# Open Fermion Systems

Joint works with

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# Contents

# 1 Introduction

## 1.1 Open systems

Open quantum systems are the basic paradigms of non-equilibrium quantum statistical mechanics. An open system consists of a "small" system $\mathcal{S}$ interacting with a number of large "environments" or "reservoirs" $\mathcal{R}_1, \ldots, \mathcal{R}_M$.

The properties of a physical system out of thermal equilibrium are usually described in term of phenomenological concepts like steady state, fluxes and entropy production. These notions are related by the fundamental laws of thermodynamics. As an illustration, consider a model describing a small system $\mathcal{S}$ coupled to two infinite heat reservoirs $\mathcal{R}_1$,$\mathcal{R}_2$ which are at temperature $T_1$, $T_2$. Under normal

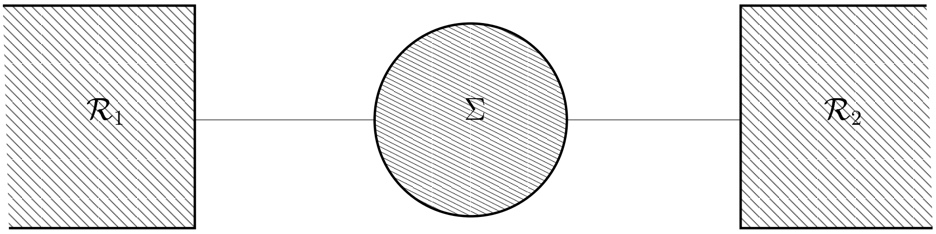


Figure 1: A system coupled to two heat reservoirs

conditions, one expects that the combined system will settle into a steady state in which there is a constant flow of heat from the hotter to the colder reservoir across the system $\mathcal{S}$. Let $\Phi_k$ be the heat current flowing from reservoir $\mathcal{R}_k$ into the small system $\mathcal{S}$, and $\mathrm{Ep}$ the entropy production rate in $\mathcal{S}$. In the steady state, the fundamental laws of thermodynamics read:

$$
\begin{aligned}
&\Phi_1 + \Phi_2 = 0, \\
&\frac{\Phi_1}{T_1} + \frac{\Phi_2}{T_2} = -\mathrm{Ep} \leq 0.
\end{aligned}
\tag{1}
$$

The first relation expresses energy conservation (the first law of thermodynamics). The second asserts that the heat flows from the hotter to the colder reservoir and that the entropy of $\mathcal{S}$ is not decreasing (the second law of thermodynamics).

Our goal is to give a precise mathematical meaning to the notions of non-equilibrium steady state, entropy production and hest flux, study their properties and prove Relations (1) from first principles.

## 1.2 Linear response

Linear response theory describes thermodynamics in the regime where the "forces" driving the system out of equilibrium are weak. In such a regime, to a very good approximation, the non-equilibrium currents depend linearly on the forces. The ultimate purpose of linear response theory is to justify well known phenomenological laws like Ohm's law for charge currents or Fick's law for heat currents. We are still far from a satisfactory derivation of these laws, even in the framework of classical mechanics; see [BLR] for a recent review on this matter. A less ambitious application of linear response theory concerns transport properties of microscopic and mesoscopic quantum devices (the advances in nanotechnologies during the last decade have triggered a strong interest in the transport properties of such devices). Linear response theory of such systems is much better understood, as we shall try to illustrate.

In the example of the previous subsection, the force that drive the system $\mathcal{S}+\mathcal{R}$ out of equilibrium is the difference $T_2 - T_1$ of temperatures of the reservoirs attached to $\mathcal{S}$. If both temperatures $T_1, T_2$ are sufficiently close to some value $T_{\rm equ}$, we expect linear response theory to give a good account of the thermodynamics of the system near thermal equilibrium at inverse temperature $T_{\rm equ}$.

In phenomenological non-equilibrium thermodynamics, the duality between the driving forces $F_\alpha$, also called *affinities*, and the steady currents $\Phi_\alpha$ they induce is expressed by the entropy production formula

$$\mathrm{Ep} = \sum_\alpha F_\alpha\,\Phi_\alpha, \tag{2}$$

(see [DGM]). The steady currents are themselves functions of the affinities $\Phi_\alpha = \Phi_\alpha(F_1, \cdots)$. In the linear response regime, these functions are given by the relations

$$\Phi_\alpha = \sum_\gamma L_{\alpha\gamma} F_\gamma, \tag{3}$$

which define the *transport coefficients* $L_{\alpha\gamma}$.

Combining (3) with the first law of thermodynamics $\sum_\alpha \Phi_\alpha = 0$ we obtain that for all $\gamma$,

$$\sum_\alpha L_{\alpha\gamma} = 0. \tag{4}$$

Similarly, (2), (3) and the second law $\mathrm{Ep} \geq 0$ imply that the quadratic form

$$\sum_{\alpha\gamma} L_{\alpha\gamma} F_\alpha F_\gamma,$$

is non-negative. Note that this does not imply that the matrix $L$ is symmetric !

Linear response theory goes far beyond the above elementary relations. Its true cornerstones are the *Onsager reciprocity relations* (ORR), the Kubo *fluctuation-dissipation* formula (KF) and the *Central Limit Theorem* (CLT). All three of them deal with the transport coefficients. The Onsager reciprocity relations assert that the matrix $L_{\alpha\gamma}$ of a time reversal invariant (TRI) system is symmetric,

$$L_{\gamma\alpha} = L_{\alpha\gamma}. \tag{5}$$

For non-TRI systems, similar relations hold between the transport coefficients of the system and those of the time reversed one. For example, if time reversal invariance is broken by the action of an external magnetic field $B$, then the Onsager-Casimir relations

$$L_{\alpha\gamma}(B) = L_{\gamma\alpha}(-B),$$

hold.

The Kubo fluctuation-dissipation formula expresses the transport coefficients of a TRI system in terms of the *equilibrium* current-current correlation function

$$C_{\alpha\gamma}(t) \equiv \frac{1}{2}\, \langle \Phi_\alpha(t)\Phi_\gamma(0) + \Phi_\alpha(0)\Phi_\gamma(t)\rangle_{\rm equ}\,, \tag{6}$$

namely

$$L_{\alpha\gamma} = \frac{1}{2}\int_{-\infty}^{\infty} C_{\alpha\gamma}(t)\,\mathrm{d}t. \tag{7}$$

The Central Limit Theorem further relates $L_{\alpha\gamma}$ to the statistics of the current fluctuations in equilibrium. In term of characteristic function, the CLT for open systems in thermal equilibrium asserts that

$$\lim_{t\to\infty}\left\langle \exp\left(\mathrm{i}\sum_\alpha \xi_\alpha \frac{1}{\sqrt{t}}\int_0^t \Phi_\alpha(s)\,\mathrm{d}s\right)\right\rangle_{\rm equ} = \mathrm{e}^{-\frac{1}{2}\sum_{\alpha\gamma} D_{\alpha\gamma}\,\xi_\alpha\xi_\gamma}, \tag{8}$$

where the covariance matrix $D_{\alpha\gamma}$ is given by

$$D_{\alpha\gamma} = 2\,L_{\alpha\gamma}.$$

Because fluxes do not commute in quantum mechanics, $[\Phi_\alpha, \Phi_\gamma] \neq 0$ for $\alpha \neq \gamma$, they can not be measured simultaneously and a simple classical probabilistic interpretation of (8) for the vector variable $\Phi = (\Phi_1, \Phi_2, \ldots)$ is not possible. Instead, the quantum fluctuations of the vector variable $\Phi$ are described by the so-called *fluctuation algebra* [GVV1, GVV2, GVV3, GVV4, GVV5, Ma]. The description and study of the fluctuation algebra involve somewhat advanced technical tools and for this reason we will not discuss the quantum CLT theorem in this lecture.

The mathematical theory of ORR, KF, and CLT is reasonably well understood in classical statistical mechanics. In the context of open quantum systems these important notions are still not completely understood (see however [AJPP, JPR2] for some recent results).

## 1.3 Reference state

The concept of reference state will play an important role in our discussion of non-equilibrium statistical mechanics. To clarify this notion, let us consider first a classical dynamical system with finitely many degrees of freedom and compact phase space $X \subset \mathbb{R}^n$. The normalized Lebesgue measure $\mathrm{d}x$ on $X$ provides a physically natural statistics on the phase space in the sense that initial configurations sampled according to it can be considered typical. Note that this has nothing to do with the fact that $\mathrm{d}x$ is invariant under the flow of the system—any measure of the form $\rho(x)\mathrm{d}x$ with a strictly positive density $\rho$ would serve the same purpose. The situation is completely different if the system has infinitely many degrees of freedom. In this case, there is no natural replacement for the Lebesgue $\mathrm{d}x$. In fact, a measure on an infinite-dimensional phase space physically describes a thermodynamical state of the system. Suppose for example that the system is Hamiltonian and is in thermal equilibrium at inverse temperature $\beta$ and chemical potential $\mu$. The statistics of such a system is described by the Gibbs measure (grand canonical ensemble). Since two Gibbs measures with different values of the intensive thermodynamic parameters $\beta$, $\mu$ are mutually singular, initial points sampled according to one of them will be atypical relative to the other. In conclusion, if a system has infinitely many degrees of freedom, we need to specify its initial thermodynamic state by choosing an appropriate reference measure. As in the finite-dimensional case, this measure may not to be invariant under the flow. It also may not be uniquely determined by the physical situation we wish to describe.

The situation in quantum mechanics is very similar. The Schrdinger representation of a system with finitely many degrees of freedom is (essentially) uniquely determined and the natural statistics is provided by any strictly positive density matrix on the Hilbert space of the system. For systems with infinitely many degrees of freedom there is no such natural choice. The consequences of this fact are however more drastic than in the classical case. There is no natural choice of a Hilbert space in which the system can be represented. To induce a representation, we must specify the thermodynamical state of the system by choosing an appropriate reference state. The algebraic formulation of quantum statistical mechanics provides a mathematical framework to study such infinite system in a representation independent way.

One may object that no real physical system has an infinite number of degrees of freedom and that, therefore, a unique natural reference state always exists. There are however serious methodological reasons to consider this mathematical idealization. Already in equilibrium statistical mechanics the fundamental phenomena of phase transition can only be characterized in a mathematically precise way within such an idealization: A quantum system with finitely many degrees of freedom has a unique thermal equilibrium state. Out of equilibrium, relaxation towards a stationary state and emergence of steady currents can not be expected from the quasi-periodic time evolution of a finite system.

In classical non-equilibrium statistical mechanics there exists an alternative approach to this idealization. A system forced by a non-Hamiltonian or time-dependent force can be driven towards a non-equilibrium steady state, provided the energy supplied by the external source is removed by some thermostating device. This *micro-canonical* point of view has a number of advantages over the *canonical*, infinite system idealization. A dynamical system with a relatively small number of degrees of freedom can easily be explored on a computer (numerical integration, iteration of Poincar sections, . . . ). A large body of "experimental facts" is currently available from the results of such investigations (see [EM, Do] for an introduction to the techniques and a lucid exposition of the results). From a more theoretical perspective, the full machinery of finite-dimensional dynamical system theory becomes available in the micro-canonical approach. The *Chaotic Hypothesis* introduced in [CG1, CG2] is an attempt to exploit this fact. It justifies phenomenological thermodynamics (Onsager relations, linear response theory, fluctuation-dissipation formulas,...) and has lead to more unexpected results like the Gallavotti-Cohen Fluctuation Theorem. The major drawback of the micro-canonical point of view is the non-Hamiltonian nature of the dynamics, which makes it inappropriate to quantum-mechanical treatment.

The two approaches described above are not completely unrelated. For example, we shall see that the signature of a non-equilibrium steady state in quantum mechanics is its singularity with respect to the reference state, a fact which is well understood in the classical, micro-canonical approach (see Chapter 10 of [EM]). More speculatively, one can expect a general *equivalence principle* for dynamical (micro-canonical and canonical) ensembles (see [Ru5]). The results in this direction are quite scarce and much work remains to be done.

# 2 Quantum dynamical systems

## 2.1 $C^*$-dynamical systems

A $C^*$- dynamical system is a pair $(\mathcal{O}, \tau)$, where

- $\mathcal{O}$ is a $C^*$-algebra. For our purposes, we can think of $\mathcal{O}$ as a norm closed self-adjoint subalgebra of bounded operators on some Hilbert space $\mathcal{H}$. In particular, $\mathcal{O}$ is a Banach space and we denote by $\mathcal{O}^\star$ its dual.

- $\tau^t$ is a strongly continuous group of $*$-automorphisms of $\mathcal{O}$. That is, $\tau^t$ is a linear map on $\mathcal{O}$ such that $\tau^t(AB) = \tau^t(A)\tau^t(B)$ and $\tau^t(A^*) = \tau^t(A)^*$. Moreover, the map $t \mapsto \tau^t(A)$ is norm-continuous and satisfies the group property $\tau^t \circ \tau^s(A) = \tau^{t+s}(A)$ for each $A \in \mathcal{O}$ .

We always assume that $I \in \mathcal{O}$. The elements of $\mathcal{O}$ describe observables of the physical system under consideration and the group $\tau$ specifies their time evolution in the Heisenberg picture $A_t = \tau^t(A)$.

From the general theory of strongly continuous semigroups, there exists a densely defined, norm closed linear operator $\delta$ on $\mathcal{O}$ such that $\tau^t = e^{t\delta}$. Since $\tau^t(I) = I$, if follows that $I \in D(\delta)$ and $\delta(I) = 0$. Differentiation of the identities $\tau^t(AB) = \tau^t(A)\tau^t(B)$ and $\tau^t(A^*) = \tau^t(A)^*$ for $A, B \in D(\delta)$ further show that $D(\delta)$ is a $*$-subalgebra of $\mathcal{O}$ and that

$$\delta(AB) = \delta(A)B + A\delta(B), \qquad \delta(A^*) = \delta(A)^*.$$

Such an operator on $\mathcal{O}$ is called $*$-derivation.

A state of the system is a linear functional $\omega \in \mathcal{O}^\star$ satisfying

- $\omega(A^*A) \geq 0$ (positivity).

- $\|\omega\| = 1$ (normalization).

A linear functional $\omega$ on $\mathcal{O}$ satisfying these two conditions is automatically continuous (hence belongs to $\mathcal{O}^\star$) and satisfies $\omega(I) = 1$.

Let us denote by $\mathcal{O}_1^\star$ the unit ball of $\mathcal{O}^\star$. The set of all states on $\mathcal{O}$ is

$$E(\mathcal{O}) = \{\omega \in \mathcal{O}_1^\star | \omega(A^*A) \geq 0 \text{ for all } A \in \mathcal{O}\},$$

from which it follows that it is a convex, weak-$\star$ compact subset of $\mathcal{O}^\star$.

Assuming that the system was initially in the state $\omega$, the expectation value of the observable $A$ at time $t$ is the number $\omega(A_t)$. Since

$$\omega(A_t) = \omega(\tau^t(A)) = \omega \circ \tau^t(A),$$

states evolve in the Schrödinger picture according to $\omega_t = \omega \circ \tau^t$.

A state $\omega \in E(\mathcal{O})$ is called $\tau$- invariant, or steady state, if $\omega \circ \tau^t = \omega$ for all $t$. A $C^*$-dynamical system has at least one (and typically many) steady states.

The thermal equilibrium states of a $C^*$-dynamical system are characterized by the KMS condition. Let $\beta > 0$ be the inverse temperature. A state $\omega$ is $(\tau, \beta)$-KMS if, for all $A, B \in \mathcal{O}$, there is a function $F_{A,B}$ analytic inside the strip $\{z \,|\, 0 < \mathrm{Im}\, z < \beta\}$, bounded and continuous on its closure, and satisfying the KMS boundary conditions

$$F_{A,B}(t) = \omega(A\tau^t(B)), \qquad F_{A,B}(t + \mathrm{i}\beta) = \omega(\tau^t(B)A),$$

for $t \in \mathbb{R}$. A KMS state is $\tau$- invariant.

**Exercise 1** *Let $\mathcal{H}$ be a finite dimensional Hilbert space and $H$ a self-adjoint operator on $\mathcal{H}$. Consider the $C^*$-dynamical system $(\mathcal{B}(\mathcal{H}), \tau)$ defined by*

$$\tau^t(A) = e^{\mathrm{i}tH} A\, e^{-\mathrm{i}tH}.$$

*Show that for any $\beta \in \mathbb{R}$, its unique $\beta$-KMS state is given by*

$$\omega_\beta(A) = \mathrm{Tr}\,(\rho_\beta A),$$

*where*

$$\rho_\beta = \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}\,\mathrm{e}^{-\beta H}}.$$

Note that a $(\tau, \beta)$-KMS state is also a $(\tau', \beta')$-KMS state for the dynamics defined by $\tau'^t = \tau^{t\beta/\beta'}$. Even though, in most systems, the physical temperature is a non-negative parameter, it is mathematically convenient to define KMS state for all $\beta \in \mathbb{R}$. The case $\beta = 0$ corresponds to infinite temperature and $(\tau, 0)$-KMS states ($\tau$- invariant traces) are sometimes called chaotic states. In the mathematical litterature, $(\tau, \beta)$-KMS states for $\beta = -1$ are simply called $\tau$-KMS states.

## 2.2 Cyclic representation and modular structure

Let $\omega$ be a positive linear functional on the $C^*$-algebra $\mathcal{O}$. We denote by $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS-representation of $\mathcal{O}$ associated to $\omega$.

A linear functional $\mu \in \mathcal{O}^*$ is called $\omega$-normal, denoted $\mu \ll \omega$, if there exists a trace class operator $\rho_\mu$ on $\mathcal{H}_\omega$ such that $\mu(\cdot) = \mathrm{Tr}(\rho_\mu \pi_\omega(\cdot))$. Any $\omega$-normal linear functional $\mu$ has a unique normal extension to the enveloping von Neumann algebra $\mathfrak{M}_\omega = \pi_\omega(\mathcal{O})''$. We denote by $\mathcal{N}_\omega$ the set of all $\omega$-normal states. $\mathcal{N}_\omega$ is a norm closed convex subset of $E(\mathcal{O})$.

If $\nu$ is another positive linear functionals on $\mathcal{O}$, then $\nu \ll \omega$ iff $\mathcal{N}_\nu \subset \mathcal{N}_\omega$. $\omega$ and $\nu$ are said to be quasi-equivalent if $\mathcal{N}_\nu = \mathcal{N}_\omega$ and disjoint if $\mathcal{N}_\nu \cap \mathcal{N}_\omega = \emptyset$.

If $\nu \geq \phi \geq 0$ for some $\omega$-normal linear functional $\phi$ implies $\phi = 0$ we say that $\nu$ and $\omega$ are mutually singular (or orthogonal), and write $\nu \perp \omega$. An equivalent (more symmetric) definition is: $\nu \perp \omega$ iff $\nu \geq \phi \geq 0$ and $\omega \geq \phi \geq 0$ imply $\phi = 0$.

If $\nu$ and $\omega$ are disjoint, then $\nu \perp \omega$. The converse does not hold— it is possible that $\nu$ and $\omega$ are mutually singular but not disjoint.

A positive linear functional $\nu$ has a unique decomposition $\nu = \nu_n + \nu_s$, where $\nu_n, \nu_s$ are positive linear functional, $\nu_n \ll \omega$, and $\nu_s \perp \omega$. Moreover, $\nu_n$ and $\nu_s$ are disjoint. The uniqueness of the decomposition implies that if $\nu$ is $\tau$-invariant, then so are $\nu_n$ and $\nu_s$.

A state $\omega$ is called factor state (or primary state) if its enveloping von Neumann algebra is a factor *i.e.*, if $\mathfrak{M}_\omega \cap \mathfrak{M}_\omega' = \mathbb{C}I$. It is called modular if $\Omega_\omega$ is a separating vector for $\mathfrak{M}_\omega$ *i.e.*, if $A\Omega_\omega = 0$ for $A \in \mathfrak{M}_\omega$ implies $A = 0$. This condition is equivalent to the cyclicity of $\Omega_\omega$ for the commutant $\mathfrak{M}_\omega'$. Any KMS state at inverse temperature $\beta \in \mathbb{R}$ is modular.

