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Mathematical Theory of Non-Equilibrium Quantum Statistical Mechanics

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We review and further develop a mathematical framework for non-equilibrium quantum statistical mechanics recently proposed in refs. 1–7. In the algebraic formalism of quantum statistical mechanics we introduce notions of non-equilibrium steady states, entropy production and heat fluxes, and study their properties. Our basic paradigm is a model of a small (finite) quantum system coupled to several independent thermal reservoirs. We exhibit examples of such systems which have strictly positive entropy production.

KEY WORDS: Nonequilibrium quantum statistical mechanics; Liouvillean; open systems; entropy production; steady state; C^*-algebra.

1. INTRODUCTION

The properties of a physical system out of thermal equilibrium are usually described in term of phenomenological concepts like steady state, entropy production and heat flux. These notions are related by the fundamental laws of thermodynamics. As an illustration, consider a model describing a small system $\mathscr{S}$ coupled to two infinite heat reservoirs $\mathscr{R}_1$, $\mathscr{R}_2$ which are at temperature T_1, T_2 (see Fig. 1).

Under normal conditions, one expects that the combined system will settle into a steady state in which there is a constant flow of heat and entropy from the hotter to the colder reservoir across the system $\mathscr{S}$. Let Φ_k be the heat current flowing from reservoir $\mathscr{R}_k$ into the small system $\mathscr{S}$, and

Dedicated to David Ruelle and Yakov Sinai on the occasion of their 65th birthday.

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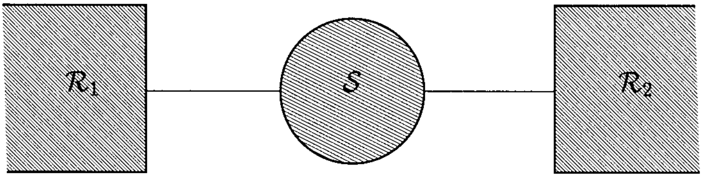

Fig. 1. A system coupled to two heat reservoirs.

Ep the entropy production rate in $\mathscr{S}$. In the steady state, the fundamental laws of thermodynamics read:

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

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 $\mathscr{S}$ 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 heat flux, study their properties and prove Relations (1) from first principles. We will also exhibit examples of combined systems $\mathscr{S} + \mathscr{R}_1 + \mathscr{R}_2$ which have strictly positive entropy production and hence non-trivial thermodynamics.

We will work in the mathematical framework of algebraic quantum statistical mechanics which appears to be particularly well-suited to the study of general structural properties of non-equilibrium steady states. The basic notions of this algebraic framework are briefly introduced in Section 2. The reader is referred to the monographs of refs. 8–12 for more detailed expositions. In Section 3, we define non-equilibrium steady states and discuss their basic structural properties. Section 4 is devoted to the notion of entropy production. Finally, a simple class of models with strictly positive entropy production is described in Section 5.

This review is based on a series of recent papers.[1–7] These works rely on a large body of knowledge previously developed by many authors in various areas of mathematical physics: Equilibrium statistical mechanics, quantum dynamical systems, quantum Markovian processes, van Hove limit, linear response theory, etc. Even though we have tried to provide the reader with the most relevant references to these earlier works, we do not claim completeness in this respect, and refer the reader to refs. 8, 9, and 13 for an extensive list of references.

2. THE FRAMEWORK

In its algebraic formulation, the quantum mechanics of a physical system is described by a C^* or a W^*-dynamical system. To avoid technicalities we will consider in this review only C^*-systems. The non-equilibrium statistical mechanics of W^*-systems will be discussed elsewhere.

C^*-dynamical systems are introduced in Sections 2.1 and 2.2 later. In Section 2.3 we describe some examples of such systems.

2.1. C^*-Dynamical Systems

A C^*-dynamical system is a pair $(\mathcal{O}, \tau)$, where $\mathcal{O}$ is a C^*-algebra and τ^t a strongly continuous group of $*$-automorphisms of $\mathcal{O}$ (that is, the map $t \mapsto \tau^t(A)$ is norm-continuous for each $A \in \mathcal{O}$). We assume that $\mathcal{O}$ has an identity $\mathbf{1}$. The elements of $\mathcal{O}$ describe observables of the physical system under consideration and the group τ specifies their time evolution. An example of a C^*-algebra is $\mathcal{B}(\mathcal{H})$, the algebra of all bounded operators on a Hilbert space $\mathcal{H}$, equipped with the operator norm topology. Any C^*-algebra is isomorphic to a subalgebra of $\mathcal{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$.

A state of the system is described by a positive linear functional $\omega \in \mathcal{O}^*$ satisfying $\omega(\mathbf{1}) = 1$. The number $\omega(\tau^t(A))$ is the expected value of the observable A at time t, assuming that the system was initially in the state ω. The set $E(\mathcal{O})$ of all states on $\mathcal{O}$ is a convex, weak-$*$ compact subset of the dual Banach space $\mathcal{O}^*$.

A state $\omega \in E(\mathcal{O})$ is called τ-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. We call quantum dynamical system a triple $(\mathcal{O}, \tau, \omega)$, where ω is a τ-invariant state.

A quantum dynamical system $(\mathcal{O}, \tau, \omega)$ is called ergodic if

$$\lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} \omega(B^* \tau^t(A)\, B)\, dt = \omega(A)\, \omega(B^* B),$$

for all $A, B \in \mathcal{O}$. It is said to have the property of return to equilibrium if

$$\lim_{|t| \to \infty} \omega(B^* \tau^t(A)\, B) = \omega(A)\, \omega(B^* B).$$

Thermal equilibrium states are characterized by the KMS condition. Let $\beta > 0$ be the inverse temperature. A state ω is (τ, β)-KMS if, for all

$A, B \in \mathcal{O}$, there is a function $F_{A,B}$ analytic inside the strip $\{z \mid 0 < \operatorname{Im} z < \beta\}$, bounded and continuous on its closure, and satisfying the KMS boundary conditions

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

for $t \in \mathbb{R}$. A KMS state is τ-invariant. The quantum dynamical system $(\mathcal{O}, \tau, \omega)$, where ω is a (τ, β)-KMS state, describes a physical system in thermal equilibrium at temperature $1/\beta$.

Note that a (τ, β)-KMS state is also a β'-KMS state for the dynamics defined by $\tau^{t\beta/\beta'}$. Even though, in most systems, the physical temperature is a non-negative parameter, it is mathematically convenient to define KMS state for all $\beta \in \mathbb{R} \cup \{\pm\infty\}$. The case $\beta = 0$ corresponds to infinite temperature and $(\tau, 0)$-KMS states (τ-invariant traces) are sometimes called chaotic states. Let δ be the generator of τ. The state ω is called $(\tau, \pm\infty)$-KMS state if $\pm i\omega(A^*\delta(A)) \geqslant 0$ for all $A \in \mathscr{D}(\delta)$. (τ, β)-KMS states at values $\beta = +\infty$ and $\beta = -\infty$ are called respectively ground states and ceiling states.

Let ω be a state on the C^*-algebra $\mathcal{O}$. We denote by $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS-representation of $\mathcal{O}$ associated to ω. An injective representation π_ω is called faithful. A state $\eta \in E(\mathcal{O})$ is called ω-normal if there is a density matrix ρ on $\mathscr{H}_\omega$ such that $\eta(\cdot) = \operatorname{Tr}(\rho\pi_\omega(\cdot))$. The set $\mathscr{N}_\omega$ of all ω-normal states is a norm closed convex subset of $E(\mathcal{O})$. $\mathscr{N}_\omega$ is sometimes called the folium of ω. Any $\eta \in \mathscr{N}_\omega$ has a unique normal extension to the enveloping von Neumann algebra $\mathfrak{M}_\omega = \pi_\omega(\mathcal{O})''$. The state ω is called factor state (or primary state) if its enveloping von Neumann algebra is a factor i.e., if its center $\mathfrak{M}_\omega \cap \mathfrak{M}'_\omega$ consists of multiples of the identity.

The effectiveness of the algebraic formalism of quantum statistical mechanics is largely due to Tomita-Takesaki modular theory of von Neumann algebras. We assume that the reader is familiar with the basic results of this theory as discussed, for example, in refs. 8–10 and 13. For notational purposes we recall some well-known facts.

The state ω is called modular if Ω_ω is a separating vector for $\mathfrak{M}_\omega$ i.e., if ω extends to a faithful normal state on $\mathfrak{M}_\omega$. Any KMS state at inverse temperature $\beta \in \mathbb{R}$ is modular. Assume that ω is a modular state on $\mathcal{O}$ and denote by $\Delta_\omega = \mathrm{e}^{\mathscr{L}_\omega}$, J and $\mathscr{P}$ the modular operator, the modular conjugation and the natural cone associated to the pair $(\mathfrak{M}_\omega, \Omega_\omega)$. The operator $\mathscr{L}_\omega$ is self-adjoint while J is an anti-unitary involution on $\mathscr{H}_\omega$. These operators are characterized by the relation

$$J\mathrm{e}^{\mathscr{L}_\omega/2}A\Omega_\omega = A^*\Omega_\omega, \tag{2}$$

which holds for any $A \in \mathfrak{M}_\omega$. The natural cone $\mathscr{P}$ is the norm closure of the set

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

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

$$\begin{aligned} \pi_\omega(\tau^t(A)) &= \mathrm{e}^{itL}\pi_\omega(A)\,\mathrm{e}^{-itL}, \\ \mathrm{e}^{-itL}\mathscr{P} &\subset \mathscr{P}. \end{aligned} \tag{3}$$

The operator L is called the standard Liouvillean. The first formula in (3) allows us to extend τ to all of $\mathfrak{M}_\omega$.

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

$$\mathscr{L}_\omega = -\beta L. \tag{4}$$

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.[14, 15] For example, if the state ω 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.

2.2. Local Perturbations

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system describing a physical system in a steady state. Our guiding physical principle is that the response of the system to local perturbations will reveal its basic thermodynamical properties. We now discuss the mathematical formalism needed to deal with local perturbations.

Let δ be the generator of the dynamical group τ^t. The operator δ is a $*$-derivation: Its domain $\mathscr{D}(\delta)$ is a $*$-subalgebra of $\mathcal{O}$ and for $A, B \in \mathscr{D}(\delta)$,

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

Let V be a local perturbation, i.e., $V = V^* \in \mathcal{O}$. The generator of the perturbed dynamics is $\delta_V(\cdot) = \delta(\cdot) + i[V, \cdot]$. The operator δ_V is also a $*$-derivation and $\mathcal{D}(\delta_V) = \mathcal{D}(\delta)$. The perturbed dynamics is given by the automorphisms $\tau_V^t = \mathrm{e}^{t\delta_V}$,

$$\tau_V^t(A) = \tau^t(A) + \sum_{n \geqslant 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n [\tau^{t_n}(V), [\cdots[\tau^{t_1}(V), \tau^t(A)]]].$$

The pair $(\mathcal{O}, \tau_V)$ is a C^*-dynamical system. If ω is modular and L is the standard Liouvillean associated to τ, then the standard Liouvillean associated to τ_V is the self-adjoint operator given by

$$L_V = L + V - JVJ,$$

with domain $\mathcal{D}(L_V) = \mathcal{D}(L)$.

2.3. Examples

2.3.1. Finite Quantum Systems

Let $\mathcal{K} \simeq \mathbb{C}^N$ be a finite dimensional Hilbert space and $\mathcal{O} = \mathcal{B}(\mathcal{K})$. A C^*-dynamics τ is determined by a self-adjoint operator (Hamiltonian) H on $\mathcal{K}$

$$\tau^t(A) = \mathrm{e}^{itH} A \mathrm{e}^{-itH}.$$

The dynamics associated with the local perturbation V is

$$\tau_V^t(A) = \mathrm{e}^{it(H+V)} A \mathrm{e}^{-it(H+V)}.$$

A states $\omega \in E(\mathcal{O})$ is determined by a density matrix on $\mathcal{K}$ which we denote by the same letter, so $\omega(A) = \mathrm{Tr}(\omega A)$. The state ω is faithful iff $\omega > 0$ and it is τ-invariant iff $[\omega, H] = 0$.

For any $\beta \in \mathbb{R}$ the density matrix

$$\mathrm{e}^{-\beta H}/\mathrm{Tr}(\mathrm{e}^{-\beta H}),$$

defines the unique (τ, β)-KMS state on $\mathcal{O}$. On the other hand, if ω is a faithful state, then for any $\beta \neq 0$ there exists a unique C^*-dynamics $\sigma_{\omega,\beta}$ such that ω is a $(\sigma_{\omega,\beta}, \beta)$-KMS state. This dynamics is generated by the Hamiltonian $-\beta^{-1} \log \omega$.

