4. *A centered observable $A \in \mathcal{O}$ is regular if $X \mapsto \omega_{X+}(A)$ is differentiable at $X = 0$ and*

$$\partial_X \omega_{X+}(A)|_{X=0} = \lim_{t\to\infty} \partial_X \omega_X \circ \tau^t(A)\big|_{X=0}.$$

Proving regularity of an observable is a difficult dynamical problem which can only be solved within specific models. In practice, it can be checked with the help of

Lemma 5. *Suppose (A1)&(A3) hold and the centered observable A is such that the function $X \mapsto \omega_X(A)$ has analytic extension to $D_\epsilon = \{X \in \mathbb{C}^M \,|\, \max_k |X_k| < \epsilon\}$ such that*

$$\sup_{t \geqslant 0, X \in D_\epsilon} |\omega_X(\tau^t(A))| < \infty,$$

then A is regular.

Keeping the exchange of limits problem out of our way we obtain

Theorem 6. *(A1)&(A2)&(A3) imply that, for any regular observable A, Kubo formula*

$$\partial_{X_k} \omega_{X+}(A)|_{X=0} = \frac{1}{\beta} \int_0^\infty ds \int_0^\beta du \; \omega_{\rm eq}(\tau^s(A) \tau^{iu}(\Phi_k)),$$

holds.

4.4. Time reversal invariance

System is TRI if there exists involutive, $*$-anti-morphism θ on $\mathcal{O}$ s.t.

$$\theta(\mathcal{O}_{\mathcal{S}}) = \mathcal{O}_{\mathcal{S}}, \quad \theta(\mathcal{O}_{\mathcal{R}_k}) = \mathcal{O}_{\mathcal{R}_k}, \quad \theta \circ \tau_0^t = \tau_0^{-t} \circ \theta, \quad \theta(V_k) = V_k.$$

A4. Mixing equilibrium state. For all $A, B \in \mathcal{O}$

$$\lim_{|t| \to \infty} \omega_{\mathrm{eq}}(A\tau^t(B)) = \omega_{\mathrm{eq}}(A)\omega_{\mathrm{eq}}(B).$$

Theorem 7. *For TRI systems (A1)&(A2)&(A3)&(A4) imply that, for any regular observable A, Kubo formula*

$$\partial_{X_k}\omega_{X+}(A)|_{X=0} = \frac{1}{2}\int_{-\infty}^{\infty} \omega_{\mathrm{eq}}(\tau^s(A)\Phi_k)\, ds, \tag{3}$$

holds.

Corollary 8. *If the fluxes Φ_k are regular then Onsager reciprocity holds*

$$\partial_{X_k}\omega_{X+}(\Phi_j)|_{X=0} = \partial_{X_j}\omega_{X+}(\Phi_k)\big|_{X=0}.$$

Proof. Onsager symmetry follows from Kubo formula (3) and the fact that (A4) implies the stability condition

$$\int_{-\infty}^{\infty} \omega_{\mathrm{eq}}([A, \tau^s(B)])\, ds = 0,$$

for all $A, B \in \mathcal{O}$.$\square$

Proof of Theorem 7. TRI and (A1) give $\omega_{\mathrm{eq}}(\theta(A)) = \omega_{\mathrm{eq}}(A^*)$ for $A \in \mathcal{O}$. KMS condition further give

$$\omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(B)) = \omega_{\mathrm{eq}}(\tau^{-s}(A)\tau^{i(\beta-u)}(B)),$$

for $0 \leqslant u \leqslant \beta$ and thus

$$\frac{1}{\beta}\int_0^{\beta}\left(\int_0^t \omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(B))\, ds\right) du = \frac{1}{2\beta}\int_0^{\beta}\left(\int_{-t}^t \omega_{\mathrm{eq}}(A\tau^{s+iu}(B))\, ds\right) du.$$

Since the integral of $z \mapsto \omega_{\mathrm{eq}}(A\tau^z(B))$ over the boundary of $[-t, t] + i[0, u]$ is zero we get

$$\frac{1}{\beta}\int_0^{\beta}\left(\int_0^t \omega_{\mathrm{eq}}(\tau^s(A)\tau^{iu}(B))\, ds\right) du = \frac{1}{2}\int_{-t}^t \omega_{\mathrm{eq}}(A\tau^s(B))\, ds + \frac{1}{2\beta}\int_0^{\beta} R(t, u)\, du,$$

where

$$R(t,u) = i \int_0^u \Big(\omega_{\rm eq}(A\tau^{t+iv}(B)) - \omega_{\rm eq}(A\tau^{-t+iv}(B))\Big)\, dv.$$

Assumption (A4) and dominated convergence yield the result.□

5. Examples

5.1. Spin-Fermion models

Small system $\mathcal{S}$. 2-level system

- Hilbert space $\mathcal{H}_{\mathcal{S}} = \mathbb{C}^2$.
- Hamiltonian $H_{\mathcal{S}} = \sigma_z$.
- Algebra $\mathcal{O}_{\mathcal{S}} = \mathcal{B}(\mathcal{H}_{\mathcal{S}})$.
- $\omega^{(0)}_{\mathcal{S}\,X}(\,\cdot\,) = Z_{\mathcal{S}}^{-1}\mathrm{tr}\,(e^{-\beta H_{\mathcal{S}}}(\,\cdot\,))$.

