

On entropy production in quantum statistical mechanics

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Abstract

We propose a definition of entropy production in the framework of algebraic quantum statistical mechanics. We relate our definition to heat flows through the system. We also prove that entropy production is non-negative in natural nonequilibrium steady states.

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1 Introduction

Let (\mathcal{O}, τ) be a C^* -dynamical system, where \mathcal{O} is a C^* -algebra with identity and τ a strongly continuous group of automorphisms of \mathcal{O} (strong continuity means that the map $\mathbf{R} \ni t \mapsto \tau^t(A)$ is continuous in norm for each $A \in \mathcal{O}$). The elements of \mathcal{O} describe observables of the physical system under consideration. The group τ specifies their time evolution. A physical state of the system is described by a mathematical state on \mathcal{O} , that is, a positive linear functional ω such that $\omega(\mathbf{1}) = 1$. The set $E(\mathcal{O})$ of all states on \mathcal{O} is a convex, weak- $*$ compact subset of the dual \mathcal{O}^* . A state ω is invariant under the group τ if $\omega \circ \tau^t = \omega$ for all t . For our purposes we assume that in addition to (\mathcal{O}, τ) we are given a τ -invariant state ω .

The triple $(\mathcal{O}, \tau, \omega)$ describes a physical system in a steady state. We are interested in effects of local perturbations on such system. A local perturbation is specified by a self-adjoint element V of \mathcal{O} and in what follows we fix such a V . The perturbed time evolution is given by

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

The pair (\mathcal{O}, τ_V) is also a C^* -dynamical system. Following Ruelle [Ru2], we call the weak- $*$ limit points of the set

$$\left\{ \frac{1}{T} \int_0^T \omega \circ \tau_V^t dt \mid T > 0 \right\} \subset E(\mathcal{O}),$$

nonequilibrium steady states (NESS) of the locally perturbed system. The set $\Sigma_V^+(\omega)$ of NESS of (\mathcal{O}, τ_V) is a non-empty, compact subset of $E(\mathcal{O})$ whose elements are τ_V -invariant.

Our first assumption is:

(A1) There exists a strongly continuous group σ_ω of automorphisms of \mathcal{O} such that ω is $(\sigma_\omega, -1)$ -KMS state.

Let δ_ω be the generator of σ_ω (i.e. $\sigma_\omega^t = e^{t\delta_\omega}$). We denote by $\mathcal{D}(\delta_\omega)$ the domain of δ_ω . $\mathcal{D}(\delta_\omega)$ is a norm-dense $*$ -subalgebra of \mathcal{O} and for $A, B \in \mathcal{D}(\delta_\omega)$,

$$\delta_\omega(A)^* = \delta_\omega(A^*), \quad \delta_\omega(AB) = \delta_\omega(A)B + A\delta_\omega(B).$$

Our second assumption is:

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

We define the observable

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

and for reasons which will soon become clear, we call

$$\text{Ep}_V(\eta) \equiv \eta(\sigma_V),$$

the entropy production (with respect to the reference state ω) of the perturbed system (\mathcal{O}, τ_V) in the state $\eta \in E(\mathcal{O})$. Note that σ_V , and hence $\text{Ep}_V(\cdot)$, depend in a non-trivial way on the state ω .

Let $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ be the GNS representation of the algebra \mathcal{O} associated to ω , and let \mathcal{N}_ω be the set of π_ω -normal states on \mathcal{O} , that is, the states represented by density matrices on \mathcal{H}_ω . Any $\eta \in \mathcal{N}_\omega$ has a continuous extension to $\mathfrak{M} \equiv \pi_\omega(\mathcal{O})''$ which we denote by the same letter. For $\eta, \xi \in \mathcal{N}_\omega$, we denote by $\text{Ent}(\eta | \xi)$ the relative entropy of η with respect to ξ . (We use the definition of relative entropy given in [BR2], Definition 6.2.29. This definition differs by a sign and the order of factors from the original Araki's definition [Ar].)