The GNS-representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ of $\mathcal{O}$ associated to the state ω can be explicitly constructed as follows. Let $0 \leqslant \lambda_1 \leqslant \cdots \leqslant \lambda_N$ be the eigenvalues of ω counted with multiplicities and denote by ψ_i the corresponding eigenvectors. Fix a complex conjugation $\psi \mapsto \bar{\psi}$ on $\mathscr{K}$, then one can take

$$\mathscr{H}_\omega = \mathscr{K} \otimes \mathscr{K},$$
$$\pi_\omega(A) = A \otimes \mathbf{1},$$
$$\Omega_\omega = \sum_{k=1}^{N} \lambda_k^{1/2}\, \psi_k \otimes \bar{\psi}_k.$$

The standard Liouvillean corresponding to the dynamics τ generated by the Hamiltonian H is

$$L = H \otimes \mathbf{1} - \mathbf{1} \otimes \bar{H},$$

where, by definition, $\bar{H}\psi = \overline{H\bar{\psi}}$. Finally, let us describe the modular structure associated to a faithful state ω. The modular conjugation acts as $J(\psi \otimes \phi) = \bar{\phi} \otimes \bar{\psi}$, and the modular operator is given by

$$\mathscr{L}_\omega = \log \Delta_\omega = \log \omega \otimes \mathbf{1} - \mathbf{1} \otimes \log \bar{\omega}.$$

Isolated finite quantum systems have no interesting thermodynamics. However, models where a finite quantum system is coupled to infinite thermal reservoirs are one of the basic paradigms of quantum statistical mechanics.

2.3.2. Free Fermi Gases

Let $\mathscr{H}$ be the Hilbert space of a single fermion and h its Hamiltonian. For example, a free non-relativistic spinless electron of mass m is described by the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^3, dp)$ and its Hamiltonian h is the operator of multiplication by $p^2/2m$. Another example is given by a spinless lattice fermion with Hilbert space $\mathscr{H} = \ell^2(\mathbb{Z}^d)$ and Hamiltonian $h = -\Delta$, the usual discrete Laplacian on $\mathbb{Z}^d$.

Let $\Gamma_-(\mathscr{H})$ be the anti-symmetric (fermionic) Fock space over $\mathscr{H}$. For $f \in \mathscr{H}$, denote by $a(f)$ and $a^*(f)$ the annihilation and creation operators on $\Gamma_-(\mathscr{H})$. They are bounded operators satisfying $\|a(f)\| = \|a^*(f)\| = \|f\|$. As usual, $a^\#$ stands for either a or a^*. Let $\mathscr{O}$ be the C^*-algebra generated by $\{a^\#(f) \mid f \in \mathscr{H}\}$. The map

$$\tau^t(a^\#(f)) = a^\#(\mathrm{e}^{ith} f),$$

extends to a C^*-dynamics on $\mathscr{O}$ which can be explicitly written as

$$\tau^t(A) = \mathrm{e}^{itH} A \mathrm{e}^{-itH},$$

where $H = \mathrm{d}\Gamma(h)$. The C^*-dynamical system $(\mathcal{O}, \tau)$ describes a free Fermi gas.

One often deals with the even subalgebra $\mathcal{O}_{\mathrm{e}}$, the C^*-algebra generated by

$$\{a^{\#}(f_1)\cdots a^{\#}(f_{2n}) \mid n = 0, 1,...; f_1,..., f_{2n} \in \mathcal{H}\}.$$

The pair $(\mathcal{O}_{\mathrm{e}}, \tau)$ is also a C^*-dynamical system.

A self-adjoint operator T on $\mathcal{H}$, such that $0 \leqslant T \leqslant \mathbf{1}$, determines a state $\omega \in E(\mathcal{O})$ by

$$\omega(a^*(f_1)\cdots a^*(f_n)\, a(g_1)\cdots a(g_m)) = \delta_{m,n} \det\{(g_i, Tf_j)\}.$$

This, so called quasi-free gauge invariant state, is completely determined by its two-point function

$$\omega(a^*(f)\, a(g)) = (g, Tf). \tag{5}$$

A quasi-free gauge invariant states ω is τ-invariant iff for all t, $\mathrm{e}^{ith}T\mathrm{e}^{-ith} = T$. In particular, the quasi-free gauge invariant state determined by $T = F(h)$ describes a free Fermi gas with energy density per unit volume $F(E)$. For any $\beta \in \mathbb{R}$, the quasi-free gauge invariant state determined by $T = (1 + \mathrm{e}^{\beta h})^{-1}$ is the unique (τ, β)-KMS state on $\mathcal{O}$.

The GNS-representation and the associated modular structure of the quasi-free gauge invariant state ω determined by T can be explicitly computed (see ref. 16). Let N be the number operator and Ω the Fock vacuum on $\Gamma_-(\mathcal{H})$. Fix a complex conjugation on $\mathcal{H}$ and extend it to a complex conjugation on $\Gamma_-(\mathcal{H})$. Set

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

The triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ is the GNS-representation of the algebra $\mathcal{O}$ associated to ω. The modular conjugation acts as $J(\Phi \otimes \Psi) = U\bar{\Psi} \otimes U\bar{\Phi}$, where $U = (-\mathbf{1})^{N(N-1)/2}$. The modular operator is

$$\mathcal{L}_\omega = \log \Delta_\omega = \mathrm{d}\Gamma(S) \otimes \mathbf{1} - \mathbf{1} \otimes \mathrm{d}\Gamma(\bar{S}),$$

where $S = \log T(\mathbf{1} - T)^{-1}$. The corresponding Liouvillean is given by

$$L = \mathrm{d}\Gamma(h) \otimes \mathbf{1} - \mathbf{1} \otimes \mathrm{d}\Gamma(\bar{h}).$$

A quasi-free gauge invariant state is primary. It is modular iff $\mathrm{Ker}\, T = \mathrm{Ker}(\mathbf{1}-T) = \{0\}$.

From the above discussion it follows easily that, if ω is a quasi-free gauge invariant and τ-invariant state, then the quantum dynamical system $(\mathcal{O}, \tau, \omega)$ is ergodic iff h has no eigenvalues. Moreover, if the spectrum of h is purely absolutely continuous, then this system returns to equilibrium.

2.3.3. Interacting Lattice Fermi Gases

Consider the C^*-dynamical system $(\mathcal{O}, \tau)$ describing the free lattice Fermi gas introduced in the previous subsection. For $x \in \mathbb{Z}^d$, we set $a^{\#}(x) = a^{\#}(\delta_x)$ and, to any finite subset $X \subset \mathbb{Z}^d$, we associate the local algebra $\mathcal{O}_X$ generated by $\{a^{\#}(x) \mid x \in X\}$. The algebra $\mathcal{O}$ is quasi-local with respect to the net $\{\mathcal{O}_X\}$, in particular $\mathcal{O}$ is the norm closure of $\bigcup_X \mathcal{O}_X$.

The fermions interact through a real valued pair potential $v \in \ell^1(\mathbb{Z}^d)$. For any finite subset $X \subset \mathbb{Z}^d$, the local perturbation

$$V_X = \sum_{x,\, y \in X} v(x-y)\, a^*(x)\, a^*(y)\, a(y)\, a(x),$$

induces a dynamics τ_X^t on $\mathcal{O}$. Moreover, there exists a dynamics τ_v on $\mathcal{O}$ such that, for any $A \in \bigcup_X \mathcal{O}_X$ and for any increasing sequence of finite subsets $\Lambda \subset \mathbb{Z}^d$ which eventually contains any finite subset of $\mathbb{Z}^d$, one has

$$\tau_v^t(A) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \tau_\Lambda^t(A).$$

The C^*-dynamical system $(\mathcal{O}, \tau_v)$ describes an interacting Fermi gas on the lattice $\mathbb{Z}^d$. This important system is little understood (see however ref. 17).

2.3.4. Lattice Spin Systems

Let $\mathcal{K}$ be a finite dimensional Hilbert space and, for each $x \in \mathbb{Z}^d$, let $\mathcal{K}_x$ be a copy of $\mathcal{K}$. To a finite domain $\Lambda \subset \mathbb{Z}^d$ we associate the Hilbert space

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{H}_x,$$

and the corresponding C^*-algebra

$$\mathcal{O}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda).$$

If $\Lambda_1 \subset \Lambda_2$, then the injection $A \mapsto A \otimes \mathbf{1}_{\mathcal{H}_{\Lambda_2 \setminus \Lambda_1}}$ allows us to identify $\mathcal{O}_{\Lambda_1}$ with a subalgebra of $\mathcal{O}_{\Lambda_2}$. Let $\mathcal{O}$ denote the C^*-algebra obtained by completing $\bigcup_\Lambda \mathcal{O}_\Lambda$. We can identify the local algebras $\mathcal{O}_\Lambda$ with subalgebras of $\mathcal{O}$.

The algebra $\mathcal{O}$ describes observables of the infinite spin system, the subalgebra $\mathcal{O}_\Lambda$ containing the observables of the spins inside the domain Λ.

An interaction is a function Φ from the finite subsets $X \subset \mathbb{Z}^d$ into self-adjoint elements of $\mathcal{O}$ such that $\Phi(X) \in \mathcal{O}_X$. The Hamiltonian

$$H(\Lambda) = \sum_{X \subset \Lambda} \Phi(X),$$

of a finite domain Λ induces a dynamics

$$\tau_\Lambda^t(A) = \mathrm{e}^{itH(\Lambda)} A \mathrm{e}^{-itH(\Lambda)},$$

on $\mathcal{O}$.

Let us denote by $|X|$ the number of points in X. If the interaction satisfies

$$\sup_{x \in \mathbb{Z}^d} \sum_{X \ni x} \|\Phi(X)\| \, \mathrm{e}^{r|X|} < \infty, \tag{6}$$

for some $r > 0$, then the limit

$$\tau^t(A) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \tau_\Lambda^t(A),$$

exists for any $A \in \bigcup_\Lambda \mathcal{O}_\Lambda$. Moreover, τ extends by continuity to a dynamics on $\mathcal{O}$. The pair $(\mathcal{O}, \tau)$ is the C^*-dynamical system describing an infinite quantum spin system.

Whenever condition (6) holds, there exist at least one (and possibly many) (τ, β)-KMS states on $\mathcal{O}$ for any $\beta \in \mathbb{R}$. Such states are constructed as thermodynamic limits of local KMS states defined on $\mathcal{O}_\Lambda$. Under some additional regularity conditions on the interaction Φ the KMS state is unique for small enough β.

We refer the reader to refs. 9, 11, 18, and 19 for detailed information on the kinematical structure and equilibrium thermodynamics of quantum spin systems, and to refs. 4–7 for their non-equilibrium statistical mechanics. The dynamical aspects of quantum spin systems are comparatively little studied. To our knowledge the only well-understood case is the one-dimensional XY model, see ref. 20 and 21.

3. NON-EQUILIBRIUM STEADY STATES

In Section 3.1, we define non-equilibrium steady states (NESS) and describe their basic structural properties. Stability properties of quantum dynamical systems are discussed in Section 3.2. Finally, in Section 3.3, we review two approaches to the study of NESS.

3.1. Definition and Basic Properties of NESS

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system and $V \in \mathcal{O}$ a local perturbation. The non-equilibrium steady states (NESS) of the locally perturbed system $(\mathcal{O}, \tau_V)$ are the weak-$*$ limit points, as $T \to +\infty$, of the states

$$\omega_V^T \equiv \frac{1}{T} \int_0^T \omega \circ \tau_V^t \, dt. \tag{7}$$

In other words, ω_V^+ is a NESS iff there is a sequence $T_n \to +\infty$ such that, for all $A \in \mathcal{O}$, one has

$$\omega_V^+(A) = \lim_n \omega_V^{T_n}(A).$$

The set $\Sigma_V^+(\omega)$ of NESS is a non-empty weak-$*$ compact subset of $E(\mathcal{O})$ whose elements are τ_V-invariant.

The set $\Sigma_V^-(\omega)$ is defined analogously, by taking $T \to -\infty$ in Eq. (7). Although states in $\Sigma_V^-(\omega)$ are non-physical, they are both technically and conceptually useful.

Obviously, the τ-invariance of ω plays no role in the above definitions, and we can define the NESS and the sets $\Sigma_V^\pm(\eta)$ for any initial state $\eta \in E(\mathcal{O})$.