Assume that $\omega$ is a modular state on $\mathcal{O}$. The formula

$$A\Omega_\omega \mapsto A^*\Omega_\omega,$$

defines an anti-linear map $S$ on the dense subspace $\mathfrak{M}_\omega\Omega_\omega$. A simple calculation show that $\mathfrak{M}_\omega'\Omega_\omega \subset D(S^*)$ and

$$S^*B\Omega_\omega = B^*\Omega_\omega.$$

Since $\mathfrak{M}_\omega'\Omega_\omega$ is dense, $S$ is closable and its closure has a polar decomposition

$$\bar{S} = J\Delta_\omega^{1/2},$$

where $J$ is anti-unitary and $\Delta$ is a positive self-adjoint operator. Also of interest is the norm closure $\mathcal{P}$ of the set

$$\{AJA\Omega_\omega | A \in \mathfrak{M}_\omega\}.$$

The main results of Tomita-Takesaki are contained in the following

**Theorem 2.1** *The anti-unitary operator $J$ is a conjugation, $J^2 = I$, such that*

$$J\Delta = \Delta^{-1}J.$$

*For any $\Psi \in \mathcal{P}$ and any $A \in \mathfrak{M}_\omega$ one has*

$$J\Psi = \Psi, \qquad AJAJ\mathcal{P} \subset \mathcal{P},$$

*moreover,*

$$J\mathfrak{M}_\omega J = \mathfrak{M}_\omega'.$$

*The unitary group $\Delta^{\mathrm{i}t}$ satisfies*

$$\Delta^{\mathrm{i}t}\Omega_\omega = \Omega_\omega, \qquad \Delta^{\mathrm{i}t}\mathcal{P} \subset \mathcal{P},$$

*for all $t \in \mathbb{R}$ and generates a group of $*$-automorphisms of $\mathfrak{M}_\omega$,*

$$\sigma_\omega^t(A) = \Delta^{\mathrm{i}t}A\Delta^{-\mathrm{i}t}.$$

*$\sigma_\omega$ is the unique group of $*$-automorphisms of $\mathfrak{M}_\omega$ for which $\omega$ is a KMS state (at inverse temperature $\beta = -1$).*

$J$ is called the modular conjugation, $\Delta$ the modular operator, $\sigma_\omega$ the modular group and $\mathcal{P}$ the natural cone.

An important property of the natural cone is that for every state $\eta \in \mathcal{N}_\omega$ there is a unique vector $\Omega_\eta \in \mathcal{P}$ such that $\eta(\cdot) = (\Omega_\eta, \pi_\omega(\cdot)\Omega_\eta)$. Moreover, if $\tau$ is a $C^*$- dynamics on $\mathcal{O}$ (not necessarily leaving the state $\omega$ invariant), then there is a unique self-adjoint operator $L$ on $\mathcal{H}_\omega$ such that, for all $t$,

$$\begin{aligned} \pi_\omega(\tau^t(A)) &= \mathrm{e}^{\mathrm{i}tL}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL}, \\ \mathrm{e}^{-\mathrm{i}tL}\mathcal{P} &\subset \mathcal{P}. \end{aligned} \tag{9}$$

The operator $L$ is called the standard Liouvillean. The first formula in (9) allows us to extend $\tau$ to all of $\mathfrak{M}_\omega$.

A state $\eta \in \mathcal{N}_\omega$ is $\tau$-invariant iff $L\Omega_\eta = 0$. Thus, the study of $\omega$-normal, $\tau$-invariant states reduces to the study of $\mathrm{Ker}\, L$. This is the first link between quantum statistical mechanics and modular theory. The second one is Takesaki's theorem: $\omega$ is a $(\tau, \beta)$-KMS state iff

$$\Delta = \mathrm{e}^{-\beta L}. \tag{10}$$

The third link is quantum Koopmanism: The spectral properties of the standard Liouvillean $L$ encode the ergodic properties of the quantum dynamical system $(\mathcal{O}, \tau, \omega)$ in complete analogy with Koopman's lemma of classical ergodic theory [JP1, JP3]. For example, if the state $\omega$ is modular, then $(\mathcal{O}, \tau, \omega)$ is ergodic iff zero is a simple eigenvalue of $L$. Moreover, the system returns to equilibrium if the singular spectrum of $L$ reduces to this simple eigenvalue.

## 2.3 Perturbation theory

Let $(\mathcal{O}, \tau^t)$ be a $C^*$-dynamical system and denote by $\delta$ its generator. A *local perturbation* of the system is obtained by perturbing its generator with the bounded $*$-derivation associated with a self-adjoint element $V$ of $\mathcal{O}$

$$\delta_V = \delta + i[V, \cdot\,],$$

with $D(\delta_V) = D(\delta)$. Since this is a bounded perturbation, there is a Dyson expansion for the perturbed group $\tau_V^t = \mathrm{e}^{t\delta_V}$

$$\begin{aligned} \tau_V^t(X) &= \tau^t(X) + \\ &+ \sum_{N=1}^{\infty} \int_0^t \mathrm{d}t_1 \cdots \int_0^{t_{N-1}} \mathrm{d}t_N \, \mathrm{i}[\tau^{t_N}(V), \mathrm{i}[\cdots, \mathrm{i}[\tau^{t_1}(V), \tau^t(X)] \cdots ]], \end{aligned} \tag{11}$$

which is norm convergent for any $t \in \mathbb{R}$ and any $X \in \mathcal{O}$. Another useful representation of the locally perturbed dynamics is the *interaction picture*. The *Ansatz*

$$\tau_V^t(X) = \Gamma_V^t \tau^t(X) \Gamma_V^{t*}. \tag{12}$$

leads to the differential equation

$$\partial_t \Gamma_V^t = i \Gamma_V^t \tau^t(V),$$

with the initial condition $\Gamma_V^0 = I$. It follows that $\Gamma_V^t$ is a unitary element of $\mathcal{O}$ which has a norm convergent expansion

$$\begin{aligned} \Gamma_V^t &= \mathrm{T}\!-\exp\left\{ i \int_0^t \tau^s(V) ds \right\} \\ &= I + \sum_{N=1}^{\infty} i^N \int_0^t \mathrm{d}t_1 \cdots \int_0^{t_{N-1}} \mathrm{d}t_N \, \tau^{t_n}(V) \cdots \tau^{t_1}(V). \end{aligned} \tag{13}$$

Moreover, $\Gamma_V^t$ satisfies the cocycle relations

$$\Gamma_V^{t+s} = \Gamma_V^t \tau^t(\Gamma_V^s) = \tau_V^t(\Gamma_V^s)\Gamma_V^t. \tag{14}$$

Let $(\mathcal{H}, \pi)$ be a representation of $\mathcal{O}$ carrying a unitary implementation $U^t$ of the unperturbed dynamics $\tau^t$

$$\pi(\tau^t(X)) = U^t \pi(X) U^{t*}.$$

The interaction picture shows that $U_V^t = \pi(\Gamma_V^t)U^t$ unitarily implement $\tau_V^t$ in this representation (the group property follows from the cocycle property (14)). From the expansion (13) we get norm convergent expansion (the integral is in the strong Riemann sense)

$$U_V^t = U^t + \sum_{N=1}^{\infty} i^N \int_0^t \mathrm{d}t_1 \cdots \int_0^{t_{N-1}} \mathrm{d}t_N \, U^{t_N} \pi(V) U^{t_{N-1}-t_N} \cdots U^{t_1-t_2} \pi(V) U^{t-t_1}.$$

Let $G_V$ be the self-adjoint generator of $U_V^t$. Applying the last formula to a vector $\Phi \in D(G_0)$ and differentiating at $t = 0$ we obtain $\Phi \in D(G_V)$ and

$$G_V = G + \pi(V). \tag{15}$$

Note however that the unitary implementation of $\tau_V^t$ in $\mathcal{H}$ is by no means unique. $e^{itK}$ is another implementation if and only if

$$e^{itG_V} \pi(X) e^{-itG_V} = e^{itK} \pi(X) e^{-itK},$$

for all $X \in \mathcal{O}$ and all $t$. Thus $e^{itK} e^{-itG_V}$ must be a unitary element of $\pi(\mathcal{O})'$ for all $t$. Such $K$ are easily obtained by setting

$$K = G_V - W = G + \pi(V) - W,$$

where $W$ is a self-adjoint element of $\pi(\mathcal{O})'$. Then $\Gamma_W'^t = e^{itK} e^{-itG_V}$ satisfies the differential equation

$$\partial_t \Gamma_W'^t = -i \Gamma_W'^t W^t,$$

with $W^t = e^{itG_V} W e^{-itG_V}$ and initial value $\Gamma_W'^0 = I$. Since $e^{itG_V} = \pi(\Gamma_V^t) e^{itG}$ and $e^{itG} W e^{-itG} \in \pi(\mathcal{O})'$ for all $t$, we have $W^t = e^{itG} W e^{-itG}$ and $\Gamma_W'^t$ is given by the norm convergent time-ordered exponential

$$\Gamma_W'^t = \mathrm{T} - \exp\left\{ -i \int_0^t W^s \mathrm{d}s \right\}.$$

In the special case of the cyclic representation of a modular state $\omega$, the choice

$$U^t = \mathrm{e}^{\mathrm{i}tL}, \qquad W = J\pi_\omega(V)J,$$

where $L$ is the standard Liouvillean of $\tau$ leads to $\Gamma'^t_W = J\Gamma^t_V J$ and hence

$$\mathrm{e}^{\mathrm{i}t(L+\pi_\omega(V)-J\pi_\omega(V)J)} = \Gamma^t_V(J\Gamma^t_V J)\mathrm{e}^{\mathrm{i}tL},$$

preserves the cone $\mathcal{P}$. It follows that

$$L + \pi_\omega(V) - J\pi_\omega(V)J,$$

is the standard Liouvillean of $\tau_V$.

Specializing even more, assume now that $\omega$ is a $\beta$-KMS state for $\tau$. It is then natural to ask for a $\beta$-KMS state for the perturbed dynamics $\tau_V$.

To gain some intuition on the problem let us consider first the finite dimensional case. Let $\mathcal{O} = \mathcal{B}(\mathcal{H})$ for some finite dimensional Hilbert space $\mathcal{H}$ and $\tau^t(X) = e^{itH}Xe^{-itH}$ for some self-adjoint $H$. Then

$$\omega(X) = \mathrm{Tr}\,(e^{-\beta H}X)/\mathrm{Tr}\,(e^{-\beta H}) = \mathrm{Tr}\,(e^{-\beta H/2}Xe^{-\beta H/2})/\mathrm{Tr}\,(e^{-\beta H}),$$

is the unique $\beta$-KMS state for $\tau$. The perturbed dynamics $\tau^t_V$ as well as the perturbed KMS state $\omega_V$ are obtained by replacing $H$ by $H+V$. Note that, in the present situation, the definition (12) of the unitary cocycle $\Gamma^t_V$ reads

$$\Gamma^t_V = e^{it(H+V)}e^{-itH},$$

which is obviously an entire function of $t$. Thus, we can express $\omega_V$ in terms of $\omega$ as

$$\omega_V(X) = \frac{\omega(X\Gamma^{i\beta}_V)}{\omega(\Gamma^{i\beta}_V)} = \frac{\omega(\Gamma^{i\beta/2\star}_V X\Gamma^{i\beta/2}_V)}{\omega(\Gamma^{i\beta/2\star}_V\Gamma^{i\beta/2}_V)}. \tag{16}$$

On the other hand, we have

$$\pi_\omega(\Gamma^{i\beta/2}_V)\Omega_\omega = \pi_\omega(\Gamma^{i\beta/2}_V)e^{-\beta L/2}\Omega_\omega = e^{-\beta(L+\pi_\omega(V))/2}\Omega_\omega, \tag{17}$$

by Equ. (15). Thus we can write Equ. (16) as

$$\omega_V(X) = \frac{(\Omega_{\omega^V}, \pi_\omega(X)\Omega_{\omega^V})}{(\Omega_{\omega^V}, \Omega_{\omega^V})},$$

where $\Omega_{\omega_V} = e^{-\beta(L+V)/2}\Omega_\omega$. The cocycle property (14) further gives

$$\Gamma_V^{i\beta/2} = \Gamma_V^{i\beta/4}\tau^{i\beta/4}(\Gamma_V^{i\beta/4}) = \Gamma_V^{i\beta/4}\tau^{i\beta/2}(\tau^{-i\beta/4}(\Gamma_V^{i\beta/4})),$$

and $\tau^{-i\beta/4}(\Gamma_V^{i\beta/4}) = (\Gamma_V^{-i\beta/4})^{-1}$. Since $\Gamma_V^{\bar{z}*}$ is analytic and equals $(\Gamma_V^z)^{-1}$ for real $z$, they are equal for all $z$ and

$$\Gamma_V^{i\beta/2} = \Gamma_V^{i\beta/4}\tau^{i\beta/2}(\Gamma_V^{i\beta/4*}).$$

We can rewrite the perturbed vector $\Omega_{\omega_V}$ as

$$\Omega_{\omega_V} = \pi_\omega(\Gamma_V^{i\beta/4})e^{-\beta L/2}\pi_\omega(\Gamma_V^{i\beta/4})^*\Omega_\omega = \pi_\omega(\Gamma_V^{i\beta/4})e^{-\beta L/2}J\Delta^{1/2}\pi_\omega(\Gamma_V^{i\beta/4})\Omega_\omega,$$

and since $J\Delta^{1/2} = Je^{-\beta L/2} = e^{\beta L/2}J$ we conclude that

$$\Omega_{\omega_V} = \pi_\omega(\Gamma_V^{i\beta/4})J\pi_\omega(\Gamma_V^{i\beta/4})J\Omega_\omega \in \mathcal{P}.$$

Thus $\Omega_{\omega_V}$ is, up to normalization, the unique standard vector representative of the perturbed KMS-state $\omega_V$.

The main difficulty in extending this formula to more general situation is to show that $\Omega_\omega \in D(e^{-\beta(L+\pi_\omega(V))/2})$. Indeed, even if $V$ is bounded, the Liouvillean $L$ is usually unbounded below and ordinary perturbation theory of quasi-bounded semi-groups fails. If $V$ is such that $\tau^t(V)$ is entire analytic, this can be done using (17) since the cocycle $\Gamma_V^t$ is then analytic, as the solution of a linear differential equation with analytic coefficients. It is possible to extend the result to general bounded perturbations using an approximation argument. The result is usually quoted as Araki's perturbation theory of $KMS$ states.

**Theorem 2.2** *Let $(\mathcal{O}, \tau^t)$ be a $C^*$-dynamical system and $V \in \mathcal{O}$ a local perturbation. There exists a bijective map $\omega \mapsto \omega_V$ between the set of $\beta$-KMS states for $\tau$ and the set of $\beta$-KMS states for $\tau_V$ such that $\omega_V \in \mathcal{N}_\omega$ and $(\omega_{V_1})_{V_2} = \omega_{V_1+V_2}$.*

*Let $\omega$ be a $\beta$-KMS state for $\tau$. Denote by $L$ the standard Liouvillean of $\tau$. For any local perturbation $V$ one has:*

1. $\Omega_\omega \in D(e^{-\beta(L+\pi_\omega(V))/2})$.
2. *Up to normalization, $\Omega_V = e^{-\beta(L+\pi_\omega(V))/2}\Omega_\omega$ is the vector representative of $\omega_V$ in $\mathcal{P}$.*
3. *$\Omega_V$ is cyclic and separating for $\mathfrak{M}_\omega$.*
4. *For any $\nu \in \mathcal{N}_\omega$ one has* $\mathrm{Ent}(\nu|\omega_V) = \mathrm{Ent}(\nu|\omega) + \nu(V) - \log\|\Omega_V\|^2$.

## 2.4 Ideal Fermi gases

In these Lectures, I will be primarily concerned with open Fermion systems. The reservoirs $\mathcal{R}_\alpha$ will be ideal Fermi gases (gases of independent electrons in the language of solid state physics). The small system $\mathcal{S}$ itself will be such an ideal gas most of the time, except in the last Section where I will present some results pertinent to the case where the Fermions are allowed to interact in the system $\mathcal{S}$ only.

Let $\mathfrak{h}$ be the Hilbert space of a single Fermion and $\Gamma_-(\mathfrak{h})$ be the anti-symmetric Fock space over $\mathfrak{h}$ and denote by $a^*(f)$, $a(f)$ the creation and annihilation operators for a single Fermion in the state $f \in \mathfrak{h}$. These operators are bounded on $\Gamma_-(\mathfrak{h})$

$$\|a(f)\| = \|a^*(f)\| = \|f\|, \tag{18}$$

and satisfy the Canonical Anticommutation Relations (CAR)

$$\{a(f), a^*(g)\} = (f, g)I, \quad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0.$$

The corresponding self-adjoint field operator

$$\varphi(f) \equiv \frac{1}{\sqrt{2}}\left(a(f) + a^*(f)\right),$$

satisfies the anticommutation relation

$$\{\varphi(f), \varphi(g)\} = \mathrm{Re}(f, g)I.$$

In the sequel $a^\#$ stands for either $a$ or $a^*$.

The norm closure in $\mathcal{B}(\Gamma_-(\mathfrak{h}))$ of the linear span of the set of monomials

$$a^\#(f_1)\cdots a^\#(f_n),$$

is a $C^*$-algebra: The CAR or Fermi algebra over $\mathfrak{h}$ which we denote by $\mathrm{CAR}(\mathfrak{h})$.

Let $h$ denotes the Hamiltonian of a single Fermion. I will always assume that $h$ is bounded below. The second quantization $H \equiv \mathrm{d}\Gamma(h)$ of $h$ generates a strongly continuous unitary group

$$\Gamma(\mathrm{e}^{ith}) = \mathrm{e}^{\mathrm{i}tH},$$

on the Fock space $\Gamma_-(\mathfrak{h})$. The induced group of $*$-automorphisms of $\mathcal{B}(\Gamma_-(\mathfrak{h}))$

$$\tau^t(A) \equiv \mathrm{e}^{\mathrm{i}tH} A\, \mathrm{e}^{-\mathrm{i}tH},$$

leaves the subalgebra $\mathrm{CAR}(\mathfrak{h})$ invariant since

$$\tau^t(a^\#(f)) = a^\#(\mathrm{e}^{\mathrm{i}th}f).$$

Moreover, Equ. (18) gives

$$\|\tau^t(a^\#(f)) - a^\#(f)\| = \|\mathrm{e}^{\mathrm{i}th}f - f\|,$$

from which one easily concludes that the restriction of $\tau^t$ to $\mathrm{CAR}(\mathfrak{h})$ is strongly continuous. Thus, the pair $(\mathrm{CAR}(\mathfrak{h}), \tau)$ is a $C^*$-dynamical system.

Recall that $N \equiv \mathrm{d}\Gamma(I)$ is the Fermion number operator on $\Gamma_-(\mathfrak{h})$. The previous argument also shows that

$$\vartheta^t(A) \equiv \mathrm{e}^{\mathrm{i}tN} A \mathrm{e}^{-\mathrm{i}tN}.$$

defines a strongly continuous group of $*$-automorphims of $\mathrm{CAR}(\mathfrak{h})$. Clearly, the gauge group $\vartheta$ commutes with the dynamical group $\tau$. For any $\mu \in \mathbb{R}$,

$$\tau_\mu^t \equiv \tau^t \circ \vartheta^{-\mu t},$$

is the strongly continuous group of $*$-automorphisms of $\mathrm{CAR}(\mathfrak{h})$ induced by $K_\mu \equiv H - \mu N$. A state on $\mathrm{CAR}(\mathfrak{h})$ is called $(\beta, \mu)$-KMS state if it is a $\beta$-KMS state for $\tau_\mu$. This state describes the free Fermi gas at thermal equilibrium in the grand canonical ensemble with inverse temperature $\beta$ and chemical potential $\mu$ (recall Exercise 1).

To every self-adjoint operator $T$ on $\mathfrak{h}$ such that $0 \leq T \leq I$ one can associate a state $\omega_T$ on $\mathrm{CAR}(\mathfrak{h})$ satisfying

$$\omega_T(a^*(f_n) \cdots a^*(f_1) a(g_1) \cdots a(g_m)) = \delta_{n,m} \mathrm{det}\{(g_i, T f_j)\}. \tag{19}$$

This $\vartheta$-invariant state is usually called the quasi-free gauge-invariant state generated by $T$. It is completely determined by its two point function

$$\omega_T(a^*(f)a(g)) = (g, Tf).$$

Alternatively, quasi-free gauge-invariant states can be described by their action on the field operators. For any integer $n$ we define $\mathcal{P}_n$ as the set of all permutations $\pi$ of $\{1, \ldots, 2n\}$ such that

$$\pi(2j-1) < \pi(2j), \quad \text{and} \quad \pi(2j-1) < \pi(2j+1),$$

for every $j \in \{1, \ldots, n\}$. Denote by $\epsilon(\pi)$ the signature of $\pi \in \mathcal{P}_n$. $\omega_T$ is the unique state on $\mathrm{CAR}(\mathfrak{h})$ satisfying the Wick relations:

$$\begin{aligned}
\omega_T(\varphi(f_1)\varphi(f_2)) &= \frac{1}{2}(f_1, f_2) - \mathrm{i}\,\mathrm{Im}(f_1, Tf_2), \\
\omega_T(\varphi(f_1)\cdots\varphi(f_{2n})) &= \sum_{\pi\in\mathcal{P}_n} \epsilon(\pi) \prod_{j=1}^{n} \omega_T(\varphi(f_{\pi(2j-1)})\varphi(f_{\pi(2j)})), \\
\omega_T(\varphi(f_1)\cdots\varphi(f_{2n+1})) &= 0.
\end{aligned}$$

Note that if $A$ is a trace class operator on $\mathfrak{h}$, then $\mathrm{d}\Gamma(A) \in \mathrm{CAR}(\mathfrak{h})$ and

$$\|\mathrm{d}\Gamma(A)\| = \|A\|_1.$$

Moreover, for any quasifree state $\omega_T$ one has

$$\omega_T(\mathrm{d}\Gamma(A)) = \mathrm{Tr}\,(TA). \tag{20}$$

Using the defining relation (19) and the CAR, one easily shows that, for any trace class operators $A, B$ on $\mathfrak{h}$, one also has

$$\omega_T(\mathrm{d}\Gamma(A)\mathrm{d}\Gamma(B)) - \omega_T(\mathrm{d}\Gamma(A))\omega_T(\mathrm{d}\Gamma(B)) = \mathrm{Tr}\,(TA(I-T)B). \tag{21}$$

If $\mathfrak{h} = \mathfrak{h}_1 \oplus \mathfrak{h}_2$ and $T = T_1 \oplus T_2$, then for $A \in \mathrm{CAR}(\mathfrak{h}_1)$ and $B \in \mathrm{CAR}(\mathfrak{h}_2)$ one has

$$\omega_T(A\,B) = \omega_{T_1}(A)\,\omega_{T_2}(B). \tag{22}$$

$\omega_T$ is a factor state. It is modular iff $\mathrm{Ker}\,T = \mathrm{Ker}\,(I-T) = \{0\}$.