Our main result, which justifies the above definition of entropy production, is:

Theorem 1.1 *Assume that (A1) and (A2) hold. Then, for any faithful state $\eta \in \mathcal{N}_\omega$ such that $\text{Ent}(\eta | \omega) > -\infty$, one has*

$$\text{Ent}(\eta \circ \tau_V^t | \omega) = \text{Ent}(\eta | \omega) - \int_0^t \text{Ep}_V(\eta \circ \tau_V^s) ds.$$

Remark. The same result (with the same proof) holds for W^* -dynamical systems.

In the rest of this section we will discuss some elementary properties of $\text{Ep}_V(\cdot)$. Let $\omega_V^+ \in \Sigma_V^+(\omega)$ and $T_n \rightarrow \infty$ be such that

$$\lim_n \frac{1}{T_n} \int_0^{T_n} \omega \circ \tau_V^t dt = \omega_V^+. \quad (1.1)$$

Then, with the particular choice $\eta = \omega$, Theorem 1.1 gives

$$\lim_n \frac{1}{T_n} \text{Ent}(\omega \circ \tau_V^{T_n} | \omega) = - \lim_n \frac{1}{T_n} \int_0^{T_n} \omega(\tau_V^s(\sigma_V)) ds = -\text{Ep}_V(\omega_V^+). \quad (1.2)$$

Since the relative entropy is non-positive, we immediately get

Theorem 1.2 *Assume that (A1) and (A2) hold. Then, for any NESS $\omega_V^+ \in \Sigma_V^+(\omega)$, one has*

$$\text{Ep}_V(\omega_V^+) \geq 0.$$

With regard to (1.2), on physical grounds one expects that the ratio

$$\text{Ent}(\eta \circ \tau_V^t | \omega) / t$$

becomes independent of the choice of the reference state ω as $t \rightarrow \infty$. More precisely, the following result holds:

Proposition 1.3 *Assume (A1) and that $\eta \in \mathcal{N}_\omega$ is faithful. Then there is a norm-dense set $\mathcal{N}'_\omega \subset \mathcal{N}_\omega$ such that for $\omega' \in \mathcal{N}'_\omega$,*

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

as $t \rightarrow \infty$.

One also expects that in thermal equilibrium the entropy production is zero, that is, if $\eta \in \mathcal{N}_\omega$ is a (τ_V, β) -KMS state then $\text{Ep}_V(\eta) = 0$. In fact, a much stronger result holds.

Proposition 1.4 *Assume (A1), (A2) and that $\eta \in \mathcal{N}_\omega$ is a faithful, τ_V -invariant state. Then*

$$\text{Ep}_V(\eta) = 0.$$

Remark. Again, this result also holds for W^* -dynamical systems.

Let \mathcal{O} be the CAR algebra over $l^2(\mathbf{Z}^3)$ describing a free Fermi gas on the lattice \mathbf{Z}^3 . Using some technical results proven in [BM] it is easy to construct a large class of quasi-free states ω and local perturbations V such that (A1)-(A2) hold, and that $\Sigma_V^+(\omega)$ consists of a single state ω_V^+ . In these examples, $\text{Ep}_V(\omega_V^+)$ can be computed perturbatively (similar calculations are done in [HTP]), and one easily constructs examples where $\text{Ep}_V(\omega_V^+) > 0$.

In the next example we relate entropy production to heat flows.

Consider two independent systems $(\mathcal{O}_i, \tau_i, \omega_i)$, $i = 1, 2$, each of which is in thermal equilibrium at temperature T_i . This means that ω_i is a (τ_i, β_i) -KMS state on \mathcal{O}_i where $\beta_i = 1/T_i$. Let

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

(\otimes is the C^* -tensor product, see Section 2.7.2 in [BR1]). Let δ be the generator of τ and δ_i the generator of τ_i . Obviously, $\delta = \delta_1 + \delta_2$ (here we write δ_1 for $\delta_1 \otimes \mathbf{1}$, etc). Let $V \in \mathcal{O}$ be such that $V \in \mathcal{D}(\delta_i)$. Then

$$\omega \circ \tau_V^t(V) - \omega(V) = \int_0^t \omega \circ \tau_V^s(\Phi) ds,$$