Remark. There is a fair amount of arbitrariness in the above definition. The ergodic mean in Eq. (7) 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 $\Sigma_V^+(\eta)$. However, most results in this section are either independent of our specific choice of averaging, or can be easily adapted to other averagings. For technical reasons, related to the use of spectral analysis (see ref. 2), a particularly useful alternative is Abelian averaging. We denote by $\Sigma_{V,\mathrm{Ab}}^\pm(\eta)$ the set of weak-$*$ limit points of the state

$$\epsilon \int_0^\infty \mathrm{e}^{-\epsilon t} \eta \circ \tau_V^{\pm t} \, dt, \tag{8}$$

as $\epsilon \downarrow 0$.

3.1.1. Dependence on the Initial State

Clearly $\Sigma_V^+(\eta)$ describes the set of steady states that can be reached starting from η, and thus depends on the particular choice of the initial state η. However, we expect that sufficiently similar initial states should be driven towards the same set of asymptotic states. Indeed, under some mild regularity assumption, $\Sigma_V^+(\eta)$ does not depend on the choice of η as long as it remains in the folium $\mathcal{N}_\omega$. The following result will be proved in ref. 3.

Theorem 3.1. Let ω be a factor state and assume that, for all $\eta \in \mathcal{N}_\omega$ and $A, B \in \mathcal{O}$,

$$\lim_{T \to \pm\infty} \frac{1}{T} \int_0^T \eta([\tau_V^t(A), B]) \, dt = 0,$$

holds (weak asymptotic abelianness in the mean). Then $\Sigma_V^\pm(\eta) = \Sigma_V^\pm(\omega)$ for all $\eta \in \mathcal{N}_\omega$. In particular, if $\mathrm{Ker}\, L_V \neq \{0\}$, then it is one-dimensional and there is a unique ω-normal τ_V-invariant state ω_V such that $\Sigma_V^\pm(\eta) = \{\omega_V\}$ for all $\eta \in \mathcal{N}_\omega$.

3.1.2. Normal and Singular NESS

From now on, we fix the initial state ω, and investigate the structural properties of the states in $\Sigma_V^\pm(\omega)$. First we remark that if the GNS-representation π_ω is not faithful, we can consider the quotient dynamical system on the algebra $\mathcal{O}/\mathrm{Ker}\pi_\omega$ (which has a faithful representation on $\mathcal{H}_\omega$). One easily sees that the NESS of the original system are obtained by lifting to $\mathcal{O}$ the NESS of the quotient system with the help of the canonical projection $\rho: \mathcal{O} \to \mathcal{O}/\mathrm{Ker}\pi_\omega$. Thus, without loss of generality, we may assume that the GNS-representation π_ω is faithful and identify $\mathcal{O}$ with $\pi_\omega(\mathcal{O})$.

A positive linear functional $\mu \in \mathcal{O}^*$ is called ω-normal iff $\mu = \lambda \nu$ for some $\nu \in \mathcal{N}_\omega$ and $\lambda > 0$. It is called ω-singular iff $\mu \geqslant \phi \geqslant 0$ for some ω-normal ϕ implies $\phi = 0$. Any state $\mu \in E(\mathcal{O})$ has a unique decomposition

$$\mu = \mu_n + \mu_s, \tag{9}$$

where μ_n and μ_s are positive linear functionals and μ_n is ω-normal while μ_s is ω-singular (in particular, μ_n and μ_s are disjoint, see refs. 22 and 23 for details). Since ω-normal states are mapped to ω-normal states by τ_V, the uniqueness of this decomposition implies that if μ is τ_V-invariant, then both μ_n and μ_s are τ_V-invariant. We say that a NESS $\mu \in \Sigma_V^\pm(\omega)$ is normal if its ω-singular part μ_s is zero and purely singular if its ω-normal part μ_n is zero.

Theorem 3.2. Assume that $\mu \in \Sigma_V^{\pm}(\omega)$, then:

1. If μ is a factor state, it is either normal or purely singular.
2. If ω is a factor state, either μ is purely singular or every ω-normal state is also μ-normal.

If the system has settled into a NESS $\mu \in \Sigma_V^{+}(\omega)$, then it is described by the quantum dynamical system $(\mathcal{O}, \tau_V, \mu)$. From the point of view of thermodynamics, a fundamental question is whether this system has a strictly positive entropy production. At this level of generality, it is far from obvious even how to define entropy production. We will return to this question in Section 4. We will prove that the entropy production of the normal part μ_n is *always zero*. Therefore, a necessary condition for non-trivial thermodynamics is that $\mu \notin \mathcal{N}_\omega$. In other words, μ must be "sufficiently far" from ω, so far in fact that it does not "live" in the same Hilbert space $\mathcal{H}_\omega$. Although physically natural, this restriction is one of the main sources of difficulty in the mathematical study of NESS.

The following result gives useful criteria for a system to have either purely singular or normal NESS.

Proposition 3.3. Assume that ω is modular, and let L_V be the Liouvillean of the locally perturbed system $(\mathcal{O}, \tau_V)$.

1. If Ker $L_V = \{0\}$, then any NESS in $\Sigma_V^{\pm}(\omega)$ is purely singular.
2. If Ker L_V contains a separating vector for $\mathfrak{M}_\omega$, then

$$\Sigma_V^{+}(\omega) = \Sigma_V^{-}(\omega) = \{\mu\} \subset \mathcal{N}_\omega.$$

We finish with a brief discussion of equilibrium vs. non-equilibrium steady states in quantum statistical mechanics. Consider a quantum dynamical system $(\mathcal{O}, \tau, \omega)$ and assume that ω is a (τ, β)-KMS state for some $\beta > 0$. The Araki perturbation theory of KMS states[9, 24, 25] yields that for any local perturbation V there exist a ω-normal (τ_V, β)-KMS state ω_V. Under normal conditions, it is expected that for any $\eta \in \mathcal{N}_\omega$, $\Sigma_V^{\pm}(\eta) = \{\omega_V\}$. There is no interesting thermodynamics in the sense that the entropy production of ω_V is zero. Hence the main question in thermal equilibrium is whether the quantum dynamical system $(\mathcal{O}, \tau_V, \omega_V)$ is ergodic or returns to equilibrium. Although it is generally expected that these properties hold for physical systems under normal conditions (the zeroth law of thermodynamics), there are very few non-trivial models for which this has been proven (see refs. 15, 26–28).

The expected scenario in the non-equilibrium case is quite different. One considers a quantum dynamical system $(\mathcal{O}, \tau, \omega)$ which is not in thermal equilibrium and a local perturbation V. Under the influence of the perturbation the system will settle into a NESS $\omega_V^+ \in \Sigma_V^+(\omega)$. One expects that under normal circumstances $\lim_{t\to+\infty} \eta \circ \tau_V^t = \omega_V^+$ for all $\eta \in \mathcal{N}_\omega$. Moreover, one expects that $\omega_V^+ \notin \mathcal{N}_\omega$ and that the entropy production associated to ω_V^+ is strictly positive. Establishing this scenario for physically relevant models is one of the central goals of non-equilibrium quantum statistical mechanics.

3.2. Stability

From a physical point of view, the prominent feature of thermal equilibrium is its stability under local perturbations. This basic phenomenon appears in two flavors: Structural and dynamical stability.

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system where ω is a (τ, β)-KMS state. It follows from Araki's theory[9, 24, 25] that for every local perturbation V there is a (τ_V, β)-KMS state $\omega_V \in \mathcal{N}_\omega$ such that

$$\|\omega_V - \omega\| = O(\|V\|). \tag{10}$$

Moreover the map $\omega \mapsto \omega_V$ is, for fixed V, a bijection from the set of (τ, β)-KMS states to the set of (τ_V, β)-KMS states. This shows that the set of thermal equilibria of the system is structurally stable under local perturbations.

Dynamical stability does not hold without further assumption. However, if we assume that

$$\lim_{T\to\pm\infty} \frac{1}{T} \int_0^T \|[V, \tau_V^t(A)]\| \, dt = 0, \tag{11}$$

for all $A \in \mathcal{O}$, then any NESS in $\Sigma_V^\pm(\omega)$ is a (τ_V, β)-KMS state (this is a simple variant of Proposition 5.4.6 in ref. 9). Moreover, if $(\mathcal{O}, \tau_V, \omega_V)$ is ergodic, then the structural isomorphism $\omega \mapsto \omega_V$ is dynamically realized as $\Sigma_V^\pm(\omega) = \{\omega_V\}$.

It is a deep fact that thermal equilibrium is actually characterized by the stability criteria (10) and (11). There are several results in this direction. We will describe one of them, for others see refs. 29–32. The following ergodicity assumption will be needed.

(E) For any self-adjoint element V of a norm-dense $*$-subalgebra $\mathcal{O}_0 \subset \mathcal{O}$ there is a $\lambda_V > 0$ such that

$$\int_{-\infty}^{\infty} \|[V, \tau_{\lambda V}^t(A)]\| \, dt < \infty, \tag{12}$$

holds for all $|\lambda| < \lambda_V$ and $A \in \mathcal{O}_0$, Under assumption (E), for any self-adjoint $V \in \mathcal{O}_0$ the strong limits

$$\gamma_{\lambda V}^{\pm} \equiv \lim_{t \to \pm\infty} \tau_{\lambda V}^{-t} \circ \tau^{t},$$

$$\alpha_{\lambda V}^{\pm} \equiv \lim_{t \to \pm\infty} \tau^{-t} \circ \tau_{\lambda V}^{t},$$

exist on $\mathcal{O}$ for all $|\lambda| < \lambda_V$. The Møller morphisms $\gamma_{\lambda V}^{\pm}$ are $*$-automorphisms of $\mathcal{O}$ and $(\gamma_{\lambda V}^{\pm})^{-1} = \alpha_{\lambda V}^{\pm}$. Since $\omega \circ \tau_{\lambda V}^{t} = \omega \circ \tau^{-t} \circ \tau_{\lambda V}^{t}$, we get

$$\Sigma_{\lambda V}^{\pm}(\omega) = \{\omega_{\lambda V}^{\pm}\},$$

with $\omega_{\lambda V}^{\pm} \equiv \omega \circ \alpha_{\lambda V}^{\pm}$. It follows that $\omega = \omega_{\lambda V}^{\pm} \circ \gamma_{\lambda V}^{\pm} = \lim_{t \to \pm\infty} \omega_{\lambda V}^{\pm} \circ \tau^{t}$, from which we get the formula

$$\omega_{\lambda V}^{+}(A) - \omega_{\lambda V}^{-}(A) = i\lambda \int_{-\infty}^{\infty} \omega_{\lambda V}^{\mathrm{sign}(t)}([V, \tau^{t}(A)])\, dt. \tag{13}$$

The stability requirement is:

(S) For any self-adjoint $V \in \mathcal{O}_0$ and λ small enough, there exists a $\tau_{\lambda V}$-invariant state $\omega_{\lambda V} \in \mathcal{N}_{\omega}$, such that

$$\Sigma_{\lambda V}^{\pm}(\omega) = \{\omega_{\lambda V}\} \qquad \text{and} \qquad \lim_{\lambda \to 0} \|\omega_{\lambda V} - \omega\| = 0.$$

Assume that (E) and (S) hold, then $\omega_{\lambda V}^{+} = \omega_{\lambda V}^{-}$ and it follows from Eq. (13) and the dominated convergence theorem that

$$\int_{-\infty}^{\infty} \omega([V, \tau^{t}(A)])\, dt = 0. \tag{14}$$

This is the famous stability criterion of ref. 30. It is a well-known result of Haag and Trych-Pohlmeyer,[31] and of Bratteli *et al.*[29] that (14) together with (E) implies that ω is a KMS state. More precisely,

Theorem 3.4. Assume that ω is a factor state and that assumption (E) holds. Then (S) holds if and only if ω is a (τ, β)-KMS state for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

An example of C^*-dynamical system satisfying condition (E) is the even subalgebra $(\mathcal{O}_{\mathrm{e}}, \tau)$ of a free Fermi gas introduced in Section 2.3.2. Let $\mathcal{O}_0$ be the $*$-subalgebra of $\mathcal{O}_{\mathrm{e}}$ consisting of finite sum of monomials

$$a^{\#}(f_1) \cdots a^{\#}(f_{2n}), \tag{15}$$

such that for all i, j,

$$(f_i, \mathrm{e}^{-ith} f_j) \in L^1(\mathbb{R}). \tag{16}$$

Then condition (12) holds for any $A \in \mathcal{O}_0$, any self-adjoint $V \in \mathcal{O}_0$ and any $\lambda \in \mathbb{R}$. Moreover, the algebra $\mathcal{O}_0$ is norm-dense in $\mathcal{O}_\mathrm{e}$ iff h has purely absolutely continuous spectrum (see ref. 33 for details).