Two states $\omega_{T_1}$ and $\omega_{T_2}$ are quasi-equivalent *i.e.*, $\mathcal{N}_{\omega_{T_1}} = \mathcal{N}_{\omega_{T_2}}$, iff the operators

$$T_1^{1/2} - T_2^{1/2} \qquad \text{and} \qquad (I-T_1)^{1/2} - (I-T_2)^{1/2}, \tag{23}$$

are Hilbert-Schmidt; see [De, PoSt, Ri]. Assume that $\mathrm{Ker}\,T_i = \mathrm{Ker}\,(I-T_i) = \{0\}$. Then the states $\omega_{T_1}$ and $\omega_{T_2}$ are unitarily equivalent iff (23) holds.

If $T = F(h)$ for some function $F\colon \mathrm{sp}(h) \to [0,1]$, then $\omega_T$ describes a free Fermi gas with energy density $F(\varepsilon)$.

The state $\omega_T$ is $\tau$-invariant iff $T$ commutes with $\mathrm{e}^{\mathrm{i}th}$ for all $t$. If the spectrum of $h$ is simple this means that $T = F(h)$ for some function $F\colon \mathrm{sp}(h) \to [0,1]$.

For any $\beta, \mu \in \mathbb{R}$, the Fermi-Dirac distribution $\rho_{\beta\mu}(\varepsilon) \equiv (1 + \mathrm{e}^{\beta(\varepsilon-\mu)})^{-1}$ induces the unique $(\beta,\mu)$-KMS state on $\mathrm{CAR}(\mathfrak{h})$, which we denote by $\omega_{\beta\mu}$.

The cyclic representation of $\mathrm{CAR}(\mathfrak{h})$ associated to $\omega_T$ can be explicitly computed as follows. Fix a complex conjugation $f \mapsto \bar{f}$ on $\mathfrak{h}$ and extend it to $\Gamma_-(\mathfrak{h})$. Denote by $\Omega$ the vacuum vector and $N$ the number operator in $\Gamma_-(\mathfrak{h})$. Set

$$\begin{aligned}\mathcal{H}_{\omega_T} &= \Gamma_-(\mathfrak{h}) \otimes \Gamma_-(\mathfrak{h}),\\ \Omega_{\omega_T} &= \Omega \otimes \Omega,\\ \pi_{\omega_T}(a(f)) &= a((I-T)^{1/2}f) \otimes I + (-I)^N \otimes a^*(\bar{T}^{1/2}\bar{f}).\end{aligned}$$

The triple $(\mathcal{H}_{\omega_T}, \pi_{\omega_T}, \Omega_{\omega_T})$ is the GNS representation of the algebra $\mathrm{CAR}(\mathfrak{h})$ associated to $\omega_T$. (This representation was constructed in [AW] and if often called Araki-Wyss representation.) If $\omega_T$ is $\tau$-invariant, the corresponding $\omega_T$-Liouvillean is

$$L = \mathrm{d}\Gamma(h) \otimes I - I \otimes \mathrm{d}\Gamma(\bar{h}).$$

If $h$ has purely (absolutely) continuous spectrum so does $L$, except for the simple eigenvalue $0$ corresponding to the vector $\Omega_{\omega_T}$. On the other hand, $0$ becomes a degenerate eigenvalue as soon as $h$ has some point spectrum. Thus the ergodic properties of $\tau$-invariant, gauge-invariant quasi-free states can be described in terms of the spectrum of $h$. If $h$ has no eigenvalues the state $\omega_T$ is ergodic

$$\lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} \nu(\tau^t(A))\,\mathrm{d}t = \omega_T(A),$$

for all $\nu \in \mathcal{N}_{\omega_T}$ and $A \in \mathrm{CAR}(\mathfrak{h})$. If $h$ has purely absolutely continuous spectrum, then $\omega_T$ is mixing

$$\lim_{|t|\to\infty} \nu(\tau^t(A)) = \omega_T(A).$$

If $\omega_T$ is modular, then its modular operator is described by

$$\log\Delta = \mathrm{d}\Gamma(s) \otimes I - I \otimes \mathrm{d}\Gamma(\bar{s}),$$

where $s = \log T(I-T)^{-1}$. The corresponding modular conjugation is $J(\Phi\otimes\Psi) = u\bar{\Psi} \otimes u\bar{\Phi}$, where $u = (-I)^{N(N+I)/2}$.

Let $\theta$ be the $*$-automorphism of $\mathrm{CAR}(\mathfrak{h})$ defined by

$$\theta(a(f)) = -a(f). \tag{24}$$

$A \in \mathrm{CAR}(\mathfrak{h})$ is called even if $\theta(A) = A$ and odd if $\theta(A) = -A$. Every element $A \in \mathrm{CAR}(\mathfrak{h})$ can be written in a unique way as a sum $A = A^+ + A^-$ where $A^\pm =$

$(A \pm \theta(A))/2$ is even/odd. The set of all even/odd elements is a vector subspace of $\mathrm{CAR}(\mathfrak{h})$ and $\mathrm{CAR}(\mathfrak{h})$ is a direct sum of these two subspaces. It follows from (19) that $\omega_T(A) = 0$ if $A$ is odd. Therefore one has $\omega_T(A) = \omega_T(A^+)$ and

$$\omega_T \circ \theta = \omega_T. \tag{25}$$

The subspace of even elements is a $C^*$-subalgebra of $\mathrm{CAR}(\mathfrak{h})$. This subalgebra is called even CAR algebra and is denoted by $\mathrm{CAR}^+(\mathfrak{h})$. It is the norm closure of the linear span of even monomials

$$a^\#(f_1)\cdots a^\#(f_{2n}).$$

The even CAR algebra plays an important role in physics. It is is preserved by $\tau$ and $\vartheta$ and the pair $(\mathrm{CAR}^+(\mathfrak{h}), \tau)$ is a $C^*$-dynamical system.

We denote the restriction of $\omega_T$ to $\mathrm{CAR}^+(\mathfrak{h})$ by the same letter. In particular, $\omega_{\beta\mu}$ is the unique $(\beta, \mu)$-KMS state on $\mathrm{CAR}^+(\mathfrak{h})$.

Let

$$A = a^\#(f_1)\cdots a^\#(f_n), \qquad B = a^\#(g_1)\cdots a^\#(g_m),$$

be two elements of $\mathrm{CAR}(\mathfrak{h})$, where $m$ is *even*. It follows from CAR that

$$\|[A, \tau^t(B)]\| \le C \sum_{i,j} |(f_i, \mathrm{e}^{\mathrm{i}th} g_j)|,$$

where one can take $C = (\max(\|f_i\|, \|g_j\|))^{n+m-2}$. If the functions $|(f_i, \mathrm{e}^{\mathrm{i}th} g_j)|$ belong to $L^1(\mathbb{R}, \mathrm{d}t)$, then

$$\int_{-\infty}^{\infty} \|[A, \tau^t(B)]\| \, \mathrm{d}t < \infty. \tag{26}$$

Let $\mathfrak{h}_0 \subset \mathfrak{h}$ be a subspace such that for any $f, g \in \mathfrak{h}_0$ the function $t \mapsto (f, \mathrm{e}^{\mathrm{i}th} g)$ is integrable. Let $\mathcal{O}_0 = \{a^\#(f_1)\cdots a^\#(f_n) \,|\, n \in \mathbb{N}, f_j \in \mathfrak{h}_0\}$ and let $\mathcal{O}_0^+$ be the even subalgebra of $\mathcal{O}_0$. Then for $A \in \mathcal{O}_0$ and $B \in \mathcal{O}_0^+$ (26) holds. If $\mathfrak{h}_0$ is dense in $\mathfrak{h}$, then $\mathcal{O}_0$ is dense in $\mathrm{CAR}(\mathfrak{h})$ and $\mathcal{O}_0^+$ is dense in $\mathrm{CAR}^+(\mathfrak{h})$.

# 3 Entropy production

## 3.1 Relative entropy

Let $\omega$ be a modular state on the $C^*$-algebra $\mathcal{O}$ and $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the induced cyclic representation.

To any state $\nu \in \mathcal{N}_\omega$ we associate its unique vector representative $\Omega_\nu \in \mathcal{P}$. We denote by $s_\nu$ the orthogonal projection on the closed subspace of $\mathcal{H}_\omega$ generated by $\mathfrak{M}_\omega'\Omega_\nu$. On the dense subspace $\mathfrak{M}_\omega\Omega_\nu \oplus (\mathfrak{M}_\omega\Omega_\nu)^\perp$ the formula

$$A\Omega_\nu \oplus \Phi \mapsto s_\nu A^*\Omega_\omega.$$

defines an anti-linear operator $S_{\omega,\nu}$. Denoting by $s_\nu'$ the orthogonal projection on the closed subspace generated by $\mathfrak{M}_\omega\Omega_\nu$, one easily checks that the dense subspace $\mathfrak{M}_\omega'\Omega_\nu \oplus (\mathfrak{M}_\omega'\Omega_\nu)^\perp$ belongs to the domain of the adjoint $S_{\omega,\nu}^*$ and that

$$S_{\omega,\nu}^*(B\Omega_\nu \oplus \Psi) = s_\nu' B^*\Omega_\omega.$$

Thus $S_{\omega,\nu}$ is closable. The positive self-adjoint operator

$$\Delta_{\omega,\nu} \equiv S_{\omega,\nu}^*\bar{S}_{\omega,\nu},$$

is called relative modular operator.

The relative entropy of two states $\omega, \nu \in E(\mathcal{O})$ has been defined by Araki in [Ar1, Ar2]. We shall however use the notation of [BR, Don] (which departs from Araki's one by the order of the arguments and the sign) and set

$$\mathrm{Ent}(\nu|\omega) \equiv \begin{cases} (\Omega_\nu, \log\Delta_{\omega,\nu}\,\Omega_\nu) & \text{if } \nu \in \mathcal{N}_\omega, \\ -\infty & \text{otherwise.} \end{cases}$$

It follows from the inequality $\log x \le x - 1$ and the fact that $(\Omega_\nu, \Delta_{\omega,\nu}\Omega_\nu) = \|s_\nu\Omega_\omega\|^2 \le 1$, that

$$\mathrm{Ent}(\nu|\omega) \le 0.$$

**Remark.** The above construction is easily adapted to the case where $\omega$ is not modular. One has then to use a standard representation of the envelopping von Neumann algebra $\mathfrak{M}_\omega$. In our applications however, $\omega$ will always be modular.

To motivate this definition, let us consider the special case of a quantum system with a finite dimensional Hilbert space $\mathcal{H}$. The $C^*$-algebra of observables is the full matrix algebra $\mathcal{O} \equiv \mathcal{B}(\mathcal{H})$ and the state space is

$$E(\mathcal{O}) = \{\omega \in \mathcal{B}(\mathcal{H}) \,|\, \omega \ge 0, \mathrm{Tr}\,\omega = 1\}.$$

To construct the cyclic representation associated with the state $\omega$ let us set $\mathcal{K} \equiv \mathrm{Ran}\,\omega = (\mathrm{Ker}\,\omega)^\perp$ and consider $\mathcal{B}(\mathcal{K}, \mathcal{H})$ as a Hilbert space equiped with the inner product $(X, Y) \equiv \mathrm{Tr}\,(X^*Y)$. We set

$$\mathcal{H}_\omega = \mathcal{B}(\mathcal{K}, \mathcal{H}), \qquad \pi_\omega(A)X = AX, \qquad \Omega_\omega = \omega^{1/2}i,$$

where $i$ denotes the canonical injection $\mathcal{K} \to \mathcal{H}$. One easily checks that $\pi_\omega(\mathcal{O})\Omega_\omega = \mathcal{H}_\omega$. Moreover, one has

$$(\Omega_\omega, \pi_\omega(A)\Omega_\omega) = \mathrm{Tr}\,(i^*\omega^{1/2}A\omega^{1/2}i) = \mathrm{Tr}\,(\omega^{1/2}ii^*\omega^{1/2}A) = \mathrm{Tr}\,(\omega A).$$

Thus $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is the cyclic representation of $\mathcal{O}$ associated to $\omega$.

Since $\pi_\omega(A)\Omega_\omega = A\omega^{1/2}i = 0$ if $\mathcal{K} \subset \mathrm{Ker}\, A$, the state $\omega$ is modular if and only if $\mathcal{K} = \mathcal{H}$, that is if $\omega > 0$. Note incidently that a Gibbs state $\omega = \mathrm{e}^{-\beta H}/\mathrm{Tr}\,(e^{-\beta H})$ is always modular.

From now on we assume that $\omega > 0$, and thus $\mathcal{H}_\omega = \mathcal{B}(\mathcal{H})$. Since $\pi_\omega$ is injective, the envelopping von Neumann algebra $\mathfrak{M}_\omega = \pi_\omega(\mathcal{O})$ is isomorphic to $\mathcal{O}$. Let us determine the modular structure associated to $\omega$. By definition we have

$$(\pi_\omega(A)\Omega_\omega, \Delta\pi_\omega(B)\Omega_\omega) = \overline{(S\pi_\omega(A)\Omega_\omega, S\pi_\omega(B)\Omega_\omega)},$$

that is

$$(A\omega^{1/2}, \Delta B\omega^{1/2}) = \overline{(A^*\omega^{1/2}, B^*\omega^{1/2})}.$$

Writing $X = B\omega^{1/2}$ and $Y = \Delta X$, we obtain

$$\mathrm{Tr}\,(\omega^{1/2}A^*Y) = \overline{\mathrm{Tr}\,(\omega^{1/2}A\omega^{-1/2}X^*\omega^{1/2})} = \mathrm{Tr}\,(\omega^{1/2}A^*\omega X\omega^{-1}),$$

from which we conclude that $Y = \Delta X = \omega X \omega^{-1}$. It follows that $\Delta^{1/2}X = \omega^{1/2}X\omega^{-1/2}$ and hence

$$JX = S\Delta^{-1/2}X = S\omega^{-1/2}X\omega^{1/2} = (\omega^{-1/2}X)^*\omega^{1/2} = X^*.$$

It is now easy to compute the natural cone

$$\mathcal{P} = \{\pi_\omega(A)J\pi_\omega(A)\Omega_\omega = A\omega^{1/2}A^* \,|\, A \in \mathcal{O}\} = \{X \in \mathcal{B}(\mathcal{H}) | X \geq 0\}.$$

We note also that the commutant $\mathfrak{M}_\omega'$ is given by

$$\mathfrak{M}_\omega' = J\mathfrak{M}_\omega J = J\pi_\omega(\mathcal{O})J = \pi_\omega'(\mathcal{O}),$$

where

$$\pi_\omega'(A) = J\pi_\omega(A)J : X \mapsto XA^*.$$

In particular the center $\mathfrak{M}_\omega \cap \mathfrak{M}_\omega'$ is trivial and therefore $\omega$ is a factor state.

If $\nu$ is another density matrix, its vector representative in $\mathcal{H}_\omega$ is just $\nu^{1/2}$. Denote by $p_\nu$ the orhogonal projection on its range. One has

$$\mathfrak{M}_\omega'\Omega_\nu = \{\nu^{1/2}A \,|\, A \in \mathcal{B}(\mathcal{H})\} = \{X \in \mathcal{B}(\mathcal{H}) \,|\, \mathrm{Ran}\, X \subset \mathrm{Ran}\, \nu\} = p_\nu\mathcal{B}(\mathcal{H}),$$

from which we conclude that $s_\nu = \pi_\omega(p_\nu)$. Similarly

$$\mathfrak{M}_\omega\Omega_\nu = \{A\nu^{1/2} \mid A \in \mathcal{B}(\mathcal{H})\} = \{X \in \mathcal{B}(\mathcal{H}) \mid \mathrm{Ker}\,\nu \subset \mathrm{Ker}\,X\} = \mathcal{B}(\mathcal{H})p_\nu,$$

and $s'_\nu = \pi'_\omega(p_\nu)$. From the definition of the relative modular operator we get, for $A, B \in \mathcal{O}$ and $\Phi, \Psi \in (\mathfrak{M}_\omega\Omega_\nu)^\perp = \mathcal{B}(\mathcal{H})(I - p_\nu)$,

$$(\pi_\omega(A)\Omega_\nu \oplus \Phi, \Delta_{\omega,\nu}(\pi_\omega(B)\Omega_\nu \oplus \Psi)) = \overline{(s_\nu\pi_\omega(A)^*\Omega_\omega, s_\nu\pi_\omega(B)^*\Omega_\omega)},$$

that is, with $X = \pi_\omega(B)\Omega_\nu \oplus \Psi = B\nu^{1/2} + \Psi(I - p_\nu)$ and $Y = \Delta_{\omega,\nu}X$,

$$\begin{array}{rcl}
\mathrm{Tr}\,((A\nu^{1/2} \oplus \Phi)^*Y) & = & \overline{\mathrm{Tr}\,((p_\nu A^*\omega^{1/2})^* p_\nu B^*\omega^{1/2})} \\
\mathrm{Tr}\,((\nu^{1/2}A^* + (I - p_\nu)\Phi^*)Y) & = & \mathrm{Tr}\,(\omega^{1/2}Bp_\nu A^*\omega^{1/2}) \\
& = & \mathrm{Tr}\,(\nu^{1/2}A^*\omega B\nu^{-1/2}p_\nu) \\
& = & \mathrm{Tr}\,(\nu^{1/2}A^*\omega X\nu^{-1}p_\nu) \\
& = & \mathrm{Tr}\,((\nu^{1/2}A^* + (I - p_\nu)\Phi^*)\omega X\nu^{-1}p_\nu),
\end{array}$$

from which we conclude that

$$\Delta_{\omega,\nu}X = \omega X\nu^{-1}p_\nu.$$

Using the spectral decomposition of $\omega$ and $\nu$, it now easy to compute the relative entropy

$$\mathrm{Ent}(\nu|\omega) = (\Omega_\nu, \log\Delta_{\omega,\nu}\Omega_\nu) = \mathrm{Tr}\,\left(\nu(\log\omega - \log\nu)\right).$$

This expression is the natural extension of the relative entropy of two probability measures

$$\mathrm{Ent}(\nu|\omega) = -\int \log\frac{\mathrm{d}\nu}{\mathrm{d}\omega}\,\mathrm{d}\nu.$$

## 3.2 Entropy balance equation

Let $\omega \in E(\mathcal{O})$ be a modular state, $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the assocaited cyclic representation and $\sigma^t_\omega$ the modular group of $\omega$. We denote by $\delta_\omega$ the generator of $\sigma^t_\omega$ and by $\mathcal{D}(\delta_\omega)$ its domain.

For unitary $U \in \mathcal{O}$ and $\eta \in E(\mathcal{O})$, we denote by $\eta_U$ the state $\eta_U(A) \equiv \eta(U^*AU)$.

**Theorem 3.1** *For any unitary* $U \in \mathcal{O} \cap \mathcal{D}(\delta_\omega)$ *and any* $\eta \in E(\mathcal{O})$,

$$\mathrm{Ent}(\eta_U|\omega) = \mathrm{Ent}(\eta|\omega) - \mathrm{i}\eta(U^*\delta_\omega(U)). \tag{27}$$

Let $\tau^t$ be a $C^*$-dynamics on $\mathcal{O}$ and assume that that $\omega$ is $\tau$-invariant. One easily checks that for any $s \in \mathbb{R}$ the state $\omega$ is KMS for $\hat{\sigma}_\omega^t \equiv \tau^{-s} \circ \sigma_\omega^t \circ \tau^s$. It follows from Theorem 2.1 that $\hat{\sigma}_\omega^t = \sigma_\omega^t$ *i.e.*, that the two groups $\tau$ and $\sigma_\omega$ commute.