Reservoirs $\mathcal{R}_k$. Free Fermi gases at thermal equilibrium.

- One particle Hilbert space $\mathfrak{h}_k = L^2(\mathbb{R}_+, d\varepsilon) \otimes \mathfrak{K}_k$.
- One particle Hamiltonian h_k is multiplication by ε.
- Algebra $\mathcal{O}_{\mathcal{R}_k} = \mathrm{CAR}(\mathfrak{h}_k)$.
- Dynamics $\tau^t_{\mathcal{R}_k}$ is Bogoliubov automorphism associated to h_k.
- $\omega^{(0)}_{\mathcal{R}_k\,X}$ is gauge-invariant quasi-free state with 2-point function

$$\omega^{(0)}_{\mathcal{R}_k\,X}(a^*(f)a(g)) = (g, (1 + e^{(\beta - X_k)h_k})^{-1} f).$$

Uncoupled joint system.

- Algebra $\mathcal{O} = \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{\mathcal{R}_1} \otimes \cdots \otimes \mathcal{O}_{\mathcal{R}_M}$.
- Dynamics $\tau_0^t = \tau_{\mathcal{S}}^t \otimes \tau_{\mathcal{R}_1}^t \otimes \cdots \otimes \tau_{\mathcal{R}_M}^t$.
- Initial state $\omega_X^{(0)} = \omega_{\mathcal{S}\,X}^{(0)} \otimes \omega_{\mathcal{R}_1\,X}^{(0)} \otimes \cdots \otimes \omega_{\mathcal{R}_M\,X}^{(0)}$.

Coupling. Trough field operators $\varphi_k(f) = 2^{-1/2}(a_k^*(f) + a_k(f))$:

$$V_k = \lambda \sigma_x \otimes \varphi_k(\alpha_k),$$

with $\alpha_k \in \mathfrak{h}_k$. Coupled dynamical system $(\mathcal{O}, \tau_\lambda^t)$.

There exists conjugation c_k on $\mathfrak{h}_k$ such that $c_k \alpha_k = \alpha_k \longrightarrow$ The system is TRI.

To $f_k \in \mathfrak{h}_k$ we associate $\tilde{f_k} \in L^2(\mathbb{R}, d\varepsilon) \otimes \mathfrak{K}_k$ given by

$$\tilde{f_k}(\varepsilon) = \begin{cases} f_k(\varepsilon) & \text{if } \ \varepsilon \geqslant 0, \\ (c_k f_k)(|\varepsilon|) & \text{if } \ \varepsilon < 0. \end{cases}$$

Denote by $H^2(\delta; \mathfrak{K}_k)$ the Hardy space of analytic function

$$f\colon \{z \in \mathbb{C} \,|\, |\mathrm{Im}\, z| < \delta\} \to \mathfrak{K}_k.$$

We shall assume:

S1. Analyticity. For some $\delta > 0$ and $\kappa > \beta$ and all k

$$e^{-\kappa z} \tilde{\alpha}_k(z) \in H^2(\delta; \mathfrak{K}_k).$$

S2. Effective coupling. $\|\alpha_k(2)\|_{\mathfrak{K}_k} > 0$ for all k.

Denote by $\tilde{\mathcal{O}}$ the $*$-subalgebra generated by elements of the form

$$Q \otimes a_k(f_k),$$

where $Q \in \mathcal{O}_{\mathcal{S}}$ and $f_k \in \mathfrak{h}_k$ is such that, for some $b > (\kappa + \beta)/2$,