The stability of thermal equilibrium can also be understood in spectral terms. Consider a quantum dynamical system $(\mathcal{O}, \tau, \omega)$, and assume that the τ-invariant state ω is modular. Since $L\Omega_\omega = 0$, zero is an eigenvalue of the standard Liouvillean L of the system. There might be other eigenvectors in $\operatorname{Ker} L$, associated to other ω-normal invariant states. In physical situations of interest, the zero eigenvalue is embedded in the continuous spectrum of L which covers the entire real line. It is a piece of folklore that, unless prevented by some symmetry, this eigenvalue will turn into complex resonances under the influence of a local perturbation V. Therefore, one expects that the standard Liouvillean $L_V = L + V - JVJ$ of the perturbed system $(\mathcal{O}, \tau_V)$ will have purely continuous spectrum and that there will be no τ_V-invariant state in the folium $\mathcal{N}_\omega$. Indeed, by computing the Fermi golden rule for $L_{\lambda V}$, the stability requirement (14) can be seen to be a condition which ensures that zero is an eigenvalue of $L_{\lambda V}$ to second order of perturbation theory. Moreover, the KMS condition Eq. (4) can be interpreted as a form of symmetry which forces L_V to have a zero eigenvalue. To see this, note that since JVJ belongs to the commutant $\mathcal{O}'$, we have

$$\mathrm{e}^{i(L+V)t} JVJ \mathrm{e}^{-i(L+V)t} = \mathrm{e}^{iLt} JVJ \mathrm{e}^{-iLt}.$$

Therefore, using Eq. (4), we can write

$$\begin{aligned} \mathrm{e}^{i(L+V)t}\, L_V\, \mathrm{e}^{-i(L+V)t} \Omega_\omega &= (L + V - \mathrm{e}^{iLt} JVJ \mathrm{e}^{-iLt})\, \Omega_\omega \\ &= V\Omega_\omega - \mathrm{e}^{iLt} JV\Omega_\omega \\ &= (V - \Delta_\omega^{-it/\beta} JV)\, \Omega_\omega. \end{aligned}$$

The analytic continuation of the right hand side of the last identity to $t = -i\beta/2$ further gives

$$(V - \Delta_\omega^{-1/2} JV)\, \Omega_\omega = (V - J\Delta_\omega^{1/2} V)\, \Omega_\omega = (V - V^*)\, \Omega_\omega = 0,$$

from which we conclude that

$$\Omega_V \equiv \mathrm{e}^{-\beta(L+V)/2} \Omega_\omega, \tag{17}$$

must be in the kernel of L_V. In fact, up to normalization, Eq. (17) is nothing but Araki's formula for the vector representative of the (τ_V, β)-KMS state ω_V, see, e.g., refs. 9, 24, and 25.

3.3. The Study of NESS

From the above discussion, it should be clear that the study of local perturbations of a quantum dynamical system $(\mathcal{O}, \tau, \omega)$ depends critically on the nature of the state ω. We can distinguish two cases:

1. If ω is a (τ, β)-KMS state, we are dealing with a system *near thermal equilibrium*. We expect that

$$\lim_{t \to \pm\infty} \eta \circ \tau_V^t(A) = \omega_V(A),$$

for any initial state η in the folium $\mathcal{N}_\omega$ and any $A \in \mathcal{O}$, where ω_V is a (τ_V, β)-KMS state. This ergodic problem can be reduced to the spectral analysis of the standard Liouvillean L_V. Although spectral theory of the standard Liouvillean has been so far understood only for very few systems, the conceptual framework of ergodic theory near thermal equilibrium is well-understood.

2. If ω does not belong to the folium of a (τ, β)-KMS state, the system is *far from equilibrium*. In contrast with the former case, the conceptual framework for the study of NESS is not well-understood. In the remaining part of this subsection, we describe the two approaches that have been adopted so far in the mathematically rigorous literature.

3.3.1. The Scattering Approach

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system and V a local perturbation such that for all A in a norm-dense $*$-subalgebra $\mathcal{O}_0 \subset \mathcal{O}$,

$$\int_{-\infty}^{\infty} \|[V, \tau^t(A)]\| \, dt < \infty, \qquad \int_{-\infty}^{\infty} \|[V, \tau_V^t(A)]\| \, dt < \infty. \tag{18}$$

As in the previous subsection, these conditions ensure that the strong limits

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

exist and define $*$-automorphisms of $\mathcal{O}$. It follows that that $\Sigma_V^{\pm}(\omega) = \{\omega_V^{\pm}\}$ and

$$\omega_V^{\pm} = \omega \circ \alpha_V^{\pm} = \lim_{t \to \pm\infty} \omega \circ \tau_V^t(A).$$

The Møller morphisms $\alpha_V^{\pm}$ induce unitary operators $U_V^{\pm}$ between the GNS spaces $\mathcal{H}_\omega$ and $\mathcal{H}_{\omega_V^{\pm}}$. These operators intertwine the representations $\pi_\omega \circ \alpha_V^{\pm}$ and $\pi_{\omega_V^{\pm}}$ and provide unitary equivalences between the standard Liouvilleans associated to ω and $\omega_V^{\pm}$. Under some additional regularity assumptions one can also show that for suitable $A \in \mathcal{O}$,

$$\omega_V^{\pm}(A) = \omega(A) + \sum_{n \geqslant 1} (\pm i)^n \int_0^\infty dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \, \omega([\tau^{\pm t_n}(V), [\ldots, [\tau^{\pm t_1}(V), A]]]). \tag{19}$$

The expansion (19) can be used for perturbative computations of basic thermodynamic quantities such as entropy production and heat fluxes.

It is important to remark that the assumptions (18) are very difficult to verify in concrete physically interesting models, and so far they have been established only for a few examples. Nevertheless, we believe that the scattering approach is a helpful tool in developing the conceptual understanding of the subject, much in the spirit of the "chaotic hypothesis" used in classical non-equilibrium statistical mechanics (see ref. 34).

An example of a system where (18) holds has been provided by Botvich and Malyshev.[33] Consider a free Fermi gas with one particle Hilbert space $\mathcal{H}$ and one particle energy h. Assume that h has purely absolutely continuous spectrum. Let $\mathcal{O}_0$ consists of finite sums of monomials

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

such that (16) holds. Set $V \equiv \lambda P$, where $P \in \mathcal{O}_0$ is an *even* polynomial. Then (18) holds for sufficiently small $\lambda \in \mathbb{R}$. In this case, each term in the expansion (19) is well-defined, and the series converges absolutely for all $A \in \mathcal{O}_0$.

3.3.2. The Spectral Approach

As already pointed out, the thermodynamically interesting NESS associated to a local perturbation V of the quantum dynamical system $(\mathcal{O}, \tau, \omega)$ are not in the folium $\mathcal{N}_\omega$. Since on the other hand the kernel of L_V, and more generally its eigenvectors, provide information about ω-normal τ_V-invariant states, the thermodynamical content of the spectral theory of L_V is not easily decoded. This explains why, for many years, scattering theory was the only available approach to the study of singular NESS.

Recently, in ref. 2, we have developed a spectral theory of NESS which we describe here in its simplest setting. According to the remark in Section 3, we define NESS using Abelian averaging (8).

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system and V a local perturbation. Assume that ω is a modular state and that the map

$$\mathbb{R} \ni t \mapsto V_t = \mathrm{e}^{it\mathcal{L}_\omega} V \mathrm{e}^{-it\mathcal{L}_\omega} \in \mathfrak{M}_\omega$$

extends to an analytic function (in norm) inside the complex strip $\{0 < \operatorname{Im} z < 1/2\}$, bounded and continuous on its closure (the set of such V is total in $\mathfrak{M}_\omega$). The C-Liouvillean of the locally perturbed system is defined by

$$L_\infty \equiv L + V - JV_{-i/2}J.$$

This operator is closed on $\mathscr{D}(L_\infty) \equiv \mathscr{D}(L)$. Its spectrum is contained in $\{|\operatorname{Im} z| \leqslant \|V_{\pm i/2}\|\}$, and its adjoint is given by

$$L_\infty^* = L + V - JV_{i/2}J.$$

The operators iL_∞ and iL_∞^* generate quasi-bounded strongly continuous groups on $\mathscr{H}_\omega$. By construction $\Omega_\omega \in \operatorname{Ker} L_\infty$, thus

$$\mathrm{e}^{itL_\infty} \Omega_\omega = \Omega_\omega,$$

(see Eq. (2)) and it follows from the Trotter product formula that

$$\tau_V^t(A) = \mathrm{e}^{itL_\infty} A \mathrm{e}^{-itL_\infty} = \mathrm{e}^{itL_\infty^*} A \mathrm{e}^{-itL_\infty^*}. \tag{20}$$

For $\operatorname{Im} z > 0$, we define linear functionals $\omega_z \in \mathcal{O}^*$ by the formula

$$\omega_z(A) \equiv i \int_0^\infty \mathrm{e}^{izt} \omega(\tau_V^t(A))\, dt.$$

Clearly, the map $z \mapsto \omega_z$ is weak-* analytic in the half-plane $\{\operatorname{Im} z > 0\}$. Moreover, for $\operatorname{Im} z > \|V_{\pm i/2}\|$, we have

$$\omega_z(A) = (\Omega_\omega, A(L_\infty^* - z)^{-1}\, \Omega_\omega).$$

This formula and the fact that Abelian NESS $\mu \in \Sigma^{\pm}_{V,\mathrm{Ab}}(\omega)$ are weak-$*$ limit points, as $\epsilon \downarrow 0$, of $(\epsilon/i)\,\omega_{i\epsilon}$ suggests that NESS are described by zero-resonance eigenvectors of L^*_∞. Indeed, it is possible to develop an abstract axiomatic complex deformation technique which allows to directly relate NESS to the zero-resonance eigenvectors of L^*_∞. This method has been used in ref. 2 to study the NESS of a finite quantum system coupled to several fermionic reservoirs at different temperatures. This analysis has led to results which could not be reached by scattering methods. In particular, it allows to obtain precise information on the relaxation to the NESS from the study of complex resonances of the C-Liouvillean. We briefly describe the model and results of ref. 2 in Section 5.3.

The spectral approach to the study of NESS is a recent development which has led to some insights into the general structure of the non-equilibrium quantum statistical mechanics and has been a useful tool in the study of some concrete models. The method is still being developed and its full potential remains to be reached. It should be noticed that this approach to the dynamical properties of quantum dynamical system is closely related to the study of the decay of correlations in classical dynamical systems, and in particular to *Ruelle resonances* of the transfer operator (see, for example, refs. 35–38).

4. ENTROPY PRODUCTION

4.1. Phenomenological Considerations

In non-equilibrium thermodynamics, the local entropy production rate σ is defined as the source term in the local entropy balance equation

$$\partial_t s + \operatorname{div} \mathbf{s} = \sigma,$$

where s is the entropy density and $\mathbf{s}$ the entropy flux. In a stationary state, the total entropy production rate in a subsystem $\mathscr{S}$ is therefore equal to the net entropy flux leaving this subsystem. If $\mathscr{S}$ interacts with independent reservoirs $\mathscr{R}_1, \mathscr{R}_2, \ldots$, which are in thermal equilibrium at inverse temperature $\beta_1, \beta_2, \ldots$, then entropy leaves $\mathscr{S}$ with a rate given by the formula

$$-\sum_k \beta_k \Phi_k,$$

where Φ_k denotes the energy current leaving the reservoir $\mathscr{R}_k$ (see Fig. 2).

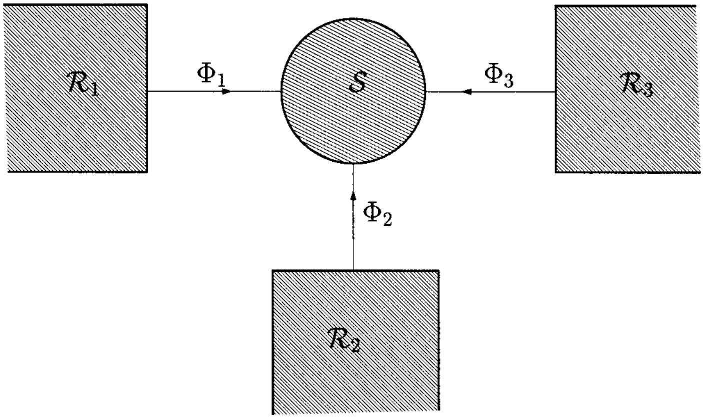

Fig. 2. The energy currents Φ_k.