where Φ is defined by

$$\tau_V^t(\Phi) = \frac{d}{dt} \tau_V^t(V).$$

Obviously, $\Phi = \Phi_1 + \Phi_2$ where $\Phi_i \equiv \delta_i(V)$ describes the energy flux out of the i -th system. Since the states ω_i are KMS, (A1) holds with $\delta_\omega = \delta_{\omega_1} + \delta_{\omega_2}$ and $\delta_{\omega_i} = -\beta_i \delta_i$. Therefore, (A1) and (A2) hold and

$$\beta_1 \Phi_1 + \beta_2 \Phi_2 = -\sigma_V.$$

It follows that in a NESS $\omega_V^+ \in \Sigma_V^+(\omega)$, the energy fluxes satisfy

$$\frac{\omega_V^+(\Phi_1)}{T_1} + \frac{\omega_V^+(\Phi_2)}{T_2} = -\text{Ep}_V(\omega_V^+) \leq 0.$$

Since $\omega_V^+(\Phi_1) + \omega_V^+(\Phi_2) = 0$, if $T_1 > T_2$, then $\Phi_1 \geq 0$ and the heat flows from the hot to the cold reservoir. This calculation is easily generalized to the case where N -level quantum system is coupled to several independent thermal reservoirs.

We finish this section with the following remarks.

In [JP1] we prove an analog of Theorem 1.1 for time-dependent perturbations and discuss the relation between entropy production and the second law of thermodynamics.

In the forthcoming paper [JP2], we will study NESS, entropy production and heat flows for a model of an N -level quantum system coupled to several independent free Fermi gas reservoirs (similar models have been studied in [D, Ru1]).

The entropy production for quantum spin systems has been studied in the recent preprint [Ru2].

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2 Proofs

We assume that the reader is familiar with the basic results of Tomita-Takesaki modular theory as discussed, for example, in [BR1, BR2, H, OP]. We begin by setting the notation and recalling some well-known facts.

$(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ denotes the GNS representation of the algebra \mathcal{O} associated to ω . By (A1), the vector Ω_ω is cyclic and separating for $\mathfrak{M} \equiv \pi_\omega(\mathcal{O})''$. Moreover, (A1) implies that π_ω is injective. We respectively denote by Δ_ω , J and \mathcal{P} the modular operator, the modular conjugation and the natural cone canonically associated to the pair $(\mathfrak{M}, \Omega_\omega)$. We also adopt the shorthands $\mathcal{L}_\omega = \log \Delta_\omega$ and $j(A) = JAJ$. Note that

$$\pi_\omega(\sigma_\omega^t(A)) = e^{it\mathcal{L}_\omega} \pi_\omega(A) e^{-it\mathcal{L}_\omega}.$$

With a slight abuse of notation, we write $\sigma_\omega^t(A) = e^{it\mathcal{L}_\omega} A e^{-it\mathcal{L}_\omega}$ for $A \in \mathfrak{M}$. By the Tomita-Takesaki theorem, $\sigma_\omega^t(\mathfrak{M}) = \mathfrak{M}$, $j(\mathfrak{M}) = \mathfrak{M}'$ and

$$e^{it\mathcal{L}_\omega} J = J e^{it\mathcal{L}_\omega}. \quad (2.3)$$

The Liouvillean L of the system $(\mathcal{O}, \tau, \omega)$ is the unique self-adjoint operator on \mathcal{H}_ω such that

$$\pi_\omega(\tau^t(A)) = e^{itL} \pi_\omega(A) e^{-itL}, \quad (2.4)$$

$$L\Omega_\omega = 0,$$

and one easily shows that

$$\begin{aligned} e^{itL} \mathcal{L}_\omega &= \mathcal{L}_\omega e^{itL} \\ e^{itL} J &= J e^{itL}. \end{aligned} \quad (2.5)$$

The self-adjoint operator

$$L_V \equiv L + \pi_\omega(V) - j(\pi_\omega(V)),$$

is uniquely specified by the following two requirements:

$$\begin{aligned} \pi_\omega(\tau_V^t(A)) &= e^{itL_V} \pi_\omega(A) e^{-itL_V} \\ e^{-itL_V} \mathcal{P} &\subset \mathcal{P}. \end{aligned} \quad (2.6)$$