Let $V$ be a local perturbation, that is a self-adjoint element of $\mathcal{O}$. The perturbed time evolution is the strongly continuous family of $*$-automorphisms of $\mathcal{O}$ given by the formula

$$\begin{aligned}\tau_V^t(A) &\equiv \tau^t(A) \\ &+ \sum_{n\geq 1} \mathrm{i}^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n\, [\tau^{t_n}(V), [\cdots, [\tau^{t_1}(V), \tau^t(A)]]].\end{aligned}$$

In the interaction representation, $\tau_V^t$ is given by

$$\tau_V^t(A) = \Gamma_V^t \tau^t(A) \Gamma_V^{t*},$$

where $\Gamma_V^t \in \mathcal{O}$ is a family of unitaries satisfying the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_V^t = \mathrm{i}\Gamma_V^t \tau^t(V), \qquad \Gamma_V^0 = \mathbf{1}.$$

If $V \in \mathcal{D}(\delta_\omega)$, then $\Gamma_V^t \in \mathcal{D}(\delta_\omega)$ and

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_V^t \delta_\omega(\Gamma_V^{t*}) = -\mathrm{i}\tau_V^t(\delta_\omega(V)). \tag{28}$$

Hence, Theorem 3.1 has the following immediate corollary

**Corollary 3.2** *Assume that $\omega$ is $\tau$-invariant and that $V \in \mathcal{D}(\delta_\omega)$. Then, for any $\eta \in E(\mathcal{O})$,*

$$\mathrm{Ent}(\eta \circ \tau_V^t | \omega) = \mathrm{Ent}(\eta | \omega) - \int_0^t \eta \circ \tau_V^s(\delta_\omega(V)) \tag{29}$$

Motivated by the entropy balance equation (29), we shall call the observable

$$\sigma_V \equiv \delta_\omega(V),$$

entropy production rate of the local perturbation $V$ w.r.t. the reference state $\omega$. Note that $\sigma_V$ not only depends on the perturbation $V$, but also on the reference state $\omega$. We will see in our applications that whenever $\omega$ has some internal structure (roughly speaking if $\omega$ is a product of KMS states), then $\sigma_V$ can be related to the fluxes of extensive quantities like energy or charges across the various components of the system.

Our definition of entropy production is motivated by classical dynamics where the rate of change of thermodynamic (Clausius) entropy can sometimes be related to the phase space contraction rate [Ga2, RC]. The latter is related to the Gibbs entropy (as shown for example in [Ru3]) which is nothing else but the relative entropy with respect to the *natural reference state* provided by Lebesgue measure; see [JPR1] for a detailed discussion in a more general context. Thus, it seems reasonable to define the entropy production as the rate of change of the relative entropy with respect to the reference state $\omega$. Within this analogy, the observable $\sigma_V$ plays the role of the phase space contraction rate.

**Proof of Theorem 3.1**. Let $\mathfrak{M}_\omega \equiv \pi_\omega(\mathcal{O})''$ be the enveloping von Neumann algebra. Since $\omega$ is a KMS state, the vector $\Omega_\omega$ is separating for $\mathfrak{M}_\omega$, and we denote by $\mathcal{P}$, $J$, $\Delta$ the corresponding natural cone, modular conjugation and modular operator. We further set

$$L \equiv \log \Delta,$$

and recall that

$$\pi_\omega(\sigma_\omega^t(A)) = \mathrm{e}^{\mathrm{i}tL}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL}, \qquad L\Omega_\omega = 0.$$

Any state $\eta \in \mathcal{N}_\omega$ has a unique normal extension to $\mathfrak{M}_\omega$ which we denote by the same letter. Obviously, $\eta$ is $\omega$-normal iff $\eta_U$ is $\omega$-normal for all unitaries $U \in \mathcal{O}$ and so, in the proof of Theorem 3.1, we may restrict ourselves to $\omega$-normal $\eta$'s.

We will use the fact that if $\gamma : \mathfrak{M}_\omega \mapsto \mathfrak{M}_\omega$ is a $*$-automorphism, then

$$\mathrm{Ent}(\eta \circ \gamma | \omega \circ \gamma) = \mathrm{Ent}(\eta|\omega).$$

In particular,

$$\mathrm{Ent}(\eta_U|\omega) = \mathrm{Ent}(\eta|\omega_{U^*}).$$

Let $\Psi_{U^*}$ be the unique vector representative of the state $\omega_{U^*}$ in the cone $\mathcal{P}$. A simple computation shows that

$$\Psi_{U^*} = \pi_\omega(U^*)J\pi_\omega(U^*)\Omega_\omega.$$

We will consider $P \equiv \pi_\omega(-\mathrm{i}U^*\delta_\omega(U))$ as a local perturbation of the modular group $\sigma_\omega^t$. Let $\alpha^t$ be the locally perturbed $W^*$-dynamics,

$$\alpha^t(A) \equiv \mathrm{e}^{\mathrm{i}t(L+P)}A\mathrm{e}^{-\mathrm{i}t(L+P)} = \Theta_P^t\sigma_\omega^t(A)\Theta_P^{t*},$$

where $\mathrm{e}^{\mathrm{i}t(L+P)}\mathrm{e}^{-\mathrm{i}tL} \equiv \Theta_P^t \in \mathfrak{M}_\omega$ is a family of unitaries satisfying

$$\frac{\mathrm{d}}{\mathrm{d}t}\Theta_P^t = \mathrm{i}\Theta_P^t\sigma_\omega^t(P), \qquad \Theta_P^0 = \mathbf{1}. \tag{30}$$

By the Araki perturbation theory, $\Omega_\omega \in \mathcal{D}(\mathrm{e}^{(L+P)/2})$ and the vector

$$\Psi = \frac{\mathrm{e}^{(L+P)/2}\Omega_\omega}{\|\mathrm{e}^{(L+P)/2}\Omega_\omega\|},$$

belongs to the natural cone $\mathcal{P}$ and defines a state $\psi$ which is KMS for $\alpha$.

Another fundamental result of Araki's theory is the relation

$$\mathrm{Ent}(\eta|\psi) = \mathrm{Ent}(\eta|\omega) + \eta(P) - \log\|\mathrm{e}^{(L+P)/2}\Omega_\omega\|^2, \tag{31}$$

which holds for all $\omega$-normal states $\eta$. (For $\eta$ faithful, this relation was proven in [Ar1, Ar2], see also [BR]. Its extension to general $\eta$ was obtained by Donald in [Don]. Hence, to finish the proof it suffices to show that $\mathrm{e}^{(L+P)/2}\Omega_\omega = \Psi_{U^*}$.

We set $T^t \equiv U^*\sigma_\omega^t(U)$ and observe that

$$\frac{\mathrm{d}}{\mathrm{d}t}T^t = \mathrm{i}T^t\sigma_\omega^t(-\mathrm{i}U^*\delta_\omega(U)), \qquad T^0 = \mathbf{1}.$$

Comparison with Equ. (30) immediately leads to $\pi_\omega(T^t) = \Theta_P^t$ and therefore

$$\begin{aligned} \mathrm{e}^{\mathrm{i}t(L+P)}\Omega_\omega &= \pi_\omega(T^t)\mathrm{e}^{\mathrm{i}tL}\Omega_\omega \\ &= \pi_\omega(U^*)\mathrm{e}^{\mathrm{i}tL}\pi_\omega(U)\Omega_\omega. \end{aligned} \tag{32}$$

Since the vector-valued function $z \mapsto \mathrm{e}^{\mathrm{i}z(L_\omega+P)}\Omega_\omega$ is analytic inside the strip $-1/2 < \mathrm{Im}\, z < 0$ and strongly continuous on its closure, analytic continuation of the identity (32) to $z = -\mathrm{i}/2$, yields

$$\begin{aligned} \mathrm{e}^{(L+P)/2}\Omega_\omega &= \pi_\omega(U^*)\Delta^{1/2}\pi_\omega(U)\Omega_\omega \\ &= \pi_\omega(U^*)J\pi_\omega(U^*)\Omega_\omega \\ &= \Psi_{U^*}, \end{aligned}$$

which is the desired relation.$\square$

# 4 Non-Equilibrium Steady States

## 4.1 Definition

Our definition of Non-Equilibrium Steady States (NESS) follows closely the idea of Ruelle that a “natural” steady state should provide the statistics, over large time intervals $[0, t]$, of initial configurations of the system which are typical with respect to the reference state [Ru3].

Let $(\mathcal{O}, \tau)$ be a $C^*$-dynamical system and $\rho$ a given initial state. The NESS associated to $\rho$ and $\tau$ are the weak-$*$ limit points of the time averages along the trajectory $\rho \circ \tau^t$. In other words, if

$$\langle \rho \rangle_t \equiv \frac{1}{t} \int_0^t \rho \circ \tau^s \, \mathrm{d}s, \tag{33}$$

then $\rho_+$ is a NESS associated to $\rho$ and $\tau$ if there exists a sequence $t_n \uparrow \infty$ such that $\langle \rho \rangle_{t_n}(A) \to \rho_+(A)$ for all $A \in \mathcal{O}$. We denote by $\Sigma_+(\rho, \tau)$ the set of such NESS. One easily sees that $\Sigma_+(\rho, \tau) \subset E(\mathcal{O}, \tau)$. Moreover, since $E(\mathcal{O})$ is weak-$\star$ compact, $\Sigma_+(\rho, \tau)$ is non-empty.

**Remark.** There is a fair amount of arbitrariness in the above definition. The ergodic mean in Equ. (33) can be replaced by another averaging procedure. Without further assumptions on the ergodic properties of the system, the resulting set of NESS will generally not coincide with $\Sigma_+(\rho, \tau)$. However, most results in this section are either independent of our specific choice of averaging, or can be easily adapted to other averagings.

In these notes, we will consider NESS of locally perturbed dynamical systems which occur naturaly in the study of open systems. Let $(\mathcal{O}, \tau)$ be a $C^*$-dynamical system and $\omega$ a modular $\tau$-invariant reference state. We denote by $\tau_V$ the dynamics induced by a local perturbation $V \in \mathcal{O}$. We shall always assume that our initial states are normal w.r.t. the reference state $\omega$. Thus, let $\rho \in \mathcal{N}_\omega$ and consider a NESS $\rho_+ \in \Sigma_+(\rho, \tau_V)$. We define the entropy production rate of $\rho_+$ by

$$\mathrm{Ep}(\rho_+) \equiv \rho_+(\sigma_V).$$

Let $t_n \to \infty$ be a sequence such that $\langle \rho \rangle_{t_n} \to \rho_+(A)$. According to the entropy balance equation (29)

$$\mathrm{Ep}(\rho_+) = - \lim_n \frac{1}{t_n} \left( \mathrm{Ent}(\rho \circ \tau_V^{t_n} | \omega) - \mathrm{Ent}(\rho | \omega) \right). \tag{34}$$

Since $\mathrm{Ent}(\rho \circ \tau_V^t|\omega) \leq 0$, an immediate consequence of this equation is that, for $\rho_+ \in \Sigma_+(\rho, \tau_V)$,

$$\mathrm{Ep}(\rho_+) \geq 0. \tag{35}$$

## 4.2 Structural properties

In this subsection we shall discuss structural properties of NESS and entropy production. Proofs can be found in [AJPP].

First, we will discuss the dependence of $\Sigma_+(\rho, \tau_V)$ on the initial state $\rho$. On physical grounds, one may expect that if the reference state $\omega$ is sufficiently regular, then $\Sigma_+(\rho, \tau_V) = \Sigma_+(\omega, \tau_V)$ for any initial state $\rho \in \mathcal{N}_\omega$.

**Theorem 4.1** *Assume that $\omega$ is a factor state on the $C^*$-algebra $\mathcal{O}$ and that, for all $\rho \in \mathcal{N}_\omega$ and $A, B \in \mathcal{O}$,*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \rho([\tau_V^t(A), B])\,\mathrm{d}t = 0,$$

*holds (weak asymptotic abelianness in mean). Then $\Sigma_+(\rho, \tau_V) = \Sigma_+(\omega, \tau_V)$ for all $\rho \in \mathcal{N}_\omega$.*

The second structural property we would like to mention is:

**Theorem 4.2** *Let*
*$rho$ be a $\omega$-normal $\tau_V$-invariant state. Then $\rho(\sigma_V) = 0$. In particular, the entropy production of the $\omega$-normal part of any NESS is equal to zero.*

If $\mathrm{Ent}(\rho|\omega) > -\infty$, then Theorem 4.2 is an immediate consequence of the entropy balance equation (34). The case $\mathrm{Ent}(\rho|\omega) = -\infty$ has been treated in [JP7] and the proof requires the full machinery of Araki's perturbation theory.

If $\omega_+$ is a factor state, then either $\omega_+ \ll \omega$ or $\omega_+ \perp \omega$. Hence, Theorem 4.2 yields:

**Corollary 4.3** *If $\omega_+$ is a factor state and $\mathrm{Ep}(\omega_+) > 0$, then $\omega_+ \perp \omega$. If $\omega$ is also a factor state, then $\omega_+$ and $\omega$ are disjoint.*

Certain structural properties can be characterized in terms of the standard Liouvillean. Let $L$ be the standard Liouvillean associated to $\tau$ and $L_V = L + \pi_\omega(V) - J\pi_\omega(V)J$ the standard Liouvillean associated to $\tau_V$.

**Theorem 4.4** *Assume that $\omega$ is modular.*
**1.** *Under the assumptions of Theorem 4.1, if $\mathrm{Ker}\, L_V \neq \{0\}$, then it is one-dimensional and there exists a unique normal, $\tau_V$-invariant state $\omega_V$ such that*

$$\Sigma_+(\omega, \tau_V) = \{\omega_V\}.$$

**2.** *If $\mathrm{Ker}\, L_V = \{0\}$, then any NESS in $\Sigma_+(\omega, \tau_V)$ is purely singular.*
**3.** *If $\mathrm{Ker}\, L_V$ contains a separating vector for $\mathfrak{M}_\omega$, then $\Sigma_+(\omega, \tau_V)$ contains a unique state $\omega_+$ and this state is $\omega$-normal.*

# 5 Open Systems

## 5.1 Setup

We consider an open system where a small system $\mathcal{S}$ interacts with $M$ reservoirs $\mathcal{R}_1, \ldots, \mathcal{R}_M$. The combined system $\mathcal{S} + \mathcal{R}_1 + \cdots + \mathcal{R}_M$ is described by a $C^*$-algebra $\mathcal{O}$. To each subsystem $\mathcal{S}, \mathcal{R}_1, \ldots, \mathcal{R}_M$ corresponds a subalgebra $\mathcal{O}_\mathcal{S}, \mathcal{O}_{\mathcal{R}_1}, \ldots, \mathcal{O}_{\mathcal{R}_M}$ of $\mathcal{O}$. Subalgebras corresponding to distinct subsystems may not commute. However, we will assume that $\mathcal{O}_a \cap \mathcal{O}_b = \mathbb{C}I$ for $a \neq b$. If $\mathcal{A}_k$, $1 \leq k \leq N$, are subsets of $\mathcal{O}$, we denote by $\langle \mathcal{A}_1, \cdots, \mathcal{A}_N \rangle$ the minimal $C^*$-subalgebra of $\mathcal{O}$ that contains all $\mathcal{A}_k$. Without loss of generality, we may assume that $\mathcal{O} = \langle \mathcal{O}_\mathcal{S}, \mathcal{O}_{\mathcal{R}_1}, \cdots, \mathcal{O}_{\mathcal{R}_M} \rangle$.

The dynamics of the joint but *decoupled* system is given by a group $\tau^t = \mathrm{e}^{t\delta}$ which preserves each subalgebras $\mathcal{O}_a$. We denote the restriction of $\tau$ to $\mathcal{O}_a$ by $\tau_a$ and its generator by $\delta_a$. The reference state $\omega$ is such that its restrictions $\omega_a \equiv \omega|\mathcal{O}_a$ are $\tau_a$-invariant.

The subsystem $\mathcal{S}$ is coupled to the reservoir $\mathcal{R}_j$ through a *junction* described by a self-adjoint perturbation $V_j \in \langle \mathcal{O}_\mathcal{S}, \mathcal{O}_{\mathcal{R}_j} \rangle$. The complete interaction, given by

$$V \equiv \sum_{j=1}^{M} V_j, \tag{36}$$

is a local perturbation and the $*$-derivation $\delta_V \equiv \delta + \mathrm{i}[V, \cdot\,]$ generates the coupled dynamics $\tau_V^t$ on $\mathcal{O}$. The *coupled* joint system is described by the $C^*$-dynamical system $(\mathcal{O}, \tau_V)$ and the reference state $\omega$.

The subsystem structure of $\mathcal{O}$ can be chosen in a number of different ways and the choice ultimately depends on the class of examples one wishes to describe. One obvious choice is the following: the small system is described by the

$C^*$-dynamical system $(\mathcal{O}_\mathcal{S}, \tau_\mathcal{S})$ with reference state $\omega_\mathcal{S}$ and the $j$-th reservoir by $(\mathcal{O}_{\mathcal{R}_j}, \tau_{\mathcal{R}_j})$ and $\omega_{\mathcal{R}_j}$. We then set

$$\begin{aligned}\mathcal{O} &\equiv \mathcal{O}_\mathcal{S} \otimes \mathcal{O}_{\mathcal{R}_1} \otimes \cdots \otimes \mathcal{O}_{\mathcal{R}_M},\\ \tau &= \tau_\mathcal{S} \otimes \tau_{\mathcal{R}_1} \otimes \cdots \otimes \tau_{\mathcal{R}_M},\\ \omega &= \omega_\mathcal{S} \otimes \omega_{\mathcal{R}_1} \otimes \cdots \otimes \omega_{\mathcal{R}_M}.\end{aligned}$$

In view of the examples we plan to cover, we are forced to allow the more general structure describd above.

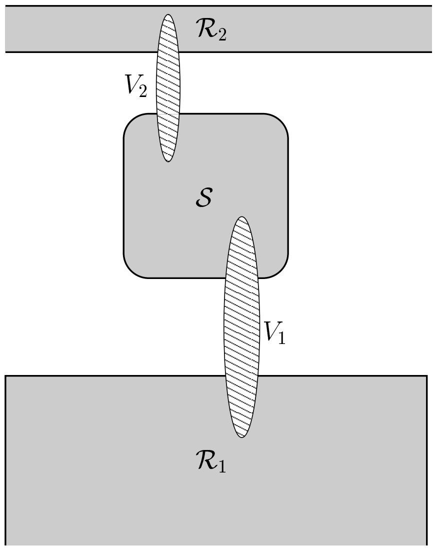


Figure 2: Junctions $V_1$, $V_2$ between the system $\mathcal{S}$ and two reservoirs.

An anti-linear, involutive, $*$-automorphism $\mathfrak{r}\colon \mathcal{O} \to \mathcal{O}$ is called a *time reversal* if it satisfies $\mathfrak{r} \circ \tau_\mathcal{S}^t = \tau_\mathcal{S}^{-t} \circ \mathfrak{r}$, $\mathfrak{r} \circ \tau_{\mathcal{R}_j}^t = \tau_{\mathcal{R}_j}^{-t} \circ \mathfrak{r}$ and $\mathfrak{r}(V_j) = V_j$. If $\mathfrak{r}$ is a time reversal, then

$$\mathfrak{r} \circ \tau^t = \tau^{-t} \circ \mathfrak{r}, \qquad \mathfrak{r} \circ \tau_V^t = \tau_V^{-t} \circ \mathfrak{r}.$$

An open quantum system described by $(\mathcal{O}, \tau_V)$ and the reference state $\omega$ is called time reversal invariant (TRI) if there exists a time reversal $\mathfrak{r}$ such that $\omega \circ \mathfrak{r} = \omega$.

## 5.2 The scattering approach

Let $(\mathcal{O}, \tau)$ be a $C^*$-dynamical system and $V$ a local perturbation. The abstract $C^*$-scattering approach to the study of NESS is based on the following assumption:

**Assumption (S)** The strong limit

$$\alpha_V^+ \equiv \mathrm{s} - \lim_{t\to\infty} \tau^{-t} \circ \tau_V^t,$$

exists.

The map $\alpha_V^+$ is an isometric $*$-endomorphism of $\mathcal{O}$, and is often called Møller morphism. $\alpha_V^+$ is one-to-one but it is generally not onto, namely

$$\mathcal{O}_+ \equiv \mathrm{Ran}\, \alpha_V^+ \neq \mathcal{O}.$$

Since $\alpha_V^+ \circ \tau_V^t = \tau^t \circ \alpha_V^+$, the pair $(\mathcal{O}_+, \tau)$ is a $C^*$-dynamical system and $\alpha_V^+$ is an isomorphism between the dynamical systems $(\mathcal{O}, \tau_V)$ and $(\mathcal{O}_+, \tau)$.