The Hamiltonian of the combined system $\mathscr{S}+\mathscr{R}_1+\cdots$ is

$$H=H_{\mathscr{S}}+\sum_k H_{\mathscr{R}_k}+V,$$

where V describes the interaction between $\mathscr{S}$ and the reservoirs. The Heisenberg equation for the total energy of the reservoir $\mathscr{R}_k$ leads to the expression $\Phi_k=-i[H, H_{\mathscr{R}_k}]=-i[V, H_{\mathscr{R}_k}]$. To make the connection with the algebraic formulation we note that

$$\Phi_k=\delta_k(V),$$

where $\delta_k\equiv i[H_{\mathscr{R}_k},\ \cdot\ ]$ is the generator of the dynamics of $\mathscr{R}_k$. The entropy production rate in a stationary state μ can now be written as

$$\mathrm{Ep}(\mu)=\mu\left(-\sum_k \beta_k\delta_k(V)\right). \tag{21}$$

Clearly, the argument leading to this formula physically makes sense only in the idealized case where the interaction V is so small that it does not affect the thermal equilibrium states of the reservoirs. In concrete models, strictly speaking this will only be the case if either $V=0$ or $\beta_1=\beta_2=\cdots$. However, if the reservoirs are initially in thermal equilibrium at different temperatures, we do not expect a local perturbation V to be strong enough to induce a global approach to thermal equilibrium in the combined system $\mathscr{S}+\mathscr{R}_1+\cdots$. In such circumstances, provided that the restriction to $\mathscr{R}_k$ of the NESS μ remains sufficiently close to the initial thermal equilibrium, the quantity defined in Eq. (21) should still carry useful information on the thermodynamics of the system.

In fact, as we shall see in the next section, $\mathrm{Ep}(\mu)$ has many of the expected properties of an entropy production. In particular, $\mathrm{Ep}(\mu) \geqslant 0$ for an NESS μ, and the strict positivity of $\mathrm{Ep}(\mu)$ is a sufficient condition for the existence of energy currents. Thus, we consider Eq. (21) as a sufficient motivation for the general definition of entropy production given below. We refer the reader to refs. 5–7 for a more detailed discussion of entropy production in spin systems.

4.2. Definition and Basic Properties

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system. For any state $\eta \in \mathcal{N}_\omega$ we denote by $\mathrm{Ent}(\eta \mid \omega)$ the relative entropy of η with respect to ω. The basic properties of the relative entropy are discussed in the monograph of ref. 13. We recall that $\mathrm{Ent}(\eta \mid \omega) \leqslant 0$ and that for finite quantum systems

$$\mathrm{Ent}(\eta \mid \omega) = \mathrm{Tr}(\eta(\log \omega - \log \eta)). \tag{22}$$

Note also that our notation for the relative entropy differs from the one originally introduced by Araki in refs. 39 and 40 by a sign and the order of its two arguments.

We shall need two assumptions. The first one concerns the state ω:

(A1) There exists a C^*-dynamics σ_ω such that ω is a $(\sigma_\omega, -1)$-KMS state.

Remark 1. The choice of the reference temperature $\beta = -1$ in (A1) is made for mathematical convenience. If (A1) holds, then for any $\beta \neq 0$ there is a C^*-dynamics $\sigma_{\omega, \beta}$ such that ω is $(\sigma_{\omega, \beta}, \beta)$-KMS state (set $\sigma^t_{\omega, \beta} = \sigma_\omega^{-t/\beta}$). Let us also point out that a state satisfying (A1) is modular and that Takesaki's theorem shows that $\sigma^t_\omega(A) = \mathrm{e}^{it\mathcal{L}_\omega} A^{\ -it\mathcal{L}_\omega}$.

Remark 2. A state which can be factorized into a product of KMS states satisfies condition (A1). Indeed, if

$$\omega = \bigotimes_{k=0}^{N} \omega_k, \tag{23}$$

where ω_k is (τ_k, β_k)-KMS, then ω is $(\bigotimes_k \tau_k^{-\beta_k t}, -1)$-KMS. Since this is a common situation in non-equilibrium statistical mechanics, our first hypothesis is quite natural.

Let δ_ω be the generator of σ_ω. Our second assumption is a regularity condition for the local perturbation V:

(A2) $V \in \mathscr{D}(\delta_\omega)$.

Remark 3. To make the connection with the discussion of the previous section and Formula (21), note that for the state (23) we get

$$\delta_\omega = -\sum_k \beta_k \delta_k,$$

where δ_k is the generator of τ_k. Thus, identifying the factor corresponding to $k=0$ with the system $\mathscr{S}$ and the remaining factors with the reservoirs $\mathscr{R}_k$, we can easily reproduce Formula (21) by setting $\beta_0 = 0$.

For a τ-invariant state ω satisfying Hypothesis (A1) and a local perturbation V satisfying (A2), we introduce the observable

$$\sigma_V \equiv \delta_\omega(V) \in \mathcal{O},$$

and define the entropy production of the locally perturbed system $(\mathcal{O}, \tau_V)$ in the stationary state $\eta \in E(\mathcal{O})$, with respect to the reference state ω, as

$$\mathrm{Ep}(\eta) \equiv \eta(\sigma_V).$$

The following theorem is a simple extension of the main result in ref. 1 (see ref. 3 for the proof).

Theorem 4.1. Assume that Hypotheses (A1) and (A2) hold. Then, for any state $\eta \in \mathscr{N}_\omega$ one has

$$\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) = \mathrm{Ent}(\eta \mid \omega) - \int_0^t \eta \circ \tau_V^s(\sigma_V)\, ds, \tag{24}$$

both sides of this equality being either finite or $-\infty$.

The proof of Theorem 4.1 is based on the Araki perturbation theory of KMS states.[24] It is however an instructive elementary exercise to verify relation (24) for finite quantum systems. We use the notation of Example 2.3.1 and set

$$\eta_t \equiv \eta \circ \tau_V^t = \mathrm{e}^{-it(H+V)} \eta\, \mathrm{e}^{it(H+V)}.$$

From Eq. (22) we get

$$\begin{aligned}\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) &= \mathrm{Tr}(\eta_t \log \omega) - \mathrm{Tr}(\eta_t \log \eta_t)\\ &= \mathrm{Tr}(\eta_t \log \omega) - \mathrm{Tr}(\eta \log \eta),\end{aligned}$$

and hence

$$\frac{d}{dt}\,\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) = i\,\mathrm{Tr}([\eta_t, H+V] \log \omega).$$

Since ω is τ-invariant, we have $[\log \omega, H] = 0$ and the cyclicity of the trace leads to

$$\frac{d}{dt}\,\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) = -i\,\mathrm{Tr}(\eta_t\, [\log \omega, V]).$$

Finally, note that $\delta_\omega(V) = i[\log \omega, V]$, from which we conclude

$$\frac{d}{dt}\,\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) = -\mathrm{Tr}(\eta_t\, \delta_\omega(V)) = -\eta \circ \tau_V^t(\delta_\omega(V)).$$

In the rest of this section we describe some basic properties of the entropy production. Let $\mu \in \Sigma_V^+(\omega)$ be such that $\mu(A) = \lim_n \omega^{T_n}(A)$, then one has

$$\lim_n \frac{1}{T_n}\,\mathrm{Ent}(\omega \circ \tau_V^{T_n} \mid \omega) = -\lim_n \frac{1}{T_n} \int_0^{T_n} \omega \circ \tau_V^t(\sigma_V)\, dt = -\mathrm{Ep}(\mu). \qquad (25)$$

The following result follows immediately from this relation.

Theorem 4.2. Assume that Hypotheses (A1) and (A2) hold. Then, any $\mu \in \Sigma_V^+(\omega)$ satisfies

$$\mathrm{Ep}(\mu) \geqslant 0.$$

Remark. Obviously $\mathrm{Ep}(\mu) \leqslant 0$ if $\mu \in \Sigma_V^-(\omega)$. In particular, $\mathrm{Ep}(\mu) = 0$ for any $\mu \in \Sigma_V^+(\omega) \cap \Sigma_V^-(\omega)$.

As displayed by Formula (25), $\mathrm{Ep}(\mu)$ describes the rate at which the relative entropy decreases along the trajectory $\omega \circ \tau_V^t$. The idea of defining entropy production as the asymptotic rate of decrease of some relative entropy was already present in the early works (see refs. 41 and 42), although in the slightly different context of quantum semigroups. For quantum dynamical systems, a similar construction can be found in refs. 43–45, where the positivity of entropy production is also discussed.

The next result shows that this asymptotic behavior, and thus the value of $\mathrm{Ep}(\mu)$, is essentially independent of the choice of the reference state used to compute the relative entropy.

Proposition 4.3. Assume that (A1) holds, then there is a norm-dense set of states $\mathcal{N}'_\omega \subset \mathcal{N}_\omega$ such that, as $t \to \infty$,

$$\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega') = \mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) + \mathrm{O}(1),$$

for any $\omega' \in \mathcal{N}'_\omega$ and any $\eta \in \mathcal{N}_\omega$.

Since we believe that a state $\mu \in \mathcal{N}_\omega$ describes the same thermodynamics as ω, we expect such a state to have vanishing entropy production. This was shown in ref. 1 under the assumption that μ is faithful. The next statement generalizes this result.

Proposition 4.4. Assume that Hypotheses (A1) and (A2) hold. Then, for any τ_V-invariant, ω-normal state μ, one has

$$\mathrm{Ep}(\mu) = 0.$$

Under the assumptions of the above proposition it follows that, for any NESS $\mu \in \Sigma_V^{\pm}(\omega)$, one has

$$\mathrm{Ep}(\mu) = \mu_{\mathrm{s}}(\sigma_V),$$

where μ_{s} denotes the ω-singular part of μ. Thus the singular part of a NESS contains the full information about its entropy production.

The reverse of Proposition 4.4 holds in a slightly weaker form:

Proposition 4.5. Assume that (A1) and the following condition hold,

$$\liminf_{t \to \infty} \mathrm{Ent}(\omega \circ \tau_V^t \mid \omega) > -\infty.$$

Then, one has

$$\Sigma_V^+(\omega) = \Sigma_V^-(\omega) = \{\mu\} \subset \mathcal{N}_\omega.$$

Under some weak ergodicity assumption, we can actually characterize ω-normality of a NESS by the vanishing of its entropy production. This result is an effective way to prove strict positivity of entropy production in some interesting examples, see Section 5.3.

Proposition 4.6. Assume that $\mu \in \Sigma_V^+(\omega)$ satisfies

$$\sup_{T>0} \left| \int_0^T (\omega \circ \tau_V^t(\sigma_V) - \mu(\sigma_V))\, dt \right| < \infty. \tag{26}$$

Then μ is ω-normal if and only if $\mathrm{Ep}(\mu) = 0$.

Finally, we wish to briefly come back to the interpretation of entropy production. For a NESS $\mu \in \Sigma_V^{\pm}(\omega)$, we have seen that $\mathrm{Ep}(\mu)$ describes the divergence rate of the entropy of $\omega \circ \tau_V^t$ relative to a "typical" reference state in $\mathcal{N}_\omega$. However, we do not yet have such an interpretation for an arbitrary τ_V-invariant state $\eta \in E(\mathcal{O})$ (we are grateful to J. L. Lebowitz for raising this question).