$$e^{-b\varepsilon} \tilde{f}_k(\varepsilon) \in H^2(\delta; \mathfrak{K}_k).$$

Using C-Liouvillean techniques one can prove the following

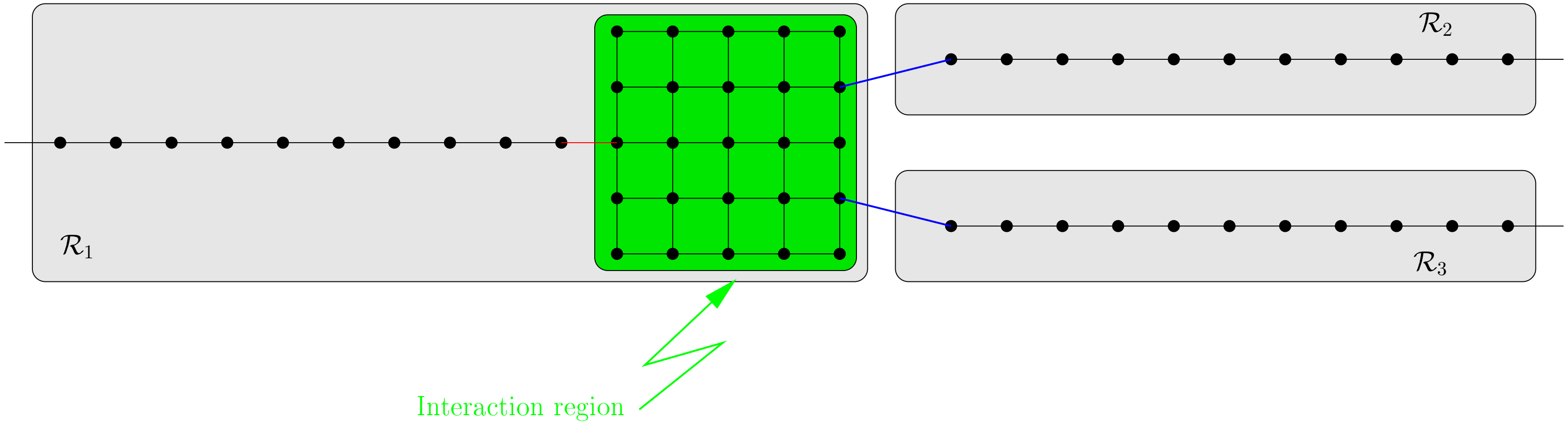
Theorem 9. *Under Assumptions (S1)&(S2) there exists $\Lambda > 0$ such that, for $0 < |\lambda| < \Lambda$, Assumptions (A1)-(A4) are satisfied and*

$$\lim_{t \to \infty} \eta(\tau_\lambda^t(A)) = \omega_{X+}(A),$$

holds for any $\omega_X^{(0)}$-normal state η. Moreover, any centered observable $A \in \tilde{O}$ is regular and $\Phi_k \in \tilde{O}$.

Similar result hold for more general N-level systems coupled to Fermionic reservoirs.

5.2. Locally interacting Fermi gases



Free Fermi gas with

- One particle Hilbert space $\mathfrak{h} = \mathfrak{h}_{\mathcal{R}_1} \oplus \cdots \oplus \mathfrak{h}_{\mathcal{R}_M}$.
- One particle Hamiltonian $h = h_{\mathcal{R}_1} \oplus \cdots \oplus h_{\mathcal{R}_M}$.
- Algebra $\mathcal{O} = \mathrm{CAR}(\mathfrak{h})$.
- Bogoliubov decoupled dynamics τ_0^t generated by h.

- Initial state $\omega_X^{(0)}$: quasi-free gauge-invariant with 2-points function

$$\omega_X^{(0)}(a^*(f)a(g)) = (g, T_X^{(0)} f),$$

$$T_X^{(0)} = \bigoplus_{k=1}^{M} (1 + e^{(\beta - X_k)h_{\mathcal{R}_k}})^{-1}.$$

- Local interaction

$$V = V^* = \lambda \sum_{k=1}^{K} \prod_{j=1}^{n_k} a^*(u_{k,j})a(v_{k,j}) \in \mathrm{CAR}^+(\mathfrak{h}),$$

with $u_{k,j}, v_{k,j} \in \mathfrak{h} \longrightarrow$ perturbed coupled dynamics τ_λ^t.

We shall assume:

L1. The channel Hamiltonians h_k have purely a.c. spectra.

L2. There exists a dense subspace $\mathcal{D} \subset \mathfrak{h}$ such that

- $u_{k,j}, v_{k,j}, h_l u_{k,j}, h_l v_{k,j} \in \mathcal{D}$ for all k, j, l.
- For any $f, g \in \mathcal{D}$

$$\int_{-\infty}^{\infty} |(f, e^{ith} g)| dt < \infty.$$

Theorem 10. *If (L1)&(L2) hold there exists $\Lambda > 0$ such that, for $0 < |\lambda| < \Lambda$ the Møller morphism*

$$\gamma_+ = s - \lim_{t \to \infty} \tau_0^{-t} \circ \tau_\lambda^t,$$

exists and is a $*$-automorphism of $\mathcal{O}$. For any $\omega_X^{(0)}$-normal state η one has

$$\lim_{t \to \infty} \eta \circ \tau_\lambda^t(A) = \omega_{X+}(A) = \omega_X^{(0)} \circ \gamma_+(A).$$

Moreover, any centered observable of the type

$$A = \sum_k a^{\#}(f_{k,1}) \cdots a^{\#}(f_{k,n_k}),$$

with $f_{k,j} \in \mathcal{D}$ is regular. In particular, the heat fluxes Φ_k are regular.