If the reference state $\omega$ is $\tau$-invariant, then $\omega_+ = \omega \circ \alpha_V^+$ is the unique NESS associated to $\omega$ and $\tau_V$ and

$$\lim_{t\to\infty} \omega \circ \tau_V^t(A) = \omega_+(A),$$

for any $A \in \mathcal{O}$. Note in particular that if $\omega$ is a $(\tau, \beta)$-KMS state, then $\omega_+$ is a $(\tau_V, \beta)$-KMS state.

The map $\alpha_V^+$ is the algebraic analog of the wave operator in Hilbert space scattering theory. A simple and useful result in Hilbert space scattering theory is the Cook criterion for the existence of the wave operator. Its algebraic analog is:

**Proposition 5.1** **1.** *Assume that there exists a dense subset $\mathcal{O}_0 \subset \mathcal{O}$ such that for all $A \in \mathcal{O}_0$,*

$$\int_0^\infty \|[V, \tau_V^t(A)]\| \,\mathrm{d}t < \infty. \tag{37}$$

*Then Assumption* (S) *holds.*

**Proof.** For all $A \in \mathcal{O}$ we have

$$\tau^{-t_2} \circ \tau_V^{t_2}(A) - \tau^{-t_1} \circ \tau_V^{t_1}(A) = \mathrm{i} \int_{t_1}^{t_2} \tau^{-t}([V, \tau_V^t(A)]) \,\mathrm{d}t, \tag{38}$$

and so

$$\|\tau^{-t_2} \circ \tau_V^{t_2}(A) - \tau^{-t_1} \circ \tau_V^{t_1}(A)\| \leq \int_{t_1}^{t_2} \|[V, \tau_V^t(A)]\| \,\mathrm{d}t, \tag{39}$$

Note that (37) and (39) imply that for $A \in \mathcal{O}_0$ the norm limit

$$\alpha_V^+(A) \equiv \lim_{t\to\infty} \tau^{-t} \circ \tau_V^t(A),$$

exists. Since $\mathcal{O}_0$ is dense and $\tau^{-t}\circ\tau_V^t$ is isometric, the limit exists for all $A\in\mathcal{O}$, and $\alpha_V^+$ is a $*$-morphism of $\mathcal{O}$. $\Box$

Until the end of this subsection we will assume that the Assumption (S) holds and that $\omega$ is $\tau$-invariant.

Let $\tilde\omega\equiv\omega|\mathcal{O}_+$ and let $(\mathcal{H}_{\tilde\omega},\pi_{\tilde\omega},\Omega_{\tilde\omega})$ be the GNS-representation of $\mathcal{O}_+$ associated to $\tilde\omega$. Obviously, if $\alpha_V^+$ is an automorphism, then $\tilde\omega=\omega$. We denote by $(\mathcal{H}_{\omega_+},\pi_{\omega_+},\Omega_{\omega_+})$ the GNS representation of $\mathcal{O}$ associated to $\omega_+$. Let $L_{\tilde\omega}$ and $L_{\omega_+}$ be the standard Liouvilleans associated, respectively, to $(\mathcal{O}_+,\tau,\tilde\omega)$ and $(\mathcal{O},\tau_V,\omega_+)$. Recall that $L_{\tilde\omega}$ is the unique self-adjoint operator on $\mathcal{H}_{\tilde\omega}$ such that for $A\in\mathcal{O}_+$,

$$L_{\tilde\omega}\Omega_{\tilde\omega}=0,\qquad \pi_{\tilde\omega}(\tau^t(A))=\mathrm{e}^{\mathrm{i}tL_{\tilde\omega}}\pi_{\tilde\omega}(A)\mathrm{e}^{-\mathrm{i}tL_{\tilde\omega}},$$

and similarly for $L_{\omega_+}$.

**Proposition 5.2** *The map*

$$U\pi_{\tilde\omega}(\alpha_V^+(A))\Omega_{\tilde\omega}=\pi_{\omega_+}(A)\Omega_{\omega_+},$$

*extends to a unitary $U:\mathcal{H}_{\tilde\omega}\to\mathcal{H}_{\omega_+}$ which intertwines $L_{\tilde\omega}$ and $L_{\omega_+}$, i.e.,*

$$UL_{\tilde\omega}=L_{\omega_+}U.$$

**Proof.** Set $\pi'_{\tilde\omega}(A)\equiv\pi_{\tilde\omega}(\alpha_V^+(A))$ and note that $\pi'_{\tilde\omega}(\mathcal{O})\Omega_{\tilde\omega}=\pi_{\tilde\omega}(\mathcal{O}_+)\Omega_{\tilde\omega}$, so that $\Omega_{\tilde\omega}$ is cyclic for $\pi'_{\tilde\omega}(\mathcal{O})$. Since

$$\omega_+(A)=\omega(\alpha_V^+(A))=\tilde\omega(\alpha_V^+(A))=(\Omega_{\tilde\omega},\pi_{\tilde\omega}(\alpha_V^+(A))\Omega_{\tilde\omega})=(\Omega_{\tilde\omega},\pi'_{\tilde\omega}(A)\Omega_{\tilde\omega}),$$

$(\mathcal{H}_{\tilde\omega},\pi'_{\tilde\omega},\Omega_{\tilde\omega})$ is also a GNS representation of $\mathcal{O}$ associated to $\omega_+$. Since GNS representations associated to the same state are unitarily equivalent, there is a unitary $U:\mathcal{H}_{\tilde\omega}\to\mathcal{H}_{\omega_+}$ such that $U\Omega_{\tilde\omega}=\Omega_{\omega_+}$ and

$$U\pi'_{\tilde\omega}(A)=\pi_{\omega_+}(A)U.$$

Finally, the identities

$$\begin{aligned}U\mathrm{e}^{\mathrm{i}tL_{\tilde\omega}}\pi'_{\tilde\omega}(A)\Omega_{\tilde\omega}&=U\pi_{\tilde\omega}(\tau^t(\alpha_V^+(A)))\Omega_{\tilde\omega}=U\pi_{\tilde\omega}(\alpha_V^+(\tau_V^t(A)))\Omega_{\tilde\omega}\\&=\pi_{\omega_+}(\tau_V^t(A))\Omega_{\omega_+}=\mathrm{e}^{\mathrm{i}tL_{\omega_+}}\pi_{\omega_+}(A)\Omega_{\omega_+}\\&=\mathrm{e}^{\mathrm{i}tL_{\omega_+}}U\pi'_{\tilde\omega}(A)\Omega_{\tilde\omega},\end{aligned}$$

yield that $U$ intertwines $L_{\tilde\omega}$ and $L_{\omega^+}$. $\Box$

**Proposition 5.3** **1.** *Assume that* $\tilde{\omega} \in E(\mathcal{O}_+, \tau)$ *is* $\tau$*-ergodic. Then* $\Sigma_+(\eta, \tau_V) = \{\omega_+\}$ *for all* $\eta \in \mathcal{N}_\omega$.
**2.** *If* $\tilde{\omega}$ *is* $\tau$*-mixing, then* $\lim_{t\to\infty} \eta \circ \tau_V^t = \omega_+$ *for all* $\eta \in \mathcal{N}_\omega$.

**Proof.** We will prove the Part 1; the proof of the Part 2 is similar. If $\eta \in \mathcal{N}_\omega$, then $\eta \upharpoonright \mathcal{O}_+ \in \mathcal{N}_{\tilde{\omega}}$, and the ergodicity of $\tilde{\omega}$ yields

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \eta(\tau^t(\alpha_V^+(A)))\, \mathrm{d}t = \tilde{\omega}(\alpha_V^+(A)) = \omega_+(A).$$

This fact, the estimate

$$\|\eta(\tau_V^t(A)) - \eta(\tau^t(\alpha_V^+(A)))\| \leq \|\tau^{-t} \circ \tau_V^t(A) - \alpha_V^+(A)\|,$$

and Assumption (S) yield the statement. □

As in the Hilbert-space scattering theory, the range of the Møller morphism $\alpha_V^+$ is related to the domain of the inverse morphism

$$\beta_V^+ \equiv \mathrm{s} - \lim_{t\to\infty} \tau_V^{-t} \circ \tau^t.$$

Since in the applications we have in mind the small system is either a finite or a confined quantum system its decoupled dynamics $\tau_\mathcal{S}$ will typically be quasiperiodic. Thus we can't expect the above limit to exists on $\mathcal{O}_\mathcal{S}$ and therefore the Møller morphism $\alpha_V^+$ will not be onto (except in trivial cases). The best one may hope for is that $\mathcal{O}_+ = \mathcal{O}_\mathcal{R} \equiv \langle \mathcal{O}_{\mathcal{R}_1}, \ldots, \mathcal{O}_{\mathcal{R}_M} \rangle$, namely that $\alpha_V^+$ is an isomorphism between the $C^*$-dynamical systems $(\mathcal{O}, \tau_V)$ and $(\mathcal{O}_\mathcal{R}, \tau_\mathcal{R})$ where $\tau_\mathcal{R} \equiv \tau | \mathcal{O}_\mathcal{R}$. The next theorem was proved in [Ru1].

**Theorem 5.4** *Suppose that Assumption (S) holds.*
**1.** *If there exists a dense set* $\mathcal{O}_{\mathcal{R}0} \subset \mathcal{O}_\mathcal{R}$ *such that for all* $A \in \mathcal{O}_{\mathcal{R}0}$,

$$\int_0^\infty \|[V, \tau^t(A)]\|\, \mathrm{d}t < \infty, \tag{40}$$

*then* $\mathcal{O}_\mathcal{R} \subset \mathcal{O}_+$.
**2.** *If there exists a dense set* $\mathcal{O}_0 \subset \mathcal{O}$ *such that for all* $X \in \mathcal{O}_\mathcal{S}$ *and* $A \in \mathcal{O}_0$,

$$\lim_{t\to+\infty} \|[X, \tau_V^t(A)]\| = 0, \tag{41}$$

*then* $\mathcal{O}_+ \subset \mathcal{O}_\mathcal{R}$.
**3.** *If both (40) and (41) hold then* $\alpha_V^+$ *is an isomorphism between the* $C^*$*-dynamical systems* $(\mathcal{O}, \tau_V)$ *and* $(\mathcal{O}_\mathcal{R}, \tau_\mathcal{R})$. *In particular, if* $\omega_\mathcal{R}$ *is a* $(\tau_\mathcal{R}, \beta)$*-KMS for some inverse temperature* $\beta$*, then* $\omega_+$ *is a* $(\tau_V, \beta)$*-KMS state.*

**Proof.** The proof of Part 1 is similar to the proof of Proposition 5.1. The assumption (40) ensures that the limits

$$\beta_V^+(A) = \lim_{t\to\infty} \tau_V^{-t} \circ \tau^t(A),$$

exist for all $A \in \mathcal{O}_{\mathcal{R}}$. Clearly, $\alpha_V^+ \circ \beta_V^+(A) = A$ for all $A \in \mathcal{O}_{\mathcal{R}}$ and so $\mathcal{O}_{\mathcal{R}} \subset \operatorname{Ran} \alpha_V^+$.

To prove Part 2 recall that $\mathcal{O}_{\mathcal{S}}$ is a $N^2$-dimensional matrix algebra. It has a basis $\{E_k \,|\, k = 1, \cdots, N^2\}$ such that $\tau^t(E_k) = \mathrm{e}^{\mathrm{i}t\theta_k} E_k$ for some $\theta_k \in \mathbb{R}$. From Assumption (S) and (41) we can conclude that

$$0 = \lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}t\theta_k} \tau^{-t}([E_k, \tau_V^t(A)]) = \lim_{t\to+\infty} [E_k, \tau^{-t} \circ \tau_V^t(A)] = [E_k, \alpha_V^+(A)],$$

for all $A \in \mathcal{O}_0$ and hence, by continuity, for all $A \in \mathcal{O}$. It follows that $\operatorname{Ran} \alpha_V^+$ belongs to the commutant of $\mathcal{O}_{\mathcal{S}}$ in $\mathcal{O}$. Since $\mathcal{O}$ can be seen as the algebra $M_N(\mathcal{O}_{\mathcal{R}})$ of $N \times N$-matrices with entries in $\mathcal{O}_{\mathcal{R}}$, one easily checks that this commutant is precisely $\mathcal{O}_{\mathcal{R}}$.

Part 3 is a direct consequence of the first two parts. □

# 6 The EBB model

We now introduce a fairly general model of mesoscopic device commonly used in quantum electronics. We will establish various well known formulas for the heat and electric currents, entropy production and transport coefficients. Even though the mathematical analysis of our model is rather straightforward and relies entirely on very well known material, rigorous proofs of these formulas can not, to the best of our knowledge, be found in the literature.

The system consists of $M$ *extended* electronic reservoirs $\mathcal{R}_1 \cdots \mathcal{R}_M$ connected to a *confined* device $\mathcal{S}$ through junctions $\mathcal{J}_1 \cdots \mathcal{J}_M$. Apart from Pauli's principle, electron-electron interactions are neglected, or more precisely treated in a mean field approximation.

Each reservoir $\mathcal{R}_k$ is described by the one-electron Hilbert space $\mathfrak{h}_k$ with one-electron Hamiltonian $h_k$. We denote by $\mathfrak{h}_{\mathcal{R}} \equiv \oplus_k \mathfrak{h}_k$ and $h_{\mathcal{R}} \equiv \oplus_k h_k$ the complete, one-electron, reservoir hilbert space and Hamiltonian. The device $\mathcal{S}$ is similarly described by $\mathfrak{h}_{\mathcal{S}}$ and $h_{\mathcal{S}}$. We set $\mathfrak{h} \equiv \mathfrak{h}_{\mathcal{R}} \oplus \mathfrak{h}_{\mathcal{S}}$ and $h_0 \equiv h_{\mathcal{R}} \oplus h_{\mathcal{S}}$. We further denote by $j_\alpha^*\colon \mathfrak{h}_\alpha \to \mathfrak{h}$, $\alpha = 1, \cdots, M, \mathcal{R}, \mathcal{S}$ the canonical imbeddings and by $1_\alpha \equiv j_\alpha^* j_\alpha$ the corresponding orthogonal projections.

> **Assumption (S1)** Each $h_k$ is bounded below and has purely absolutely continuous spectrum. $h_\mathcal{S}$ is bounded below and its resolvent belongs to the trace ideal $\mathcal{L}^p(\mathfrak{h}_\mathcal{S})$ for some $p \geq 1$.

We will denote by $a$ a positive constant such that $h_\mathcal{S} + a$ and each $h_k + a$ are strictly positive.

To each junction $\mathcal{J}_k$, we associate a hilbert space $\mathfrak{K}_k$ and two coupling operators $r_k \colon \mathfrak{h}_k \to \mathfrak{K}_k$ and $s_k \colon \mathfrak{h}_\mathcal{S} \to \mathfrak{K}_k$. The coupling of the system with the $k$-th reservoir is given by

$$v_k \equiv j_\mathcal{S}^* s_k^* r_k j_k + j_k^* r_k^* s_k j_\mathcal{S}, \tag{42}$$

and the coupled one-electron Hamiltonian is

$$h \equiv h_0 + v \equiv h_0 + \sum_k v_k.$$

> **Assumption (C)** The operators $r_k(h_k+a)$ and $s_k$ belong to the Hilbert-Schmidt class. Moreover, $r_k(h_k + a)^{(p-1)/2}$ and $s_k(h_\mathcal{S} + a)^{(p-1)/2}$ are bounded.

The corresponding many-electrons system is described by the Fermi algebra $\mathcal{O} \equiv \mathrm{CAR}(\mathfrak{h})$ and the two groups of Bogoliubov automorphisms $\tau_0^t$ and $\tau^t$ induced by the one-electron Hamiltonians $h_0$ and $h$. We shall denote by $\mathcal{O}_{\mathcal{R}_k}, \mathcal{O}_\mathcal{R}, \mathcal{O}_\mathcal{S}$ the $*$-subalgebras of $\mathcal{O}$ corresponding to subsystems, and by $\tau_k^t$, $\tau_\mathcal{R}^t$, $\tau_\mathcal{S}^t$ the restrictions of $\tau_0^t$ to these algebras.

Note that, under Assumption (C), each $v_k$ is trace class. Since $\mathrm{d}\Gamma$ is a bounded map from $\mathcal{L}^1(\mathfrak{h})$ into $\mathcal{O}$ (see [Araki-Wyss]), $V_k \equiv \mathrm{d}\Gamma(v_k)$ is a self-adjoint element of $\langle \mathcal{O}_\mathcal{S}, \mathcal{O}_{\mathcal{R}_k} \rangle$. Clearly, $\tau$ is the local perturbation of $\tau_0$ by $V = \sum_k V_k$ and its generator $\delta$ is related to the generator $\delta_0$ of $\tau_0$ by $\delta = \delta_0 + i[V, \cdot]$.

> **Assumption (R1)** The reference state is a $\tau_0$-invariant, gauge invariant quasi-free state $\omega$ generated by $T = T_\mathcal{R} \oplus T_\mathcal{S}$ where
>
> $$T_\mathcal{R} \equiv \bigoplus_k \rho_k(h_k),$$
>
> for some measurable functions $\rho_k \colon \mathrm{sp}(h_k) \to ]0, 1[$ satisfying
>
> $$\sup_{\lambda \in \mathrm{sp}(h_k)} \lambda \rho_k(\lambda) < \infty.$$

As we shall see below, the choice of $T_\mathcal{S}$ is irrelevant for the purpose of computing the NESS. It does however affect the entropy production observable $\sigma_V$. We will denote by $\omega_\mathcal{R}$ the restriction of $\omega$ to $\mathcal{O}_\mathcal{R}$.

## 6.1 Heat and Electric Currents. Conservation Laws

Strictly speaking, the total charge and the total energy of the device $\mathcal{S}$ are not observables if $\mathfrak{h}_\mathcal{S}$ is infinite dimensional. However, if we denote by by $\chi_n$ an eigenbasis of $h_\mathcal{S}$ and by $\varepsilon_n$ the corresponding eigenvalues, the (possibly infinite) quantities

$$\begin{aligned} Q_\mathcal{S}(\mu) &\equiv \sum_{j=0}^{\infty} \mu(a^*(\chi_j)a(\chi_j)), \\ E_\mathcal{S}(\mu) &\equiv \sum_{j=0}^{\infty} \varepsilon_j\, \mu(a^*(\chi_j)a(\chi_j)). \end{aligned}$$

are well defined for any $\mu \in E(\mathcal{O})$. Recall that, to such an $\mu$, one can associate a two-point operator $T_\mu$ by the formula $\mu(a^*(g)a(f)) = (f, T_\mu g)$. By linearity and continuity, this formula extends to $\mu(\mathrm{d}\Gamma(q)) = \mathrm{Tr}\,(T_\mu\, q)$ for any $q \in \mathcal{L}^1(\mathfrak{h})$. In terms of $T_\mu$, the above definitions can be rewritten as

$$\begin{aligned} Q_\mathcal{S}(\mu) &= \mathrm{Tr}_{\,\mathfrak{h}_\mathcal{S}}(1_\mathcal{S} T_\mu 1_\mathcal{S}), \\ E_\mathcal{S}(\mu) &= \mathrm{Tr}_{\,\mathfrak{h}_\mathcal{S}}(1_\mathcal{S}(h_\mathcal{S}+a)^{1/2} T_\mu (h_\mathcal{S}+a)^{1/2} 1_\mathcal{S}) - aQ_\mathcal{S}(\mu), \end{aligned}$$

from which the following Lemma follows easily.

**Lemma 6.1** *Let $\mu$ be a state and denote by $T_\mu$ its two-point operator. There exists a constant $C$, depending only on $h_0$ and $v$, such that*

$$\begin{aligned} Q_\mathcal{S}(\mu\circ\tau^t) &\le C\|(h_0+a)^{p/2} T_\mu^{1/2}\|^2, \\ E_\mathcal{S}(\mu\circ\tau^t) &\le C\|(h_0+a)^{(p+1)/2} T_\mu^{1/2}\|^2. \end{aligned}$$

*Moreover, for any $\mu_+ \in \Sigma_+(\mu,\tau)$ one has*

$$\begin{aligned} Q_\mathcal{S}(\mu_+) &\le \limsup_{t\to+\infty} Q_\mathcal{S}(\mu\circ\tau^t), \\ E_\mathcal{S}(\mu_+) &\le \limsup_{t\to+\infty} E_\mathcal{S}(\mu\circ\tau^t), \end{aligned}$$

Note in particular that if $\rho_k(\lambda) = (1+\mathrm{e}^{\beta_k(\lambda-\mu_k)})^{-1}$ with $\beta_k > 0$ and $h_\mathcal{S}^{p+1}T_\mathcal{S}$ is bounded, then $Q_\mathcal{S}(\omega\circ\tau^t)$ and $E_\mathcal{S}(\omega\circ\tau^t)$ are uniformly bounded in time. Consequently $Q_\mathcal{S}(\omega_+)$ and $E_\mathcal{S}(\omega_+)$ are finite for any $\omega_+ \in \Sigma_+(\omega,\tau)$.