Let $\eta \in E(\mathcal{O})$ be an arbitrary state. Since $\mathcal{N}_\omega$ is weak-$*$ dense in $E(\mathcal{O})$, there is a sequence $\eta_n \in \mathcal{N}_\omega$ which converges towards η in the weak-$*$ topology. Moreover, one easily arranges that sequence to satisfy $\mathrm{Ent}(\eta_n \mid \omega) > -\infty$. By Theorem 4.1, the limit

$$\Delta S(\eta, t) \equiv \lim_n \, (\mathrm{Ent}(\eta_n \circ \tau_V^t \mid \omega) - \mathrm{Ent}(\eta_n \mid \omega)), \tag{27}$$

exists, is independent of the choice of the approximating sequence η_n and satisfies

$$\Delta S(\eta, t) = -\int_0^t \eta \circ \tau_V^s(\sigma_V)\, ds.$$

Hence, if η is τ_V-invariant, then $\mathrm{Ep}(\eta)$ is the rate of divergence of the entropy differential ΔS,

$$\Delta S(\eta, t) = -t\, \mathrm{Ep}(\eta).$$

4.3. Stability and Entropy Production

Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system such that $(\mathcal{O}, \tau)$ satisfies Assumption (E) of Section 3.2 for some $*$-subalgebra $\mathcal{O}_0$. It follows that for any self-adjoint $V \in \mathcal{O}_0$ and $|\lambda| < \lambda_V$, one has $\Sigma_{\lambda V}^{\pm}(\omega) = \{\omega_{\lambda V}^{\pm}\}$. Assume that ω satisfies Hypothesis (A1) and that (A2) holds for all self-adjoint $V \in \mathcal{O}_0$. Finally suppose that the following assumption also holds:

(A3) For all self-adjoint $V \in \mathcal{O}_0$

$$\sup_{|\lambda|<\lambda_V,\, t>0} \left| \int_0^t (\omega \circ \tau_{\lambda V}^s(\sigma_V) - \omega_{\lambda V}^+(\sigma_V))\, ds \right| < \infty.$$

By Theorem 4.1, if $\mathrm{Ep}(\omega_{\lambda V}^+) = 0$ the assumptions of Proposition 4.5 hold and therefore

$$\omega_{\lambda V}^+ = \omega_{\lambda V}^- \in \mathcal{N}_\omega.$$

Moreover, the well-known entropic inequality

$$\|\omega_{\lambda V}^+ - \omega\|^2 \leqslant -2\, \mathrm{Ent}(\omega_{\lambda V}^+ \mid \omega),$$

together with the upper semi-continuity of the relative entropy, yields the estimate

$$\|\omega_{\lambda V}^+ - \omega\|^2 = \mathrm{O}(\lambda).$$

Thus the stability assumption (S) is satisfied and, provided ω is a factor state, Theorem 3.4 yields that ω is a (τ, β)-KMS state for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

Hence, under sufficient regularity assumptions, ω is a KMS state if and only if the entropy production vanishes for sufficiently many local perturbations V. More precisely:

Theorem 4.7. Let $(\mathcal{O}, \tau, \omega)$ be a quantum dynamical system where ω is a factor state satisfying (A1). Assume that (E) holds and that (A2) holds for all self-adjoint $V \in \mathcal{O}_0$. Finally assume that (A3) holds. Under these hypotheses, ω is a (τ, β)-KMS state for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$ if and only if $\mathrm{Ep}(\mu) = 0$ for all $\mu \in \Sigma_{\lambda V}^+(\omega)$, all local perturbations $V \in \mathcal{O}_0$ and all sufficiently small $\lambda \in \mathbb{R}$.

Examples where all conditions of Theorem 4.7 are satisfied can be constructed using the even subalgebra of a free Fermi gas. We omit the details.

4.4. Time-Dependent Perturbations

In this section we consider time-dependent local perturbations of a quantum dynamical system $(\mathcal{O}, \tau, \omega)$. The response of the system to such perturbations will shed an additional light on the notion of entropy production.

The entropy production for time-dependent perturbations of C^*-dynamical systems have been previously studied in refs. 43–45. Some of the basic formulas of this section seem to be known for a long time (see Remark on p. 281 in ref. 46).

A time-dependent local perturbation is specified by a norm-continuous, self-adjoint, $\mathcal{O}$ valued function $V(t)$ on $\mathbb{R}$. The perturbed time evolution is a family of norm-continuous automorphisms of $\mathcal{O}$ given by the formula

$$\tau_V^t(A) \equiv \tau^t(A) + \sum_{n \geqslant 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \, [\tau^{t_n}(V(t_n)), [\dots, [\tau^{t_1}(V(t_1)), \tau^t(A)]]].$$

Note that in general τ_V^t is not a group.

The usual *interaction representation* of this time evolution is given by

$$\tau_V^t(A) = \Gamma_V^t \tau^t(A) \, \Gamma_V^{t*}, \tag{28}$$

where Γ_V^t is the unitary element of $\mathcal{O}$ satisfying the differential equation

$$\frac{d}{dt} \Gamma_V^t = i \Gamma_V^t \tau^t(V(t)), \tag{29}$$

with the initial condition $\Gamma_V^0 = \mathbf{1}$.

Throughout this section, we assume that the state ω satisfies (A1) and that $V(t)$ satisfies (A2) for all t. Moreover, the maps $t \mapsto V(t)$ and $t \mapsto \delta_\omega(V(t))$ are assumed to be respectively $C^1(\mathbb{R}, \mathcal{O})$ and $C(\mathbb{R}, \mathcal{O})$. We set

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

and for any state $\eta \in E(\mathcal{O})$, we define the rate of entropy production by

$$\mathrm{Ep}(\eta, t) \equiv \eta(\sigma_V(t)). \tag{30}$$

The analog of the Theorem 4.1 is the following result.

Theorem 4.8. For any state $\eta \in \mathcal{N}_\omega$, such that $\mathrm{Ent}(\eta \mid \omega) > -\infty$, one has

$$\mathrm{Ent}(\eta \circ \tau_V^t \mid \omega) - \mathrm{Ent}(\eta \mid \omega) = -\int_0^t \eta \circ \tau_V^s(\sigma_V(s)) \, ds = -i\eta(\Gamma_V^t \delta_\omega(\Gamma_V^{t*})). \tag{31}$$

Its proof follows closely the proof of Theorem 4.1. Time-dependent local perturbations allow us to discuss some physical aspects of entropy production which could not be discussed within the framework of Section 4.2. The most interesting of those aspects involves the relation between entropy production and Carnot's version of the second law of thermodynamics.

Assume that the system $(\mathcal{O}, \tau, \omega)$ is initially in thermal equilibrium —this means that ω is a (τ, β)-KMS state, where $\beta > 0$ is the inverse temperature. The KMS condition implies that $\delta_\omega = -\beta\delta$. Assume also that $V(t)$ vanishes outside of the interval $[0, T]$. Relation (31) yields that

$$\mathrm{Ent}(\omega \circ \tau_V^T \mid \omega) = i\beta\omega(\Gamma_V^T \delta(\Gamma_V^{T*})). \tag{32}$$

On the other hand, the quantity $W \equiv -i\omega(\Gamma_V^T \delta(\Gamma_V^{T*}))$ is precisely the work done on the system by the time-dependent force V. Let us briefly elaborate this well-known point (see Section V.3.3 in ref. 10 and Appendix to Section IV.5 in ref. 11). Assume that our system is finite, that is, that $\mathcal{O}$ is a finite dimensional algebra. Denote by H the Hamiltonian of the unperturbed system, so that $\delta(\cdot) = i[H, \cdot]$. The Hamiltonian of the perturbed system is $H(t) = H + V(t)$, and its energy at time t is

$$e(t) = \omega(\tau_V^t(H(t)).$$

Since $H(T) = H$, the total amount of work done on the system is given by

$$\begin{aligned} W = e(T) - e(0) &= \omega(\tau_V^T(H)) - \omega(H) \\ &= -\int_0^T \omega \circ \tau_V^t(\delta(V(t)))\, dt \\ &= -i\omega(\Gamma_V^T \delta(\Gamma_V^{T*})), \end{aligned} \tag{33}$$

where the last relation is easily derived with the help of (29) and (28). For infinite systems, the total energy is infinite and H is not well-defined. However, the work W remains a well-defined quantity given by one of the two last formulas in (33). In particular, Eq. (33) yields the following expression for the instantaneous power dissipated into the system:

$$\Phi_V(t) \equiv -\omega \circ \tau_V^t(\delta(V(t))).$$

Equation (32) is the integrated form of the relation

$$\mathrm{Ep}(\omega \circ \tau_V^t, t) = \beta\Phi_V(t). \tag{34}$$

Obviously, (32) and (34) are expressions of the thermodynamical relation $dS = \beta\, dQ$.

We further remark that since the relative entropy is always non-positive and $\beta > 0$, (32) implies that the energy W transfered by the external perturbations is always non-negative—this is Carnot's version of the second law of thermodynamics which says that one cannot extract work from a system in thermal equilibrium. With regard to the usual discussion of passivity, energy transfer and the second law of thermodynamics (see refs. 9–12), we emphasize the relation of these notions with entropy production.

Consider now two independent systems $(\mathcal{O}_k, \tau_k, \omega_k)$, each of which is in thermal equilibrium at inverse temperature β_k (ω_k is a (τ_k, β_k)-KMS state). We set

$$\mathcal{O} = \mathcal{O}_1 \otimes \mathcal{O}_2, \qquad \tau = \tau_1 \otimes \tau_2, \qquad \omega = \omega_1 \otimes \omega_2,$$

and denote by δ_k the generator of τ_k. The generator of τ is given by $\delta = \delta_1 + \delta_2$. As already noticed, Assumption (A1) holds and $\delta_\omega = -(\beta_1\delta_1 + \beta_2\delta_2)$. Let $V(t)$ be a time-dependent local perturbation of $(\mathcal{O}, \tau, \omega)$, vanishing outside of the time interval $[0, T]$, and establishing a temporary link between the two subsystems. In accordance with the above discussion, the total work done by the external perturbation is

$$W = -i\omega(\Gamma_V^T \delta(\Gamma_V^{T^*})).$$

Obviously, $W = W_1 + W_2$, where

$$W_k = -i\omega(\Gamma_V^T \delta_k(\Gamma_V^{T^*})),$$

is interpreted as the work done on the kth subsystem. As in the previous example, it follows from Theorem 4.8 that

$$\beta_1 W_1 + \beta_2 W_2 = -\mathrm{Ent}(\omega \circ \tau_V^T \mid \omega). \tag{35}$$

Relation (35) has an interesting consequence.[46] If $T_k \equiv \beta_k^{-1}$ denotes the temperature of the kth subsystem and $T_1 > T_2$, then ω is not a thermal equilibrium state, and in principle it is possible to have $W_1 < 0$, which means that the first system produces a positive amount of work during a cyclic process. Since the relative entropy is non-positive, we get from (35) that $W < 0$ and

$$\frac{W}{W_1} \leqslant \frac{T_1 - T_2}{T_1}.$$

This is the well-known Carnot's formula which states that the efficiency of a heat engine is limited by $(T_1 - T_2)/T_1$, where T_1 is the temperature of the heat source and T_2 the temperature of the heat sink (compare with remark on p. 216 of refs. 9 and 46).

A deep result of Pusz and Woronowicz[46] asserts that (under a mild additional regularity condition and assuming $T_1 > T_2$) there exist perturbations $V(t)$ satisfying all our conditions and such that $W_1 < 0$ (see also Theorem 5.4.28 in ref. 46). It suffices, for example, that the systems $(\mathcal{O}_k, \tau_k, \omega_k)$ have the property of return to equilibrium.

5. THERMODYNAMICS OF FINITE QUANTUM SYSTEMS COUPLED TO THERMAL RESERVOIRS

In this section we consider a more specific class of models where a finite quantum system $\mathcal{S}$ interacts with several extended reservoirs $\mathcal{R}_k$ which are at thermal equilibrium at different inverse temperatures β_k. This class of models is a basic paradigm of non-equilibrium quantum statistical mechanics.[2, 4, 42] The classical statistical mechanics of such systems has been developed in refs. 47–49.

We define these models and describe their basic properties in Section 5.1. The general features of the scattering approach and spectral analysis of these models are described in Section 5.2. Finally, in Section 5.3, we discuss a concrete example.

5.1. The Model

The system $\mathcal{S}$ is a finite quantum system, as described in Section 2.3.1. We denote its Hilbert space by $\mathcal{H}_{\mathcal{S}}$ and its Hamiltonian by $H_{\mathcal{S}}$. The corresponding C^*-dynamical system is $(\mathcal{O}_{\mathcal{S}}, \tau_{\mathcal{S}})$ and we denote its $(\tau_{\mathcal{S}}, 0)$-KMS state (i.e., the normalized trace on $\mathcal{O}_{\mathcal{S}}$) by $\omega_{\mathcal{S}0}$.

Each reservoir $\mathcal{R}_k$, $k = 1,..., M$, is a quantum dynamical system $(\mathcal{O}_k, \tau_k, \omega_k)$, in thermal equilibrium at inverse temperature β_k. Thus ω_k is a (τ_k, β_k)-KMS state. We denote by δ_k the generator of τ_k.

The combined system $\mathcal{S} + \mathcal{R}_1 + \cdots + \mathcal{R}_M$ is described by the quantum dynamical system $(\mathcal{O}, \tau, \omega)$ where

$$\mathcal{O} \equiv \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_1 \otimes \cdots \otimes \mathcal{O}_M,$$

and the free (i.e., decoupled) dynamics is given by

$$\tau = \tau_{\mathcal{S}} \otimes \tau_1 \otimes \cdots \otimes \tau_M.$$

We are interested in initial states of the form

$$\omega = \omega_{\mathscr{S}} \otimes \omega_1 \otimes \cdots \otimes \omega_M, \tag{36}$$

where $\omega_{\mathscr{S}}$ is a faithful, $\tau_{\mathscr{S}}$-invariant state on $\mathscr{O}_{\mathscr{S}}$. We denote the set of such product states by $\mathscr{N}_{\mathscr{S}}$. If $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ is the GNS-representation associated to $\omega \in \mathscr{N}_{\mathscr{S}}$, then $\mathscr{H}_\omega$ and π_ω do not depend on the choice of ω.

The coupling of the finite system $\mathscr{S}$ with the reservoir $\mathscr{R}_k$ is specified by a self-adjoint element $V_k \in \mathscr{O}_{\mathscr{S}} \otimes \mathscr{O}_k$. Note that V_k is naturally identified with an element of $\mathscr{O}$. We will use such obvious identification without further comment. The complete interaction is given by the local perturbation

$$\lambda V = \lambda \sum_{k=1}^{M} V_k,$$

where λ is a coupling constant. We assume that $V_k \in \mathscr{D}(\delta_k)$ for all k, and therefore $V \in \bigcap_k \mathscr{D}(\delta_k)$. The generator of the locally perturbed dynamics $\tau_{\lambda V}$ is given by

$$\delta_{\lambda V} = \sum_{k=1}^{M} \delta_k + i[H_{\mathscr{S}} + \lambda V, \cdot\,]. \tag{37}$$

The goal is to study the NESS of $(\mathscr{O}, \tau_{\lambda V})$ associated to the initial states $\omega \in \mathscr{N}_{\mathscr{S}}$. As remarked in Section 4.1, the observable describing the heat flux from the $\mathscr{R}_k$ into the system $\mathscr{S}$ is

$$\Phi_k \equiv \lambda \delta_k(V) = \lambda \delta_k(V_k).$$

It follows from Eq. (37) that the heat fluxes satisfy the energy balance relation

$$\sum_{k=1}^{M} \Phi_k = \delta_{\lambda V}(H_{\mathscr{S}} + \lambda V),$$

from which we immediately obtain the following expression of the first law of thermodynamics

Proposition 5.1. For any τ_V-invariant state η, one has

$$\sum_{k=1}^{M} \eta(\Phi_k) = 0.$$

It is also possible to define the heat flux from the kth reservoir into the system $\mathscr{S}$ as the "change of energy" of $\mathscr{S}$ due to the coupling to $\mathscr{R}_k$. We then obtain the observables

$$\tilde{\Phi}_k \equiv \frac{d}{dt} \tau^t_{\lambda V_k}(H_{\mathscr{S}})|_{t=0} = i[\lambda V_k, H_{\mathscr{S}}], \tag{38}$$

which satisfy the energy balance relation

$$\sum_{k=1}^{M} \tilde{\Phi}_k = \delta_{\lambda V}(H_{\mathscr{S}}). \tag{39}$$

The relation with the previously defined heat flux is given by

$$\tilde{\Phi}_k = \Phi_k - \lambda \delta_{\lambda V}(V_k) + i\lambda^2 [V, V_k]. \tag{40}$$

Note that both Φ_k and $\tilde{\Phi}_k$ are $O(\lambda)$, while $\Phi_k - \tilde{\Phi}_k$ is $O(\lambda^2)$, up to a total derivative. From Eqs. (39) and (40) we obtain the following result.

Proposition 5.2. For any τ_V-invariant state η, one has

$$\sum_{k=1}^{M} \eta(\tilde{\Phi}_k) = 0.$$

Moreover, if $[V, V_k] = 0$, then $\eta(\Phi_k) = \eta(\tilde{\Phi}_k)$.

Finally, we relate the heat fluxes to entropy production. For this purpose, it is convenient to choose the reference state

$$\omega_0 = \omega_{\mathscr{S}0} \otimes \omega_1 \otimes \cdots \otimes \omega_M,$$

where $\omega_{\mathscr{S}0}$ is the KMS state of $\mathscr{S}$ at $\beta = 0$. Then we have $\delta_{\omega_0} = -\sum_k \beta_k \delta_k$. One shows that for any $\omega \in \mathscr{N}_{\mathscr{S}}$,

$$\mathrm{Ent}(\omega \circ \tau^t_V \mid \omega) = \mathrm{Ent}(\omega \circ \tau^t_V \mid \omega_0) + O(1),$$

as $t \to \infty$, and the following result is immediate.

Proposition 5.3. Assume that $\omega \in \mathscr{N}_{\mathscr{S}}$, then for any $\mu \in \Sigma^+_V(\omega)$ one has

$$\sum_{k=1}^{M} \beta_k \mu(\Phi_k) = -\mathrm{Ep}(\mu). \tag{41}$$

Formula (41) is the basic thermodynamic relation between heat fluxes and entropy production. In particular, if $\mathrm{Ep}(\mu) > 0$, the NESS μ carries non-vanishing energy currents.

5.2. The Study of NESS

In Section 3.3 we have discussed the scattering and spectral approaches to the study of NESS for general quantum systems. In this subsection we describe features of these methods which are particular to the specific model $\mathcal{S} + \mathcal{R}_1 + \cdots + \mathcal{R}_M$.

5.2.1. The Scattering Approach

The scattering approach described in Section 3.3.1 has to be slightly modified to accommodate for the finite subsystem $\mathcal{S}$. The necessary changes are described in ref. 4. Setting

$$\mathcal{O}_{\mathcal{R}} \equiv \mathcal{O}_1 \otimes \cdots \otimes \mathcal{O}_M,$$

$$\tau_{\mathcal{R}} \equiv \tau_1 \otimes \cdots \otimes \tau_M,$$

$$\omega_{\mathcal{R}} \equiv \omega_{\beta_1} \otimes \cdots \otimes \omega_{\beta_M},$$

the C^*-dynamical system $(\mathcal{O}_{\mathcal{R}}, \tau_{\mathcal{R}})$ describes free non-interacting reservoirs. Assume that there exists norm-dense subalgebras $\mathcal{O}_0 \subset \mathcal{O}$ and $\mathcal{O}_{\mathcal{R}0} \subset \mathcal{O}_{\mathcal{R}}$ such that, for $A \in \mathcal{O}_0$ and $A_{\mathcal{R}} \in \mathcal{O}_{\mathcal{R}0}$,

$$\int_{-\infty}^{\infty} \|[V, \tau^t(\mathbf{1}_{\mathcal{S}} \otimes A_{\mathcal{R}})]\| \, dt < \infty, \qquad \int_{-\infty}^{\infty} \|[V, \tau_V^t(A)]\| \, dt < \infty. \tag{42}$$

The first condition ensures that the limits

$$\gamma_V^{\pm}(A_{\mathcal{R}}) \equiv \lim_{t \to \pm\infty} \tau_V^{-t} \circ \tau^t(\mathbf{1}_{\mathcal{S}} \otimes A_{\mathcal{R}}),$$

exist in norm and define $*$-morphisms $\gamma_V^{\pm}: \mathcal{O}_{\mathcal{R}} \to \mathcal{O}$. The second condition ensures that the strong limits

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

exist and define $*$-morphisms $\alpha_V^{\pm}: \mathcal{O} \to \mathcal{O}$. One shows that for $A \in \mathcal{O}$,

$$\alpha_V^{\pm}(A) = \mathbf{1}_{\mathcal{S}} \otimes \alpha_{V\mathcal{R}}^{\pm}(A),$$

where $\alpha^{\pm}_{V\mathscr{R}} = (\gamma^{\pm}_{V})^{-1}$. Thus $\alpha^{\pm}_{V\mathscr{R}}$ are in fact $*$-isomorphisms. The sets $\Sigma^{\pm}_{V}(\omega)$ consist of single NESS $\omega^{\pm}_{V}$ and

$$\omega^{\pm}_{V} = \omega \circ \alpha^{\pm}_{V} = \omega_{\mathscr{R}} \circ \alpha^{\pm}_{V\mathscr{R}}.$$

Under some additional assumption one can also construct perturbative expansions of $\omega^{\pm}_{V}$ analogous to (19). For details and additional information we refer the reader to ref. 4.

The abstract scattering method is elegant and provides a fairly complete framework for the study of NESS. However, in concrete models, the verification of conditions (42) (or suitable variants of them) is a rather difficult mathematical problem.

There exists a number of interesting, essentially exactly solvable models, for which conditions (42) (or suitable variants of them) can be verified. One such model is the extensively studied XY spin chain.[20, 21] Another one involves a single spin coupled to free fermionic reservoirs.[50] It would be interesting to study the NESS of these models in detail and show that they have strictly positive entropy production.

5.2.2. The Spectral Approach

In this section we take into account the additional structure of the model $\mathscr{S}+\mathscr{R}_1+\cdots+\mathscr{R}_M$ to elaborate the spectral theory of NESS described in Section 3.3.2. Let $(\mathscr{H}_{\mathscr{S}}, \pi_{\mathscr{S}}, \Omega_{\mathscr{S}})$ be the GNS-representation of $\mathcal{O}_{\mathscr{S}}$ associated to the $(\tau_{\mathscr{S}}, 0)$-KMS state $\omega_{\mathscr{S}0}$. The Liouvillean $L_{\mathscr{S}}$ is then given by

$$L_{\mathscr{S}} = H_{\mathscr{S}} \otimes \mathbf{1} - \mathbf{1} \otimes \bar{H}_{\mathscr{S}},$$

and if $\{E_i\}$ is the spectrum of $H_{\mathscr{S}}$, the spectrum of $L_{\mathscr{S}}$ consists of the eigenvalue differences $\{E_i - E_j\}$. In particular, 0 is an eigenvalue whose multiplicity is at least equal to the dimension of $\mathscr{H}_{\mathscr{S}}$. Let $(\mathscr{H}_k, \pi_k, \Omega_k)$ be the GNS-representation of $\mathcal{O}_k$ associated to ω_k and let L_k be the corresponding Liouvillean. We assume that the reservoirs are sufficiently ergodic so that L_k has a simple eigenvalue zero, the rest of its spectrum being purely absolutely continuous and filling the entire real line. The GNS-representation $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ associated to a state $\omega \in \mathcal{N}_{\mathscr{S}}$ is obtained by taking tensor products of the GNS-representations of individual subsystems. In particular,

$$\mathscr{H}_\omega = \mathscr{H}_{\mathscr{S}} \otimes \mathscr{H}_1 \otimes \cdots \otimes \mathscr{H}_M.$$

The corresponding Liouvillean is

$$L = L_{\mathscr{S}} + L_1 + \cdots + L_M.$$

Fig. 3. The spectrum of the Liouvillean L.

The eigenvalues of L coincide with the eigenvalues of $L_{\mathcal{S}}$ and the rest of its spectrum is purely absolutely continuous and covers the real line, see Fig. 3.

The standard Liouvillean for the locally perturbed dynamics $\tau_{\lambda V}$ is

$$L_\lambda = L + \lambda V - \lambda JVJ.$$

If the temperatures of the reservoirs are different, then one expects that for small non-zero λ all the eigenvalues of L turn into resonances and that the spectrum of L_λ is purely absolutely continuous (see Fig. 4). This implies that in non-equilibrium situations there is no ω-normal, τ_V-invariant state. In fact, by Theorem 3.3, any NESS is purely singular. To prove the above spectral results in concrete models one uses either complex deformation techniques or Mourre theory, see ref. 27 for a general description of these methods.

If the temperatures of all the reservoirs are equal, 0 remains an eigenvalue of L_λ with an eigenvector corresponding to the perturbed KMS state $\omega_{\lambda V}$. Apart from this simple eigenvalue, the spectrum of L_λ is expected to be purely absolutely continuous, all the other eigenvalues of L turning into complex resonances, see Fig. 5. This yields that, in thermal equilibrium, the combined system enjoys strong ergodic properties and in particular, has the property of return to equilibrium. See refs. 15 and 27 and the next section for application of this strategy to concrete models.