In the one-electron picture, the energy of the reservoir $\mathcal{R}_k$ is given by

$$h_k(t) = \mathrm{e}^{ith} h_k \mathrm{e}^{-ith},$$

from which we conclude that the heat current flowing from this reservoir into the device $\mathcal{S}$ is

$$\varphi_k^{(1)}(t) \equiv -\partial_t h_k(t) = \mathrm{e}^{ith} \varphi_k^{(1)} \mathrm{e}^{-ith}$$

with the one-electron heat current

$$\varphi_k^{(1)} \equiv -i[h, h_k] = i[h_k, v] = i[h_k, v_k] = i[h_{\mathcal{R}}, v_k]. \tag{43}$$

The heat current in the many-electrons model is therefore given by

$$\Phi_k^{(1)} \equiv \mathrm{d}\Gamma(\varphi_k^{(1)}) = i[\mathrm{d}\Gamma(h_k), V] = \delta_k(V).$$

Electric currents are obtained in a similar way, substituting the energy $h_k$ with the orthogonal projection $1_k$. Thus the one-electron electric current is

$$\varphi_k^{(0)} \equiv -i[h, 1_k] = i[1_k, v] = i[1_k, v_k] = i[1_{\mathcal{R}}, v_k], \tag{44}$$

and its many-electron counterpart is

$$\Phi_k^{(0)} \equiv \mathrm{d}\Gamma(\varphi_k^{(0)}) = i[\mathrm{d}\Gamma(1_k), V] = \tilde{\delta}_k(V),$$

where $\tilde{\delta}_k$ is the generator of the gauge group of $\mathcal{R}_k$.

Energy and charge conservation holds in the following precise form.

**Lemma 6.2** *If $Q_{\mathcal{S}}(\mu \circ \tau^t) < \infty$ for $t$ in some open interval, it is differentiable there and its derivative is given by*

$$\partial_t Q_{\mathcal{S}}(\mu \circ \tau^t) = \sum_k \mu \circ \tau^t(\Phi_k^{(0)}).$$

*In particular, if $\mu$ is an invariant state such that $Q_{\mathcal{S}}(\mu) < \infty$, then*

$$\sum_k \mu(\Phi_k^{(0)}) = 0.$$

*A similar statement holds for the energy.*

**Proof.** One has an absolutely convergent series

$$Q_{\mathcal{S}}(\mu\circ\tau^t)=\sum_j q_j(t),$$

where each term $q_j(t)=(\mathrm{e}^{ith}\chi_j,T_\mu\mathrm{e}^{ith}\chi_j)$ is continuously differentiable since $\chi_j\in D(h)$. An explicit calculation shows that $\dot{q}_j(t)=2\,\mathrm{Im}\,(\chi_j,v\,T_{\mu\circ\tau^t}\chi_j)$ from which one easily obtains the estimate

$$\sum_j\sup_t|\dot{q}_j(t)|\le 2\sum_k\|r_k\|_2\,\|s_k\|_2.$$

This allows us to conclude that

$$\partial_t Q_{\mathcal{S}}(\mu\circ\tau^t)=\sum_j\dot{q}_j(t)=\mathrm{Tr}\,(T_{\mu\circ\tau^t}\,i[v,1_{\mathcal{S}}]).$$

Finaly, since $i[v,1_{\mathcal{S}}]=i[1_{\mathcal{R}},v]=\sum_k i[1_k,v]=\sum_k\varphi_k^{(0)}$, the result follows. □

## 6.2 Entropy Production

To compute the entropy production we need a modular reference state $\omega$. Thus, we strengthen Assumption (R1) by the following requirements

> **Assumption (R2)** $T_{\mathcal{S}}=(1+\mathrm{e}^{-\xi_{\mathcal{S}}})^{-1}$ where $\xi_{\mathcal{S}}$ is a self-adjoint operator commuting with $h_{\mathcal{S}}$, bounded above, with resolvent in a trace ideal $\mathcal{L}^q(\mathfrak{h}_{\mathcal{S}})$ for some $q\ge 1$. Moreover, there exists $\mu>1$ such that $\sum_k\|(a-\xi_{\mathcal{S}})^\mu s_k^*\|_2<\infty$.

We set $\xi_k(\lambda)=\log\rho_k(\lambda)-\log(1-\rho_k(\lambda))$. The reference state $\omega$ is $\tau_0$ invariant and modular. Its modular dynamics is the group of Bogoliubov automorphisms associated with the Hamiltonian

$$\xi\equiv\left(\bigoplus_k\xi_k(h_k)\right)\oplus\xi_{\mathcal{S}}.$$

Hence, the entropy production observable is

$$\sigma_V=\delta_\omega(V)=\mathrm{d}\Gamma(i[\xi,v])=\sum_k\mathrm{d}\Gamma(i[\xi_k(h_k),v_k])+\mathrm{d}\Gamma(i[\xi_{\mathcal{S}},v]).$$

The last expression clearly displays the dependence of entropy production on the choice of the reference state $\omega_{\mathcal{S}}$. However, one has

**Lemma 6.3** *Under Assumptions (R1), (R2),*

$$\eta(\sigma_V) = \sum_k \eta(\mathrm{d}\Gamma(i[\xi_k(h_k), v_k])),$$

*for any $\tau$-invariant state $\eta$. In particular, if $\rho_k(\lambda) = (1 + \mathrm{e}^{\beta_k(\lambda-\mu_k)})^{-1}$ then,*

$$\eta(\sigma_V) = -\sum_k \beta_k(\eta(\Phi_k^{(1)}) - \mu_k \eta(\Phi_k^{(0)})).$$

**Proof.** Without loss of generality, we may assume that $\xi_{\mathcal{S}} < 0$ and that $(-\xi_{\mathcal{S}})^{-q}$ is trace class. We first note that if $k$ is a trace class operator commuting with $h_0$ one has $i[\mathrm{d}\Gamma(k), V] = \mathrm{d}\Gamma(i[k, v]) = -\mathrm{d}\Gamma(i[h, k]) = -\delta(\mathrm{d}\Gamma(k))$ and hence

$$\eta(i[\mathrm{d}\Gamma(k), V]) = 0,$$

for all $\tau$-invariant states $\eta$. In particular, since

$$\xi_{\mathcal{S}}^{(\epsilon)} \equiv \frac{\xi_{\mathcal{S}}}{1 + \epsilon(-\xi_{\mathcal{S}})^{q+1}},$$

is trace class for $\epsilon > 0$, one has

$$|\eta(i[\mathrm{d}\Gamma(\xi_{\mathcal{S}}), V])| \leq \|[\xi_{\mathcal{S}} - \xi_{\mathcal{S}}^{(\epsilon)}, v]\|_1.$$

Writing

$$\xi_{\mathcal{S}} - \xi_{\mathcal{S}}^{(\epsilon)} = -\epsilon^\alpha \left(\frac{\epsilon(-\xi_{\mathcal{S}})^{q+1}}{1 + \epsilon(-\xi_{\mathcal{S}})^{q+1}}\right)^{1-\alpha} \frac{(-\xi_{\mathcal{S}})^{1+\alpha(q+1)}}{(1 + \epsilon(-\xi_{\mathcal{S}})^{q+1})^\alpha},$$

with $0 < \alpha < 1$ leads to the estimate

$$|[k_{\mathcal{S}} - k_{\mathcal{S}}^{(\epsilon)}, v]\|_1 \leq 2\epsilon^\alpha \sum_k \|r_k\|_2 \|(-\xi_{\mathcal{S}})^{1+\alpha(q+1)} s_k^*\|_2,$$

which, for sufficiently small $\alpha$, allows to conclude.□

## 6.3 NESS

Let us denote by $1_{ac}(h)$ the orthogonal projection on the subspace of $\mathfrak{h}$ corresponding to the absolutely continuous spectrum of $h$. Under Hypotheses (S1) and (C), it follows from the Kato-Rosenblum trace class scattering theory that the Møller operators

$$w_{\pm} = \mathrm{s}-\lim_{t\to\pm\infty} e^{ith}e^{-ith_0}1_{\mathcal{R}},$$

exist and are complete *i.e.*, $w_{\pm}$ are unitary operators from $\mathfrak{h}_{\mathcal{R}}$ onto $\mathrm{Ran}\ 1_{\mathrm{ac}}(h)$. In particular, the inverse Møller operators are given by

$$w_{\pm}^* = \mathrm{s}-\lim_{t\to\pm\infty} e^{ith_0}e^{-ith}1_{\mathrm{ac}}(h),$$

with $w_{\pm}^* w_{\pm} = 1_{\mathcal{R}}$ and $w_{\pm}w_{\pm}^* = 1_{\mathrm{ac}}(h)$. Let us make the following Hypothesis

**Assumption (S2)** $h$ has purely absolutely continuous spectrum.

Then, for elements of the form

$$A = a^{\#}(\psi_1)\cdots a^{\#}(\psi_n), \tag{45}$$

of $\mathcal{O}$ one has

$$\tau_0^{-t}\circ\tau^t(A) = a^{\#}(\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th}\psi_1)\cdots a^{\#}(\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th}\psi_n),$$

and therefore

$$\lim_{t\to\infty}\tau_0^{-t}\tau^t(A) = a^{\#}(w_-^*\psi_1)\cdots a^{\#}(w_-^*\psi_n).$$

Since the linear span of the set of elements of the form (45) is dense in $\mathcal{O}$, we derive that the limit

$$\alpha^+ = \lim_{t\to\infty}\tau_0^{-t}\circ\tau^t,$$

exists in the strong topology on $\mathcal{O}$. Hence,

$$\omega_+ = \omega\circ\alpha^+,$$

is the unique NESS associated to $\omega$ and $\tau$. From (19) it is clear that $\omega_+$ is the gauge-invariant quasi-free state generated by

$$T_+ = w_- T_{\mathcal{R}} w_-^*.$$

Since $\mathrm{Ran}\, w_-^* = \mathfrak{h}_{\mathcal{R}}$, one has $\mathrm{Ran}\,\alpha^+ = \mathcal{O}_{\mathcal{R}}$, and $\omega_+ = \omega_{\mathcal{R}}\circ\alpha^+$. The map $\alpha^+$ is an isomorphism of $C^*$-dynamical systems between $(\mathcal{O},\tau)$ and $(\mathcal{O}_{\mathcal{R}},\tau_{\mathcal{R}})$. Since it follows from Assumptions (S1) and (R1) that $\omega_{\mathcal{R}}$ is $\tau_{\mathcal{R}}$ mixing (see Subection 2.4), Proposition 5.3 allows to conclude that

$$\lim_{t\to\infty} \eta \circ \tau^t = \omega_+,$$

for any $\eta \in \mathcal{N}_\omega$. We thus have shown

**Theorem 6.4** *Under Assumptions (S1), (S2), (R1), and (C), $\Sigma_+(\eta, \tau)$ does not depend of the choice of the initial state $\eta \in \mathcal{N}_\omega$. It contains a unique NESS $\omega_+$ which is the gauge-invariant, quasi-free state on $\mathcal{O}$ generated by*

$$T_+ \equiv w_- \, T_{\mathcal{R}} \, w_-^*.$$

*Moreover, for any $\eta \in \mathcal{N}_\omega$ one has*

$$\lim_{t\to\infty} \eta \circ \tau^t = \omega_+.$$

*In particular, for any $q \in \mathcal{L}^1(\mathfrak{h})$,*

$$\omega_+(\mathrm{d}\Gamma(q)) = \mathrm{Tr}_{\,\mathfrak{h}_{\mathcal{R}}}(T_{\mathcal{R}} w_-^* \, q \, w_-).$$

*If $\omega$ is such that $h_0^{p+1} T$ is bounded, then*

$$\sum_k \omega_+(\Phi_k^{(l)}) = 0,$$

*for $l = 0, 1$.*

If all the energy densities $\rho_j(\varepsilon)$ are the same and equal to $\rho(\varepsilon)$, then one has

$$T_+ = \rho(h).$$

Since $h_\lambda - h_{\mathcal{R}}$ is a finite rank operator, one easily verifies that the operators

$$(T_+)^{1/2} - T^{1/2} \qquad \text{and} \qquad (1 - T_+)^{1/2} - (1 - T)^{1/2}$$

are Hilbert-Schmidt. The Powers-Stormer theorem yields that $\omega_{\lambda+} \ll \omega$ and the model has trivial thermodynamics in the sense that its entropy production is equal to zero.

These observations require a comment. By the general principles of statistical mechanics, one may expect that $\mathrm{Ep}(\omega_+) = 0$ iff all the resevoirs are in thermal equilibrium at the same inverse temperature $\beta$. This is not the case in EBB model since the perturbations $V_j$ are chosen in a very special way. One can show that the Planck law can be deduced from the stability requirement $\mathrm{Ep}(\omega_+) = 0$ for a slightly more general class of interactions $V_j$.

We remark that our last Assumption (S2) is quite strong. In particular, it will fail (even at small coupling) if spectral gap $\mathbb{C}\setminus\cup_k \mathrm{sp}(h_k)$ of the reservoirs contains some eigenvalues of $h_{\mathcal{S}}$. On the other hand, (S2) can not be avoided since the presence of point spectrum of $h$ generates a quasi-periodic component in the time evolution $\tau$ which prevents the convergence of $\eta \circ \tau^t$. In this case, one is forced to use time-averaging to reach a steady state. As the following result shows, point spectrum does not affect the steady currents.

**Theorem 6.5** *Assume besides (S1), (R1) and (C) that $h$ has empty singular continuous spectrum. Then there is a unique NESS $\omega_+$ in $\Sigma_+(\omega, \tau)$. Moreover,*

$$\omega_+(\Phi_k^{(l)}) = \mathrm{Tr}_{\,\mathfrak{h}_{\mathcal{R}}}(T_{\mathcal{R}}\, w_-^*\, \varphi_k^{(l)}\, w_-). \tag{46}$$

*The last statement of Theorem 6.4 remains valid.*

**Remark.** As we shall see in the next section, Equ. (46) is an abstract form of the Büttiker-Landauer formula.

**Proof.** Denote by $1_{\mathrm{ac}}$ and $1_{\mathrm{pp}}$ the spectral projections of $h$ on the absolutely continuous and pure point spectral subspaces. We start with the two-point functions. For $f, g \in \mathfrak{h}$ we have

$$\omega(\tau^t(a^*(g)a(f))) = (\mathrm{e}^{\mathrm{i}th}f, T\mathrm{e}^{\mathrm{i}th}g) = \sum_{j=1}^{3} N_j(\mathrm{e}^{\mathrm{i}th}f, \mathrm{e}^{\mathrm{i}th}g),$$

where

$$\begin{aligned} N_1(f,g) &\equiv (1_{\mathrm{ac}}f, T1_{\mathrm{ac}}g), \\ N_2(f,g) &\equiv 2\mathrm{Re}\,(1_{\mathrm{pp}}f, T1_{\mathrm{ac}}g), \\ N_3(f,g) &\equiv (1_{\mathrm{pp}}f, T1_{\mathrm{pp}}g). \end{aligned}$$

Since $\mathrm{e}^{-\mathrm{i}th_0}T = T\mathrm{e}^{-\mathrm{i}th_0}$, we have

$$N_1(\mathrm{e}^{\mathrm{i}th}f, e^{\mathrm{i}th}g) = (\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th}1_{\mathrm{ac}}f, T\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th}1_{\mathrm{ac}}g),$$

and so

$$\lim_{t\to\infty} N_1(\mathrm{e}^{\mathrm{i}th}f, e^{\mathrm{i}th}g) = (w_-^* f, T w_-^* g).$$

Since $\mathfrak{h}$ is separable, there exists a sequence $P_n$ of finite rank projections commuting with $h$ such that $\mathrm{s} - \lim P_n = 1_{\mathrm{pp}}$. The Riemann-Lebesgue lemma yields that for all $n$

$$\lim_{t\to\infty} \|P_n T \mathrm{e}^{\mathrm{i}th} 1_{\mathrm{ac}} g\| = 0.$$

The relation

$$N_2(\mathrm{e}^{\mathrm{i}th}f, \mathrm{e}^{\mathrm{i}th}g) = (\mathrm{e}^{\mathrm{i}th}1_{\mathrm{pp}}f, P_n T \mathrm{e}^{\mathrm{i}th}1_{\mathrm{ac}}g) + (\mathrm{e}^{\mathrm{i}th}(I - P_n)1_{\mathrm{pp}}f, T\mathrm{e}^{\mathrm{i}th}1_{\mathrm{ac}}g),$$

yields that

$$\lim_{t\to\infty} N_2(\mathrm{e}^{\mathrm{i}th}f, \mathrm{e}^{\mathrm{i}th}g) = 0.$$

Since $N_3(\mathrm{e}^{\mathrm{i}th}f, \mathrm{e}^{\mathrm{i}th}g)$ is either a periodic or a quasi-periodic function of $t$ it does not have a limit as $t \to \infty$. However, one easily shows that

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t N_3(\mathrm{e}^{\mathrm{i}sh}f, \mathrm{e}^{\mathrm{i}sh}g)\,\mathrm{d}s = \sum_{e\in \mathrm{sp}_{\mathrm{pp}}(h)} (P_e f, T P_e g),$$

where $P_e$ denotes the spectral projection of $h$ associated with the eigenvalue $e$. Hence,

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \omega(\tau^s(a^*(g)a(f)))\,\mathrm{d}s = \sum_{e\in \mathrm{sp}_{\mathrm{pp}}(h)} (P_e f, T P_e g) + (w_-^* f, T w_-^* g). \tag{47}$$

In a similar way one concludes that for any observable of the form

$$A = a^*(g_n)\cdots a^*(g_1)a(f_1)\cdots a(f_m), \tag{48}$$

the limit

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \omega(\tau^s(A))\mathrm{d}s = \delta_{n,m} \lim_{t\to\infty} \frac{1}{t}\int_0^t \det\{(\mathrm{e}^{\mathrm{i}sh}f_i, T\mathrm{e}^{\mathrm{i}sh}g_j)\}\,\mathrm{d}s$$

exists and is equal to the limit

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \det\left\{(\mathrm{e}^{\mathrm{i}sh}1_{\mathrm{pp}}f_i, T\mathrm{e}^{\mathrm{i}sh}1_{\mathrm{pp}}g_j) + (w_-^* 1_{\mathrm{ac}}f_i, T w_-^* 1_{\mathrm{ac}}g_j)\right\}\,\mathrm{d}s. \tag{49}$$

Since the linear span of the set of observables of the form (48) is dense in $\mathfrak{h}$, we conclude that for all $A \in \mathrm{CAR}(\mathfrak{h})$ the limit

$$\omega_+(A) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \omega(\tau^s(A))\,\mathrm{d}s$$

exists. This shows that $\Sigma_+(\omega,\tau) = \{\omega_+\}$.

For a trace class operator $A$ on $\mathfrak{h}$, Equ. (47) yields

$$\omega_+(\mathrm{d}\Gamma(A)) = \mathrm{Tr}\left\{T\left(\sum_{e\in\mathrm{sp}_{\mathrm{pp}}(h_\lambda)} P_e A P_e + w_-^* A w_-\right)\right\}. \tag{50}$$

Note that if for some operator $q$, $A = \mathrm{i}[h_\lambda, q]$ in the sense of quadratic forms on $D(h)$, then $P_e A P_e = 0$ and eigenvalues do not contribute to $\omega_+(\mathrm{d}\Gamma(A))$. This is the case of the current observables $\mathrm{d}\Gamma(\varphi_k^{(l)})$. $\Box$

# 7 Scattering with a trace condition

In this Section, we further investigate Equ. (46) and show that it is equivalent to a generalization of the well-known Büttiker-Landauer formula which expresses the currents in terms of the scattering data (reflection and transmission coefficients). To proceed, we need some further notation. We denote by $r_0(z) \equiv (z - h_0)^{-1}$ and $r(z) \equiv (z-h)^{-1}$ the resolvent of the decoupled and coupled Hamiltonians. We define the full junction space as $\mathfrak{K} \equiv \mathfrak{K}_{\mathcal{R}} \oplus \mathfrak{K}_{\mathcal{S}}$, where $\mathfrak{K}_{\mathcal{R}} = \mathfrak{K}_{\mathcal{S}} \equiv \oplus_k \mathfrak{K}_k$. We also introduce the canonical projections $j_k\colon \mathfrak{h} \to \mathfrak{h}_k$ as well as $j_k^{\mathcal{R}}\colon \mathfrak{K} \to \mathfrak{K}_k$ and $j_k^{\mathcal{S}}\colon \mathfrak{K} \to \mathfrak{K}_k$.

The formula

$$(f_1, \cdots, f_M, f_{\mathcal{S}}) \mapsto (r_1 f_1, \cdots, r_M f_M, s_1 f_{\mathcal{S}}, \cdots, s_M f_{\mathcal{S}}),$$

defines a Hilbert-Schmidt map $G$ from $\mathfrak{h}$ to the full junction space $\mathfrak{K}$. Denoting by $M$ the involution of $\mathfrak{K}$ defined by

$$M\colon (u_1, \cdots, u_M, v_1, \cdots, v_M) \mapsto (v_1, \cdots, v_M, u_1, \cdots, u_M),$$

we can factorize the coupling as

$$v = G^* M G. \tag{51}$$

By the spectral theorem, each reservoir space $\mathfrak{h}_k$ can be written as a direct integral

$$\mathfrak{h}_k = \int_{\mathrm{sp}(h_k)}^{\oplus} \mathfrak{h}_k(\lambda)\, d\lambda. \tag{52}$$

For a bounded measurable function $F$ on $\mathrm{sp}(h_k)$ one has

$$F(h_k)\colon \int_{\mathrm{sp}(h_k)}^{\oplus} f(\lambda)\, d\lambda \mapsto \int_{\mathrm{sp}(h_k)}^{\oplus} F(\lambda) f(\lambda)\, d\lambda \tag{53}$$

If $\mathcal{K}$ is a separable Hilbert space and $A : \mathcal{K} \to \mathfrak{h}$ a Hilbert-Schmidt oparator, then for almost all $\lambda \in \mathrm{sp}(h_k)$ there exists a Hilbert-Schmidt operator $A(\lambda) : \mathcal{K} \to \mathfrak{h}(\lambda)$ such that

$$Au = \int_{\mathrm{sp}(h_k)}^{\oplus} A(\lambda) u\, d\lambda,$$

for all $u \in \mathcal{K}$. Moreover, if $A, B$ are two such operators one has

$$\mathrm{Tr}_{\,\mathfrak{h}}(A^* B) = \int_{\mathrm{sp}(h_k)} \mathrm{Tr}_{\,\mathfrak{h}(\lambda)}(B(\lambda) A(\lambda)^*)\, \mathrm{d}\lambda. \tag{54}$$

The following Theorem summarizes the results of stationary trace class scattering theory that we shall need to derive the ususal Büttiker-Landauer Formula from its abstract version (46) (see [Yaffaev]).

**Theorem 7.1** *Under Assumptions (S1) and (C), the following hold:*

1. *The non-tangential limits*

$$B^0_{\pm}(\lambda) \equiv G r_0(\lambda \pm \mathrm{i}0) G^*,$$

*exist in $\mathcal{L}^2(\mathfrak{K})$ for almost all $\lambda \in \mathbb{R}$.*

2. $(1 - M B^0_{\pm}(\lambda))^{-1}$ *exists for almost all $\lambda \in \mathbb{R}$.*

3. *For almost all $\lambda \in \mathbb{R}$, there exists a bounded linear map $z_k(\lambda)\colon \mathfrak{K} \to \mathfrak{h}_k(\lambda)$ such that, for any $u \in \mathfrak{K}$ one has*

$$j_k G^* u = \int_{\mathrm{sp}(h_k)}^{\oplus} z_k(\lambda) u\, d\lambda.$$

*Moreover, one has*

$$z_k(\lambda)^* z_k(\lambda) = \frac{1}{2\pi\mathrm{i}} j_k^{\mathcal{R}*} j_k^{\mathcal{R}} (B^0_{-}(\lambda) - B^0_{+}(\lambda)) j_k^{\mathcal{R}*} j_k^{\mathcal{R}} = j_k^{\mathcal{R}*} r_k^* \delta(\lambda - h_k) r_k j_k^{\mathcal{R}}. \tag{55}$$

4. *The scattering matrix* $s \equiv w_+^* w_-|_{\mathfrak{h}_\mathcal{R}}$ *is unitary on* $\mathfrak{h}_\mathcal{R}$*. For almost all* $\lambda \in \mathrm{sp}(h_k) \cap \mathrm{sp}(h_l)$*, there exists a map* $s_{kl}(\lambda)\colon \mathfrak{h}_l(\lambda) \to \mathfrak{h}_k(\lambda)$ *such that*

$$s\colon\ \oplus_k \int_{\mathrm{sp}(h_k)}^{\oplus} f_k(\lambda)\, d\lambda \mapsto \oplus_k \sum_l \int_{\mathrm{sp}(h_k)\cap\mathrm{sp}(h_l)}^{\oplus} s_{kl}(\lambda) f_l(\lambda)\, d\lambda.$$

5. *One has* $s_{kl}(\lambda) = \delta_{kl} + t_{kl}(\lambda)$*, where*

$$t_{kl}(\lambda) = -2\pi\mathrm{i} z_k(\lambda) M (1 - B_+^0(\lambda) M)^{-1} z_l(\lambda)^*, \tag{56}$$

*for almost all* $\lambda \in \mathrm{sp}(h_k) \cap \mathrm{sp}(h_l)$*.*

6. *For almost all* $\lambda \in \cup_k \mathrm{sp}(h_k)$*, one has*

$$\sum_j t_{ij}(\lambda) t_{kj}(\lambda)^* = \sum_j t_{ji}(\lambda)^* t_{jk}(\lambda) = -(t_{ik}(\lambda) + t_{ki}(\lambda)^*). \tag{57}$$

7. *Let* $\|v\|_1$ *denote the trace norm of* $v$*. Then, the following estimate holds*

$$\sum_{ij} \int \mathrm{Tr}\,(t_{ij}(\lambda)^* t_{ij}(\lambda))\, \frac{d\lambda}{2\pi} \le \|v\|_1. \tag{58}$$

8. *For all* $u \in \mathfrak{K}$ *one has*

$$j_l w_\pm^* G^* u = \int_{\mathrm{sp}(h_l)}^{\oplus} z_l(\lambda)(1 - M B_\pm^0(\lambda))^{-1} u\, d\lambda. \tag{59}$$

# 8 The Büttiker-Landauer formula

**Proposition 8.1** *Under the assumptions of Theorem 6.5, the steady currents are given by*

$$\omega_+(\Phi_k^{(n)}) = -\sum_l \int_{\mathrm{sp}(h_k)\cap\mathrm{sp}(h_l)} \rho_l(\lambda) \lambda^n\, D_{l,k}(\lambda) \frac{d\lambda}{2\pi}, \tag{60}$$

*where*

$$D_{lk}(\lambda) \equiv \mathrm{Tr}\,(t_{kl}(\lambda)^* t_{kl}(\lambda)) - \delta_{kl} \sum_j \mathrm{Tr}\,(t_{kj}(\lambda)^* t_{kj}(\lambda)). \tag{61}$$

**Proof.** For the electric current, from Equ. (44), using the factorization (51), one easily obtain the formula

$$\varphi_k^{(0)} = G^* \left\{ \mathrm{i}(j_k^{\mathcal{R}*} j_k^{\mathcal{S}} - j_k^{\mathcal{S}*} j_k^{\mathcal{R}}) \right\} G,$$

from which it follows that

$$j_l \, w_-^* \, \varphi_k^{(0)} w_- \, j_l^* = 2 \,\mathrm{Im}\, (q_{lk}^{\mathcal{S}} q_{lk}^{\mathcal{R}*}),$$

where the $q_{lk}^\alpha \equiv j_l w_-^* G^* j_k^{\alpha *}$ are Hilbert-Schmidt operators from $\mathfrak{K}_k$ to $\mathfrak{h}_l$. Thus, we can rewrite (46) as

$$\omega_+(\Phi_k^{(0)}) = 2 \,\mathrm{Im} \sum_l \mathrm{Tr}\, (q_{lk}^{\mathcal{R}*} \rho_l(h_l) q_{lk}^{\mathcal{S}}).$$

Using the fact that $\varphi_k^{(1)} = \mathrm{i}[h_k, v] = \mathrm{i}(h 1_k v - v 1_k h)$ and the intertwinning property of the Møller operators, $h w_- = w_- h_0$, we derive a similar formula for the energy currents. Both formulas are summarized in

$$\omega_+(\Phi_k^{(n)}) = 2 \,\mathrm{Im} \sum_l \mathrm{Tr}\, (q_{lk}^{\mathcal{R}*} h_l^n \rho_l(h_l) q_{lk}^{\mathcal{S}}), \tag{62}$$

for $n = 0, 1$. Using the represention (59), Equ. (53) and the identity $j_k^{\mathcal{S}*} = M j_k^{\mathcal{R}*}$ we obtain the representations

$$\begin{aligned} h_l^n \rho_l(h_l) q_{lk}^{\mathcal{S}} &= \int_{\mathrm{sp}(h_l)} \lambda \rho_l(\lambda) z_l(\lambda) (1 - M B_-^0(\lambda))^{-1} M j_k^{\mathcal{R}*} \, \mathrm{d}\lambda, \\ q_{lk}^{\mathcal{R}} &= \int_{\mathrm{sp}(h_l)} z_l(\lambda) (1 - M B_-^0(\lambda))^{-1} j_k^{\mathcal{R}*} \, \mathrm{d}\lambda. \end{aligned}$$

From Equ. (54) we conclude that

$$\omega_+(\Phi_k^{(n)}) = \sum_l \int_{\mathrm{sp}(h_l)} \lambda^n \rho_l(\lambda) D_{lk}(\lambda) \frac{d\lambda}{2\pi},$$

where, using the fact that $B_-^0(\lambda)^* = B_+^0(\lambda)$,

$$D_{lk}(\lambda) \equiv 4\pi \,\mathrm{Im}\, \mathrm{Tr}\, (z_l(\lambda)(1 - M B_-^0(\lambda))^{-1} M j_k^{\mathcal{R}*} j_k^{\mathcal{R}} (1 - B_+^0(\lambda) M)^{-1} z_l(\lambda)^*).$$

Expanding $(1 - B_+^0(\lambda) M)^{-1} = 1 + B_+^0(\lambda) M (1 - B_+^0(\lambda) M)^{-1}$ we can rewrite $D_{lk}$ as a sum of two terms. Using the identity $j_k^{\mathcal{R}*} j_k^{\mathcal{R}} z_l(\lambda)^* = \delta_{kl} z_k(\lambda)^*$, the first term becomes

$$D_{lk}^{(1)}(\lambda) = 4\pi \delta_{kl} \,\mathrm{Im}\, \mathrm{Tr}\, (z_l(\lambda)(1 - M B_-^0(\lambda))^{-1} M z_k(\lambda)^*),$$

which, due to Equ. (56), can also be written as

$$D_{lk}^{(1)}(\lambda) = -2\delta_{kl}\,\mathrm{Re}\ \mathrm{Tr}\,(t_{kl}(\lambda)) = -\delta_{kl}\mathrm{Tr}\,(t_{kl}(\lambda) + t_{lk}(\lambda)^*).$$

Finaly, the unitarity relation (57) yields

$$D_{lk}^{(1)}(\lambda) = \delta_{kl}\sum_j \mathrm{Tr}\,(t_{kj}(\lambda)^* t_{kj}(\lambda)).$$

To deal with the second term

$$D_{kl}^{(2)}(\lambda) =$$
$$4\pi\,\mathrm{Im}\,\mathrm{Tr}\,(z_l(\lambda)(1 - MB_-^0(\lambda))^{-1}M\{j_k^{\mathcal{R}*}j_k^{\mathcal{R}}B_+^0(\lambda)\}M(1 - B_+^0(\lambda)M)^{-1}z_l(\lambda)^*),$$

we note that $j_k^{\mathcal{R}*}j_k^{\mathcal{R}}$ is an orthogonal projection which commutes with $B_\pm^0(\lambda)$. Hence, Equ. (55) can be written as

$$\mathrm{Im}\,\{j_k^{\mathcal{R}*}j_k^{\mathcal{R}}B_+^0(\lambda)\} = -\pi z_k(\lambda)^* z_k(\lambda),$$

from which it follows that

$$D_{kl}^{(2)}(\lambda) =$$
$$-4\pi^2\,\mathrm{Im}\,\mathrm{Tr}\,(z_l(\lambda)(1 - MB_-^0(\lambda))^{-1}Mz_k(\lambda)^* z_k(\lambda)M(1 - B_+^0(\lambda)M)^{-1}z_l(\lambda)^*).$$

Using again Equ. (56) we finaly obtain

$$D_{lk}^{(1)}(\lambda) = -\mathrm{Tr}\,(t_{kl}(\lambda)^* t_{kl}(\lambda)).$$

□

**Remark.** Writing Equs. (60), (61) as

$$\omega_+(\Phi_k^{(n)}) = \int \lambda^n \sum_l (\rho_k(\lambda) - \rho_l(\lambda))\mathrm{Tr}\,(t_{kl}(\lambda)^* t_{kl}(\lambda))\frac{d\lambda}{2\pi},$$

it immediately follows that there are no currents if all reservoirs are in the same state, *i.e.*, if $\rho_k(\lambda) = \rho_l(\lambda)$ for almost all $\lambda \in \mathrm{sp}(h_k) \cap \mathrm{sp}(h_l)$. From the unitarity relation (57) and the cyclicity of the trace, it also follows that

$$\begin{aligned}
\sum_k \omega_+(\Phi_k^{(n)}) &= \sum_{lk}\int \rho_l(\lambda)\lambda^n \mathrm{Tr}\ (t_{lk}(\lambda)^* t_{lk}(\lambda) - t_{kl}(\lambda)^* t_{kl}(\lambda))\,\frac{d\lambda}{2\pi} \\
&= \sum_{lk}\int \rho_l(\lambda)\lambda^n \mathrm{Tr}\ (t_{kl}(\lambda)^* t_{kl}(\lambda) - t_{kl}(\lambda) t_{kl}(\lambda)^*)\,\frac{d\lambda}{2\pi} \\
&= 0.
\end{aligned}$$

## 8.1 Strict positivity on entropy production

To compute the entropy production in the steady state for non-equilibrium reservoir densities $\rho_l$, we shall need the following generalization of the Büttiker-Landauer formula.

**Lemma 8.2** *Let $f \in C^{2+\delta}(\mathbb{R})$ for some $\delta > 0$ be such that $f(h_k)r_k^*$ and $f(h_{\mathcal{S}})s_k^*$ are Hilbert-Schmidt. Under the assumptions of Theorem 6.5 one has*

$$\mathrm{d}\Gamma(\mathrm{i}[h, j_k^* f(h_k) j_k]) \in \mathcal{O},$$

*and if*

$$f \rho_l \in L^\infty(\mathrm{sp}(h_k) \cap \mathrm{sp}(h_l)),$$

*for $l = 1, \cdots, M$, the following formula holds*

$$\omega_+(\mathrm{d}\Gamma(\mathrm{i}[h, j_k^* f(h_k) j_k])) = -\sum_l \int_{\mathrm{sp}(h_k)\cap\mathrm{sp}(h_l)} \rho_l(\lambda) f(\lambda) D_{lk}(\lambda) \frac{d\lambda}{2\pi},$$

*for all $\omega_+ \in \Sigma_+(\omega, \tau)$.*

Recall that we have defined

$$\xi_k(\lambda) = \log \rho_k(\lambda) - \log(1 - \rho_k(\lambda)).$$

We shall now assume that these functions, defined on $\mathrm{sp}(h_k)$, can be extended to $\mathbb{R}$. Applying Lemmas 6.3 and 8.2, we obtain

**Corollary 8.3** *Let $\xi_k \in C^{2+\delta}(\mathbb{R})$ for some $\delta > 0$ and $k = 1, \cdots, M$ be such that $\xi_k(h_k)r_k^*$ and $\xi_k(h_{\mathcal{S}})s_k^*$ are Hilbert-Schmidt. Assume also that*

$$\sup_{\lambda\in\mathbb{R}} |\xi_k(\lambda)|\rho_l(\lambda) < \infty.$$

*Then, under the assumptions of Theorem 6.5, one has*

$$\mathrm{E}p(\omega_+) = \sum_{kl} \int_{\mathrm{sp}(h_k)\cap\mathrm{sp}(h_l)} \xi_k(\lambda) F(\xi_l(\lambda)) D_{lk}(\lambda) \frac{d\lambda}{2\pi}, \tag{63}$$

*where $F(x) \equiv (1 + \mathrm{e}^x)^{-1}$.*

Assume that all components of the system are TRI *i.e.,* that there are anti-unitary involutions $\mathfrak{r}_1, \cdots, \mathfrak{r}_M$, $\mathfrak{r}_\mathcal{S}$ of $\mathfrak{h}_1, \cdots, \mathfrak{h}_M$, $\mathfrak{h}_\mathcal{S}$, commuting with $h_1, \cdots, h_M$, $h_\mathcal{S}$ and such that $\mathfrak{r} \equiv \mathfrak{r}_\mathcal{R} \oplus \mathfrak{r}_\mathcal{S} \equiv (\oplus_k \mathfrak{r}_k) \oplus \mathfrak{r}_\mathcal{S}$ commutes with $v$. One has

$$\mathfrak{r}\, w_\pm \mathfrak{r} = w_\mp,$$

and hence

$$\mathfrak{r}_\mathcal{R} s\, \mathfrak{r}_\mathcal{R} = s^*.$$

$\mathfrak{r}_\mathcal{R}$ has a direct integral decomposition with fibers $\mathfrak{r}_k(\lambda)$ corresponding to Equ. (52) and one has

$$\mathfrak{r}_l(\lambda) t_{lk}(\lambda) \mathfrak{r}_k(\lambda) = t_{kl}(\lambda)^*.$$

Hence, the trace

$$\mathrm{Tr}\,(t_{kl}(\lambda)^* t_{kl}(\lambda)),$$

is a symmetric expression in $l, k$. Formula (63) thus takes the symmetrized form

$$\mathrm{E}p(\omega_+) = \sum_{k\neq l} \int_{\mathrm{sp}(h_k)\cap\mathrm{sp}(h_l)} (\xi_k - \xi_l)(F(\xi_l) - F(\xi_k))\mathrm{Tr}\,(t_{kl}^* t_{kl}) \frac{d\lambda}{4\pi},$$

which is obviously non-negative since $F$ is decreasing.

For each pair $(l, k)$ of reservoirs, let us define the *transmission spectrum* as

$$\tau(l, k) = \overline{\{\lambda \in \mathrm{sp}(h_l) \cap \mathrm{sp}(h_k) | t_{kl}(\lambda) \neq 0\}}.$$

Then one has $\mathrm{E}p(\omega_+) = 0$ if and only if, for each pair $(k, l)$,

$$\xi_k(\lambda) = \xi_l(\lambda),$$

for almost all $\lambda \in \tau(k, l)$. In particular, in the case $\xi_k(\lambda) = \beta_k(\lambda - \mu_k)$, the entropy production is strictly positive as soon as there exists a pair $(k, l)$ such that $\tau(k, l)$ has positive measure and either $\beta_k \neq \beta_l$ or $\mu_k \neq \mu_l$.

The conclusions of the previous paragraph still hold without the TRI assumption. They follow from the following Proposition.

**Proposition 8.4** *Under the assumptions of Corollary 8.3, one has*

$$\mathrm{E}p(\omega_+) \geq \frac{1}{M} \int_{\mathrm{sp}(h_k)\cap\mathrm{sp}(h_l)} F(|\xi_l|)F(|\xi_k|)(\xi_k - \xi_l)^2 \mathrm{Tr}\,(t_{kl}^* t_{kl}) \frac{d\lambda}{2\pi},$$

*for any pair* $(k, l)$.

The proof uses essentially the unitarity of the $S$-matrix. As far as we know and according to Stückelberg [Stu] the idea of deriving positivity of entropy production (Boltzmann's H-Theorem) from the unitarity of the scattering matrix goes back to Pauli. Here, we follow the implementation of this idea given by Inagaki, Wanders and Piron in [IWP].