In the non-equilibrium case the above argument shows that, for small non-zero coupling, there is no normal NESS. To study singular NESS one uses the C-Liouvillean defined by

$$L_{\lambda,\infty} = L + \lambda V - \lambda J \Delta^{\frac{1}{2}} V \Delta^{-\frac{1}{2}} J, \tag{43}$$

where Δ and J are the modular operator and conjugation of the unperturbed system. For sufficiently regular V, the operator $L_{\lambda,\infty}$ is well-defined and closed. It is not self-adjoint and satisfies $L_{\lambda,\infty}\Omega_\omega = 0$. The expected spectral picture is now more delicate. Roughly, there is a Banach space $\mathcal{B}$,

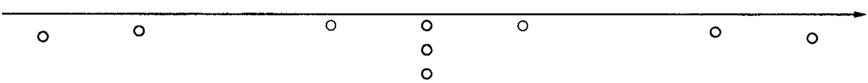

Fig. 4. The spectrum and resonances of L_λ far from equilibrium.

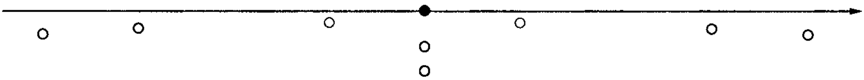

Fig. 5. The spectrum and resonances of L_λ near equilibrium.

densely and continuously embedded in $\mathscr{H}_\omega$, with the following property. For all $\Phi \in \mathscr{B}$, the matrix elements

$$(\Phi, (z - L_{\lambda,\infty})^{-1} \Phi), \tag{44}$$

originally defined for large $\operatorname{Im} z > 0$, have an analytic continuation to the entire half-plane $\operatorname{Im} z > 0$, and a meromorphic continuation across the real axis to a second Riemann sheet. The only singularity on the real axis is a simple pole at 0. The residue at this pole is given by $(\Phi, \Omega_\omega)(\Omega_\lambda, \Phi)$, where $\Omega_\lambda \in \mathscr{B}^*$ is a "resonance eigenvector" of $L^*_{\lambda,\infty}$. For a norm-dense subset $\mathscr{A} \subset \mathscr{O}$ such that $\pi_\omega(\mathscr{A})\, \Omega_\omega \subset \mathscr{B}$, the formula

$$\omega^+_\lambda(A) = (\Omega_\lambda, \pi_\omega(A)\, \Omega_\omega),$$

defines the unique NESS of the perturbed system. Moreover, Ω_λ and hence ω^+_λ will have convergent expansions in powers of λ.

For details and additional information concerning the above heuristic description of spectral theory of NESS we refer the reader to ref. 2. In the next section we describe a non-trivial model to which the above spectral approach can be effectively applied.

5.3. An Example

In this section we consider a concrete model $\mathscr{S} + \mathscr{R}_1 + \cdots + \mathscr{R}_M$, where the reservoirs are identical free Fermi gases. For concreteness, we assume that the Hilbert space of a single fermion (in momentum representation) is $\mathscr{H} = L^2(\mathbb{R}^3, dp)$ and that its Hamiltonian is the operator of multiplication by $\omega(p) = |p|^2/2m$. Denote by $\varphi_k(f) \equiv a_k(f) + a_k^*(f)$ the field operator of $\mathscr{R}_k$. The coupling V_k is given by

$$V_k = Q_k \otimes \varphi_k(\alpha_k),$$

where $\alpha_k \in \mathscr{H}$ is a form-factor and $Q_k = Q_k^* \in \mathscr{O}_{\mathscr{S}}$. The total perturbation is

$$\lambda V = \lambda \sum_k V_k,$$

where λ is a coupling constant.

To our knowledge, the dynamical system $(\mathcal{O}, \tau_{\lambda V})$ was first studied by Davies.[51] Davies investigated the van Hove weak coupling limit $\lambda \downarrow 0$, $t \uparrow \infty$ with $\bar{t} \equiv \lambda^2 t = \mathcal{O}(1)$. This limit yields information in the first non-trivial order of perturbation theory. The paper[51] was followed by a substantial body of literature concerning dynamics of open quantum systems in the van Hove limit (for references and additional information see ref. 52). In particular, the non-equilibrium thermodynamics in the van Hove limit have been studied in detail in ref. 42, while the linear response theory was developed in ref. 53.

The tools to study the dynamical system $(\mathcal{O}, \tau_{\lambda V})$ for finite small λ have been developed only recently. In the case where all the reservoirs have the same temperature, it has been shown in ref. 15 that the system enjoys strong ergodic properties. In fact, the system studied in ref. 15 differs from the one considered here by the bosonic nature of the reservoir. However the techniques extend immediately to the fermionic case (see also refs. 26–28 for additional developments). The non-equilibrium case has been considered in ref. 2, using the spectral approach outlined in the previous section. In the rest of this section, we briefly summarize the results of ref. 2. For reasons of space, we will not specify here all the technical conditions we need—the interested reader may consult ref. 2 for precise statements and additional information.

We need two assumptions on the model. The first one is a non-degeneracy condition which ensures the uniqueness of the NESS.

(ND) The commutant $\{H_{\mathcal{S}}, Q_1,..., Q_M\}'$ in $\mathcal{O}_{\mathcal{S}}$ is trivial, namely consists only of multiples of the identity. Moreover

$$\int_{-\infty}^{\infty} \mathrm{e}^{-it(E_m - E_n)}\, \omega_k(\varphi_k(\alpha_k)\, \tau_k^t(\varphi_k(\alpha_k)))\, dt \neq 0, \tag{45}$$

for $E_m, E_n \in \sigma(H_{\mathcal{S}})$.

Note that if $X \in \{H_{\mathcal{S}}, Q_1,..., Q_M\}'$, then $\tau_V^t(X) = X$. Thus, the non-triviality of the above commutant would lead to an artificial multiplicity of NESS. Relations (45) ensure that the reservoirs induces transitions between eigenstates of the small system.

The second assumption we need is of a more technical nature. It requires the form-factors α_k to be analytic in a suitable sense. This condition allows us to use a complex deformation technique to investigate the analytic structure of the resolvent (44). It is possible that some of the technical developments in refs. 26 and 27 can be used to relax this condition.

Fix an initial state $\omega \in \mathcal{N}_{\mathcal{S}}$ and assume that not all β_k are the same. The main results of ref. 2 are summarized as follows: there exists a constant $\Lambda > 0$ such that, for $0 < |\lambda| < \Lambda$, the following holds:

(1) $\Sigma^+_{\lambda V}(\omega)$ consists of a unique purely singular NESS $\omega^+_{\lambda V}$. Moreover, for all $\eta \in \mathcal{N}_\omega$ and $A \in \mathcal{O}$,

$$\lim_{t\to\infty} \eta \circ \tau^t_{\lambda V}(A) = \omega^+_{\lambda V}(A). \tag{46}$$

(2) The limit (46) is exponentially fast in the following sense. There exist $\gamma(\lambda) > 0$, a norm-dense set of states $\mathcal{N}_0 \subset \mathcal{N}_\omega$ and a norm-dense $*$-subalgebra $\mathcal{O}_0 \subset \mathcal{O}$ such that, for $\eta \in \mathcal{N}_0$ and $A \in \mathcal{O}_0$,

$$|\eta \circ \tau^t_{\lambda V}(A) - \omega^+_{\lambda V}(A)| \leqslant C_{A,\eta,\lambda}\, \mathrm{e}^{-\gamma(\lambda)\, t}. \tag{47}$$

Moreover, $\gamma(\lambda) = \gamma_0 \lambda^2 + \mathcal{O}(\lambda^4)$ as $\lambda \to 0$, where $\gamma_0 > 0$ is a computable constant. In fact, $-\gamma(\lambda)$ is equal to the imaginary part of the non-zero resonance of the operator $L_{\lambda,\infty}$ closest to the real axis.

(3) $\Phi_k, \tilde{\Phi}_k, \sigma_V \equiv \delta_{\omega_0}(V) \in \mathcal{O}_0$. Hence, Proposition 4.6 applies and gives

$$\mathrm{Ep}(\omega^+_{\lambda V}) > 0.$$

(4) There exist operators $K_{\mathcal{S},k}\colon \mathcal{O}_{\mathcal{S}} \to \mathcal{O}_{\mathcal{S}}$, completely determined by the second order perturbation theory (Fermi Golden Rule) of the resonances of $L_{\lambda,\infty}$ and such that $K_{\mathcal{S}} \equiv \sum_k K_{\mathcal{S},k}$ is precisely the generator of the Markovian dynamics in the van Hove limit. Namely, for any $A_{\mathcal{S}} \in \mathcal{O}_{\mathcal{S}}$ and any initial state $\omega = \omega_{\mathcal{S}} \otimes \omega_1 \otimes \cdots \otimes \omega_M \in \mathcal{N}_{\mathcal{S}}$ we have

$$\lim_{\lambda\to 0} \omega \circ \tau^{-\bar{t}/\lambda^2} \circ \tau^{\bar{t}/\lambda^2}_{\lambda V}(A_{\mathcal{S}} \otimes \mathbf{1}_{\mathcal{R}}) = \omega_{\mathcal{S}}(\mathrm{e}^{-\bar{t}K_{\mathcal{S}}} A_{\mathcal{S}}).$$

(5) For $A \in \mathcal{O}_0$, the function $\lambda \mapsto \omega^+_{\lambda V}(A)$ is analytic for $|\lambda| < \Lambda$. More precisely, there exist linear functionals $\omega^+_k\colon \mathcal{O}_0 \to \mathbb{C}$ such that, for $A \in \mathcal{O}_0$,

$$\omega^+_{\lambda V}(A) = \sum_{k\geqslant 0} \lambda^k \omega^+_k(A). \tag{48}$$

The first term ω^+_0 belongs to $\mathcal{N}_{\mathcal{S}}$ and hence has the form

$$\omega^+_0 = \omega_{\mathcal{S},\mathrm{eq}} \otimes \omega_1 \otimes \cdots \otimes \omega_M. \tag{49}$$

The state $\omega_{\mathcal{S},\mathrm{eq}}$ is $\tau_{\mathcal{S}}$-invariant. It is a solution of the equation $K^*_{\mathcal{S}}(\omega_{\mathcal{S},\mathrm{eq}}) = 0$. The non-degeneracy condition (ND) ensures that scalar multiples of the density matrix $\omega_{\mathcal{S},\mathrm{eq}}$ are the only solution of this equation. Although the formulas for the higher order terms in Eq. (48) become quickly very complicated, in principle it is possible to compute all terms of this expansion.

The proofs of (1)–(5) are based on the spectral analysis of the C-Liouvillean $L_{\lambda,\infty}$ and follow the strategy described in Section 3.3.2. The necessary modular structures needed to compute the C-Liouvillean are described in Sections 2.3.1 and 2.3.2. The technical analysis is based on the complex deformation technique previously developed in refs. 15 and 54. Condition (ND) is related to the ergodic properties of the Markovian semigroup e^{-tK_s} (see refs. 52, 55–57).

The results (3)–(5) allow to compute heat fluxes and entropy production perturbatively. Since ω_0^+ is invariant under the unperturbed dynamics, we have $\omega_0^+(\sigma_{\lambda V}) = \omega_0^+(\Phi_k) = 0$. Hence,

$$\mathrm{Ep}(\omega_\lambda^+) = \lambda^2\omega_1^+(\delta_{\omega_0}(V)) + \lambda^3\omega_2^+(\delta_{\omega_0}(V)) + \cdots,$$
$$\omega_\lambda^+(\Phi_k) = \lambda^2\omega_1^+(\delta_k(V)) + \lambda^3\omega_2^+(\delta_k(V)) + \cdots.$$

Of particular importance are the λ^2-contributions (we will call them the Fermi Golden Rule terms). They can be used to give a perturbative proof of the strict positivity of the entropy production, as we will describe below. With

$$\overline{\mathrm{Ep}} = \omega_1^+(\delta_{\omega_0}(V)),$$
$$\bar{\Phi}_k = \omega_1^+(\delta_k(V)),$$

we can write

$$\overline{\mathrm{Ep}} = -\sum_k \beta_k \bar{\Phi}_k.$$

From Eqs. (38) and (40) it easily follows that

$$\bar{\Phi}_k = \omega_{\mathcal{S},\mathrm{eq}}(K_{\mathcal{S},k}(H_{\mathcal{S}})).$$

The operators $K_{\mathcal{S},k}$ can be explicitly computed and a somewhat long computation shows that, as long as the β_k are not all identical, one has

$$\overline{\mathrm{Ep}} > 0.$$

This gives another proof of the strict positivity of the entropy production for small λ, which has the advantage of providing a concrete estimate.

Some of the principles of phenomenological thermodynamics hold for the state $\omega_{\mathscr{S}, \mathrm{eq}}$. Of particular interest are the Onsager reciprocity relations. For the proof of these relations and additional discussion we refer the reader to ref. 42.

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