**Proof.** We will estimate the integrand in Equ. (63) for fixed $\lambda$ and thus we omit it. First note that, by the unitarity relation 57 and the cyclicity of the trace one has

$$\begin{aligned} D_{lk} &\equiv \mathrm{Tr}\,(t_{kl}^* t_{kl}) - \delta_{kl} \sum_j \mathrm{Tr}\,(t_{kj}^* t_{kj}) \\ &\equiv \mathrm{Tr}\,(t_{kl}^* t_{kl}) - \delta_{kl} \sum_j \mathrm{Tr}\,(t_{jl}^* t_{jl}), \end{aligned}$$

from which it follows that

$$\sum_l D_{lk} = \sum_k D_{lk} = 0. \tag{64}$$

We note also that

$$D_{lk} \geq 0 \quad \text{for} \quad l \neq k. \tag{65}$$

For fixed $\xi_1, \cdots, \xi_M \in \mathbb{R}$ we consider the sum (compare with Equ. (63))

$$S \equiv \sum_{lk} D_{lk} \xi_k F(\xi_l).$$

Let $\pi$ be a permutation such that

$$\xi_{\pi(1)} \leq \xi_{\pi(2)} \leq \cdots \leq \xi_{\pi(M)},$$

then we can write

$$S = \sum_{lk} \tilde{D}_{lk} \tilde{\xi}_k F(\tilde{\xi}_l)$$

where $\tilde{\xi}_i \equiv \xi_{\pi(i)}$ and the matrix $\tilde{D}_{lk} \equiv D_{\pi(l)\pi(k)}$ also satisfies (64) and (65). In particular, from Equ. (64), it follows that

$$\begin{aligned} \sum_k \tilde{D}_{lk} \tilde{\xi}_k &= \sum_k \tilde{D}_{lk} (\tilde{\xi}_k - \tilde{\xi}_1) = \sum_k \tilde{D}_{lk} \sum_{j<k} (\tilde{\xi}_{j+1} - \tilde{\xi}_j) \\ &= \sum_j \left( \sum_{k>j} \tilde{D}_{lk} \right) (\tilde{\xi}_{j+1} - \tilde{\xi}_j) = \sum_j C_{lj} (\tilde{\xi}_{j+1} - \tilde{\xi}_j). \end{aligned}$$

Since Equ. (64) allows to rewrite the matrix $C$ as

$$C_{lj} = \begin{cases} \sum_{k>j} \tilde{D}_{lk} & \text{for} \quad l \le j \\ -\sum_{k\le j} \tilde{D}_{lk} & \text{for} \quad l > j \end{cases}$$

it follows from Equ. (65) that $C_{lj} \ge 0$ for $l \le j$ and $C_{lj} \le 0$ otherwise. Rewriting $S$ as

$$S = \sum_{l\le j} C_{lj}(\tilde{\xi}_{j+1} - \tilde{\xi}_j)F(\tilde{\xi}_l) + \sum_{l>j} C_{lj}(\tilde{\xi}_{j+1} - \tilde{\xi}_j)F(\tilde{\xi}_l),$$

and using the facts that $\tilde{\xi}_{j+1} - \tilde{\xi}_j \ge 0$ and $F(\tilde{\xi}_l) \ge F(\tilde{\xi}_j)$ in the first sum while $F(\tilde{\xi}_l) \le F(\tilde{\xi}_{j+1})$ in the second we obtain

$$S \ge \sum_j \left( \sum_{l\le j} C_{lj}F(\tilde{\xi}_j) + \sum_{l>j} C_{lj}F(\tilde{\xi}_{j+1}) \right) (\tilde{\xi}_{j+1} - \tilde{\xi}_j).$$

Since $\sum_l C_{lj} = 0$, this is the same as

$$S \ge \sum_j \left( \sum_{l\le j} C_{lj}F(\tilde{\xi}_j) - \sum_{l\le j} C_{lj}F(\tilde{\xi}_{j+1}) \right) (\tilde{\xi}_{j+1} - \tilde{\xi}_j),$$

and we obtain

$$S \ge \sum_j (F(\tilde{\xi}_j) - F(\tilde{\xi}_{j+1}))(\tilde{\xi}_{j+1} - \tilde{\xi}_j) \sum_{l\le j} C_{lj} \ge 0. \tag{66}$$

We further note that, by Equ. (64),

$$\begin{aligned} B_j &\equiv \sum_{l\le j} C_{lj} = \sum_{l\le j}\sum_{k>j} \tilde{D}_{lk} \\ &= \sum_{l\le j}\left( -\sum_{k\le j} \tilde{D}_{lk} \right) = \sum_{l>j}\sum_{k\le j} \tilde{D}_{lk}, \end{aligned}$$

from which it follows that, if $m \le j < n$, one has

$$B_j \ge \tilde{D}_{mn}, \quad \text{and} \quad B_j \ge \tilde{D}_{nm}. \tag{67}$$

Given a pair of reservoirs $(m, n)$, with $m \ne n$, let us set $m' \equiv \min(\pi^{-1}(m), \pi^{-1}(n))$ and $n' \equiv \max(\pi^{-1}(m), \pi^{-1}(n))$. From the estimate (66), we get

$$S \ge \sum_{m'\le j<n'} (F(\tilde{\xi}_j) - F(\tilde{\xi}_{j+1}))(\tilde{\xi}_{j+1} - \tilde{\xi}_j)B_j,$$

and from Equ. (67) we conclude

$$S \geq D_{mn} \sum_{m' \leq j < n'} (F(\tilde{\xi}_j) - F(\tilde{\xi}_{j+1}))(\tilde{\xi}_{j+1} - \tilde{\xi}_j).$$

The remaining sum is easily estimated, using the fact that $F'(x) = -F(x)F(-x)$ and Jensen inequality

$$\begin{aligned}
\sum_{m' \leq j < n'} (F(\tilde{\xi}_j) - F(\tilde{\xi}_{j+1}))(\tilde{\xi}_{j+1} - \tilde{\xi}_j) &\geq \min_{x \in [\tilde{\xi}_{m'}, \tilde{\xi}_{n'}]} (-F'(x)) \sum_{m' \leq j < n'} (\tilde{\xi}_{j+1} - \tilde{\xi}_j)^2 \\
&\geq F(|\tilde{\xi}_{n'}|) F(|\tilde{\xi}_{m'}|) \frac{1}{n' - m'} (\tilde{\xi}_{n'} - \tilde{\xi}_{m'})^2 \\
&\geq F(|\xi_n|) F(|\xi_m|) \frac{1}{M} (\xi_n - \xi_m)^2.
\end{aligned}$$

Inserting the resulting estimate

$$S = \sum_{lk} D_{lk} \xi_k F(\xi_l) \geq \frac{1}{M} D_{mn} F(|\xi_n|) F(|\xi_m|)(\xi_n - \xi_m)^2,$$

into Equ. (63) lead to the desired inequality.□

# 9 Kubo formula and Onsager reciprocity

In this Subsection, we prove a general Kubo Formula for the transport coefficients of the EBB model. We will therefore restrict the reference state to equilibrium reservoirs

**Assumption (R3)** $\rho_j(\lambda) = (1 + \mathrm{e}^{\beta_j(\lambda - \mu_j)})^{-1}$ for $j = 1, \cdots, M$.

We also assume that the system is TRI

**Assumption (TRI)** There exists a anti-unitary involution $C$ on $\mathfrak{h}$ such that

$$Ch_0 = h_0 C, \quad Cv = vC \quad \text{and} \quad C1_j = 1_j C \quad \text{for } j = 1 \ldots M.$$

Let us introduce relative coordinates for the affinities

$$X_j \equiv \beta - \beta_j, \qquad X_{M+j} \equiv \beta_j \mu_j - \beta \mu,$$

for $j = 1, \dots, M$ where $\beta, \mu$ are the equilibrium parameters. We denote by $\omega_{\rm eq}$ the $(\beta, \mu)$-KMS state for $\tau$ and set

$$\Phi_j \equiv \Phi_j^{(1)}, \qquad \Phi_{M+j} \equiv \Phi_j^{(0)},$$

for $j = 1, \dots, M$. Remark that the entropy production then takes the form

$$\mathrm{Ep}(\omega_+) = \sum_\alpha X_\alpha \omega_+(\Phi_\alpha),$$

to be compared with the phenomenological expression (2).

We also introduce *time averaged* current observables

$$\bar{\Phi}_\alpha \equiv \mathrm{d}\Gamma(1_{\rm ac}(h)\varphi_\alpha 1_{\rm ac}(h)).$$

According to Theorem 6.5, one has

$$\omega_+(\bar{\Phi}_\alpha) = \omega_+(\Phi_\alpha).$$

**Proposition 9.1** *For a EBB model satisfying the assumptions of Theorem 6.5 and (R3), (TRI), one has*

$$L_{\alpha\gamma} \equiv \partial_{X_\gamma} \omega_+(\Phi_\alpha)|_{X=0} = \int_0^\infty \omega_{\rm eq}(\tau^t(\bar{\Phi}_\gamma)\bar{\Phi}_\alpha)\,\mathrm{d}t, \tag{68}$$

*for any* $\omega_+ \in \Sigma_+(\omega, \tau)$.

**Proof.** For $j = 1, \dots, M$, we set

$$q_j \equiv j_j^* h_j j_j, \qquad q_{M+j} \equiv 1_j = j_j^* j_j,$$

so that $\Phi_\alpha = \mathrm{d}\Gamma(\varphi_\alpha)$ with $\varphi_\alpha = -\mathrm{i}[h, q_\alpha]$. According to Theorem 6.5 one has

$$\omega_+(\Phi_\alpha) = \mathrm{Tr}\,(T(X) w_-^* \varphi_\alpha w_-),$$

where

$$T(X) = \bigoplus_k (1 + \mathrm{e}^{\beta(h_k - \mu) - X_k q_k - X_{M+k} q_{M+k}})^{-1}$$

It is not hard to see that $T(X)$ is norm-differentiable and that

$$\partial_{X_\gamma} T(X)|_{X=0} = T_{\mathcal{R}} q_\gamma (I - T_{\mathcal{R}}),$$

where $T_{\mathcal{R}} \equiv T(0) = (1 + \mathrm{e}^{\beta(h_{\mathcal{R}}-\mu)})^{-1}$ (remark that $q_\gamma$ and $T_{\mathcal{R}}$ commutes). Hence the transport coefficients

$$L_{\alpha\gamma} \equiv \partial_{X_\gamma}\omega_+(\Phi_\alpha)|_{X=0} = \mathrm{Tr}\,(T_{\mathcal{R}} q_\gamma (I - T_{\mathcal{R}}) w_-^* \varphi_\alpha w_-),$$

are well defined. By the cyclicity of the trace

$$L_{\alpha\gamma} = \mathrm{Tr}\,(w_- T_{\mathcal{R}} q_\gamma (I - T_{\mathcal{R}}) w_-^* \varphi_\alpha) = \mathrm{Tr}\,(w_- T_{\mathcal{R}} (h_0 + a)\tilde{q}_\gamma (I - T_{\mathcal{R}}) w_-^* \varphi_\alpha),$$

where $\tilde{q}_\gamma = (h_0 + a)^{-1} q_\gamma$. The intertwinning property of the Møller operator further yields

$$L_{\alpha\gamma} = \mathrm{Tr}\,(T(h + a) w_- \tilde{q}_\gamma w_-^* (I - T)\varphi_\alpha),$$

where $T = (1 + \mathrm{e}^{\beta(h-\mu)})^{-1}$ generates the $(\beta, \mu)$-KMS state $\omega_{\mathrm{eq}}$.

Since $\tilde{q}_\gamma$ is bounded and commutes with $h_0$, we have

$$w_- \tilde{q}_\gamma w_-^* = \mathrm{w} - \lim_{t\to\infty} 1_{\mathrm{ac}}(h)\mathrm{e}^{-ith}\tilde{q}_\gamma\, \mathrm{e}^{ith} 1_{\mathrm{ac}}(h).$$

From the second resolvent identity we obtain

$$\tilde{q}_\gamma = (h + a)^{-1} q_\gamma + (h + a)^{-1} v \tilde{q}_\gamma.$$

and since the second term on the right hand side of this identity is compact we get

$$\begin{aligned} w_- \tilde{q}_\gamma w_-^* &= \mathrm{w} - \lim_{t\to\infty} 1_{\mathrm{ac}}(h)\mathrm{e}^{-ith}(h + a)^{-1} q_\gamma\, \mathrm{e}^{ith} 1_{\mathrm{ac}}(h) \\ &= 1_{\mathrm{ac}}(h)(h + a)^{-1} q_\gamma 1_{\mathrm{ac}}(h) + \int_0^\infty 1_{\mathrm{ac}}(h)\mathrm{e}^{-\mathrm{i}th}(h + a)^{-1}\varphi_\gamma \mathrm{e}^{\mathrm{i}th} 1_{\mathrm{ac}}(h)\,\mathrm{d}t, \end{aligned}$$

where the integral is understood in the weak sense. It follows that

$$\begin{aligned} L_{\alpha\gamma} &= \mathrm{Tr}\,(T 1_{\mathrm{ac}}(h) q_\gamma 1_{\mathrm{ac}}(h)(I - T)\varphi_\alpha) \\ &+ \int_0^\infty \mathrm{Tr}\,(T 1_{\mathrm{ac}}(h)\mathrm{e}^{-ith}\varphi_\gamma \mathrm{e}^{\mathrm{i}th} 1_{\mathrm{ac}}(h)(I - T)\varphi_\alpha)\,\mathrm{d}t. \end{aligned} \tag{69}$$

Since the system is TRI, one has

$$C q_\alpha C = q_\alpha, \quad CTC = T, \quad C\varphi_\alpha C = -\varphi_\alpha,$$

from which it follows that the first term in the right hand side of Equ. (69) vanishes. Using Equ. (21), and the fact that currents wanish at equilibrium in TRI systems ($\omega_{\mathrm{eq}}(\bar{\Phi}_\alpha) = 0$) we conclude that

$$L_{\alpha\gamma} = \int_0^\infty \omega_{\mathrm{eq}}(\tau^t(\bar{\Phi}_\gamma)\bar{\Phi}_\alpha)\,\mathrm{d}t.$$

□

We note that, because of the $\tau$-invariance of $\omega_{\rm eq}$, we can rewrite

$$L_{\alpha\gamma} = \int_0^\infty \omega_{\rm eq}(\bar\Phi_\gamma \tau^{-t}(\bar\Phi_\alpha))\,{\rm d}t = \int_{-\infty}^0 \omega_{\rm eq}(\bar\Phi_\gamma \tau^{t}(\bar\Phi_\alpha))\,{\rm d}t,$$

and therefore

$$L_{\alpha\gamma} = \frac{1}{2}\int_{-\infty}^\infty \omega_{\rm eq}(\tau^t(\bar\Phi_\gamma)\bar\Phi_\alpha)\,{\rm d}t.$$

Finaly, since $L_{\alpha\gamma}$ is real we have

$$\begin{aligned} L_{\alpha\gamma} = \bar L_{\alpha\gamma} &= \frac{1}{2}\int_{-\infty}^\infty \omega_{\rm eq}(\bar\Phi_\alpha \tau^{t}(\bar\Phi_\gamma))\,{\rm d}t \\ &= \frac{1}{2}\int_{-\infty}^\infty \omega_{\rm eq}(\tau^{-t}(\bar\Phi_\alpha)\bar\Phi_\gamma)\,{\rm d}t \\ &= \frac{1}{2}\int_{-\infty}^\infty \omega_{\rm eq}(\tau^{t}(\bar\Phi_\alpha)\bar\Phi_\gamma)\,{\rm d}t \\ &= L_{\gamma\alpha}, \end{aligned}$$

which proves

**Corollary 9.2** *Under the assumptions of Theorem 9.1, the Onsager reciprocity relations*

$$L_{\alpha\gamma} = L_{\gamma\alpha},$$

*hold.*

# 10 Interacting Fermions

In this section, we consider a TRI, interacting EBB model where electrons are allowed to interact in the small system $\mathcal{S}$. That is, the coupled dynamics $\tau^t$ is generated by a local perturbation $V$ of $\tau_0$. It is therefore not necessarily Bogoliubov.

To simplify the exposition, we shall only consider the 2 reservoir case and set $\mu_1 = \mu_2 = 0$. The extension to more than 2 reservoirs and to non-zero chemical potentials is simple. We parametrise the temperatures by

$$\beta_1 = \beta, \quad \beta_2 = \beta(1+\epsilon).$$

We set $\delta_V = \mathrm{i}[V, \cdot\,]$. Besides the two dynamics $\tau_0^t = \mathrm{e}^{t\delta_0}$ and $\tau^t = \mathrm{e}^{t\delta}$, with $\delta = \delta_0 + \delta_V$, we will also consider the modular group

$$\sigma_{0,\epsilon}^t = \mathrm{e}^{t(\delta_0 + \epsilon\delta_2)},$$

for which the reference state $\omega_{0,\epsilon}$ is $\beta$-KMS, and its local perturbation

$$\sigma_\epsilon^t = \mathrm{e}^{t(\delta + \epsilon\delta_2)}.$$

By Araki perturbation theory, there is a unique $\beta$-KMS state $\omega_\epsilon$ for $\sigma_\epsilon$. Since $\sigma_0 = \tau$, the state $\omega_0$ is also the $\beta$-KMS state of $\tau$.

We assume that the two Møller morphisms

$$\alpha \equiv \mathrm{s} - \lim_{t\to\infty} \tau_0^{-t} \circ \tau^t, \qquad \gamma_\epsilon \equiv \mathrm{s} - \lim_{t\to\infty} \sigma_{0,\epsilon}^{-t} \circ \sigma_\epsilon^t,$$

exist as well as the inverse morphism

$$\gamma_\epsilon^{-1} = \mathrm{s} - \lim_{t\to\infty} \sigma_\epsilon^{-t} \circ \sigma_{0,\epsilon}^t|\mathcal{O}_{\mathcal{R}},$$

Then the unique NESS in $\Sigma_+(\omega_{0,\epsilon}, \tau)$ is

$$\omega_{\epsilon+} = \omega_{0,\epsilon} \circ \alpha,$$

while

$$\omega_\epsilon = \omega_{0,\epsilon} \circ \gamma_\epsilon.$$

Therefore, one has

$$\omega_{\epsilon+}(\Phi_1) = \omega_\epsilon \circ \gamma_\epsilon^{-1} \circ \alpha(\Phi_1).$$

Since

$$\gamma_\epsilon^{-1} \circ \alpha(\Phi_1) = \lim_{t\to\infty} \sigma_\epsilon^{-t} \circ \sigma_{0,\epsilon}^t \circ \tau_0^{-t} \circ \tau^t(\Phi_1) = \lim_{t\to\infty} \sigma_\epsilon^{-t} \circ \mathrm{e}^{t\epsilon\delta_2} \circ \tau^t(\Phi_1),$$

and

$$\partial_t \sigma_\epsilon^{-t} \circ \mathrm{e}^{t\epsilon\delta_2} \circ \tau^t(\Phi_1) = \sigma_\epsilon^{-t}(\mathrm{i}[\mathrm{e}^{t\epsilon\delta_2}(V) - V, \mathrm{e}^{t\epsilon\delta_2}(\tau^t(\Phi_1))]),$$

we can write

$$\omega_{\epsilon+}(\Phi_1) = \omega_\epsilon(\Phi_1) + \int_0^\infty \omega_\epsilon(\mathrm{i}[\mathrm{e}^{t\epsilon\delta_2}(V) - V, \mathrm{e}^{t\epsilon\delta_2}(\tau^t(\Phi_1))])\, \mathrm{d}t.$$

By TRI, the first term in the right hand side of this identity vanishes (recall that $\omega_\epsilon$ is a unique KMS state for the TRI dynamics $\sigma_\epsilon$). In particular $\omega_{0,+}(\Phi_1) = \omega_0(\Phi_1) = 0$. We conclude that

$$L_{12} = \partial_\epsilon \omega_{\epsilon +}(\Phi_1)|_{\epsilon=0} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_0^\infty \omega_\epsilon(\mathrm{i}[\mathrm{e}^{t\epsilon\delta_2}(V) - V, \mathrm{e}^{t\epsilon\delta_2}(\tau^t(\Phi_1))])\,\mathrm{d}t.$$

Assuming that

$$\frac{1}{\epsilon}\omega_\epsilon(\mathrm{i}[\mathrm{e}^{t\epsilon\delta_2}(V) - V, \mathrm{e}^{t\epsilon\delta_2}(\tau^t(\Phi_1))]) = \int_0^t \omega_\epsilon(\mathrm{i}[\mathrm{e}^{t\epsilon\delta_2}(\Phi_2), \mathrm{e}^{t\epsilon\delta_2}(\tau^t(\Phi_1))])\,\mathrm{d}t,$$

is $L^1(\mathrm{d}t)$ uniformly in $\epsilon$, we obtain

$$L_{12} = \int_0^\infty t\,\omega_0(\mathrm{i}[\Phi_2, \tau^t(\Phi_1)])\,\mathrm{d}t.$$

By the KMS condition, one has

$$\begin{aligned} I_T &\equiv \int_0^T t\,\omega_0(\mathrm{i}[\Phi_2, \tau^t(\Phi_1)])\,\mathrm{d}t \\ &= \mathrm{i}\int_0^T t\,\omega_0(\Phi_2\tau^t(\Phi_1) - \Phi_2\tau^{t+\mathrm{i}\beta}(\Phi_1))\,\mathrm{d}t \\ &= \mathrm{i}\int_0^T \big(t\,\omega_0(\Phi_2\tau^t(\Phi_1)) - (t+\mathrm{i}\beta)\omega_0(\Phi_2\tau^{t+\mathrm{i}\beta}(\Phi_1))\big)\,\mathrm{d}t \\ &- \beta\int_0^T \omega_0(\Phi_2\tau^t(\Phi_1))\,\mathrm{d}t. \end{aligned}$$

The first term on the right hand side of the last identity can be interprted as a contour integral and by Cauchy Theorem, rewritten as

$$-\int_0^\beta \big(u\,\omega_0(\Phi_2\tau^{\mathrm{i}u}(\Phi_1)) - (T+\mathrm{i}u)\omega_0(\Phi_2\tau^{T+\mathrm{i}u}(\Phi_1))\big)\,\mathrm{d}u.$$

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