The dynamical groups τ and τ_V have natural extensions to \mathfrak{M} for which we use the same notation. Note also that $JL_V + L_V J = 0$, and therefore

$$e^{itL_V} J = J e^{itL_V}. \quad (2.7)$$

A state $\eta \in \mathcal{N}_\omega$ has a unique vector representative $\Omega_\eta \in \mathcal{P}$. Relations (2.6) yield that

$$\Omega_{\eta \circ \tau_V^t} = e^{-itL_V} \Omega_\eta. \quad (2.8)$$

The relative entropy of two faithful states $\eta, \xi \in \mathcal{N}_\omega$ is defined as

$$\text{Ent}(\eta | \xi) \equiv (\Omega_\eta | \log \Delta_{\xi|\eta} \Omega_\eta),$$

where $\Delta_{\xi|\eta}$ is the relative modular operator. Relative entropy is more conveniently expressed in terms of the Radon-Nikodym cocycle $[D\xi : D\eta]^s$ as

$$\text{Ent}(\eta | \xi) = \lim_{s \downarrow 0} \frac{\eta([D\xi : D\eta]^s - \mathbf{1})}{is}. \quad (2.9)$$

Proof of Theorem 1.1. Let us denote by

$$U(t) \equiv e^{-itL} e^{it(L + \pi_\omega(V))},$$

the propagator in the interaction representation. $U(t)$ is the unique solution of

$$\frac{1}{i} \frac{d}{dt} U(t) = \pi_\omega(\tau^{-t}(V)) U(t),$$

with initial data $U(0) = \mathbf{1}$. It has a norm convergent Dyson expansion

$$U(t) = \mathbf{1} + \sum_{n=1}^{\infty} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \pi_\omega(\tau^{-t_1}(V)) \cdots \pi_\omega(\tau^{-t_n}(V)),$$

from which we conclude that $U(t) \in \pi_\omega(\mathcal{O})$. With a slight abuse of notation, we will write δ_ω for $\pi_\omega \circ \delta_\omega$. A simple calculation shows that $U(t) \in \mathcal{D}(\delta_\omega)$ and

$$U^*(t) \delta_\omega(U(t)) = -\delta_\omega(U^*(t)) U(t) = i \int_0^t \pi_\omega(\tau_V^{-s}(\sigma_V)) ds. \quad (2.10)$$

We claim that

$$e^{-itL}e^{itL_V} = U(t)j(U(t)). \quad (2.11)$$

To prove this fact, note that after differentiation with respect to t both sides satisfy the same differential equation with the same initial condition at $t = 0$.

To compute the relative entropy $\text{Ent}(\eta \circ \tau_V^t | \omega)$, we will use Equation (2.9) and the fact that the Radon-Nikodym cocycle can be expressed as

$$[D\omega : D\eta \circ \tau_V^t]^s = \Delta_{\omega|\omega \circ \tau_V^t}^{\text{is}} \Delta_{\eta \circ \tau_V^t|\omega \circ \tau_V^t}^{-\text{is}}. \quad (2.12)$$

By definition of the relative modular operator, for any $A \in \mathfrak{M}$ we have

$$J\Delta_{\eta \circ \tau_V^t|\omega \circ \tau_V^t}^{1/2} A\Omega_{\omega \circ \tau_V^t} = A^* \Omega_{\eta \circ \tau_V^t}.$$

Using Relations (2.6) and (2.8), we further obtain

$$J\Delta_{\eta \circ \tau_V^t|\omega \circ \tau_V^t}^{1/2} A e^{-itL_V} \Omega_{\omega} = A^* e^{-itL_V} \Omega_{\eta}.$$

It follows that

$$\begin{aligned} J\Delta_{\eta \circ \tau_V^t|\omega \circ \tau_V^t}^{1/2} e^{-itL_V} \tau_V^t(A)\Omega_{\omega} &= e^{-itL_V} \tau_V^t(A)^* \Omega_{\eta} \\ &= e^{-itL_V} J\Delta_{\eta|\omega}^{1/2} \tau_V^t(A)\Omega_{\omega} \\ &= J e^{-itL_V} \Delta_{\eta|\omega}^{1/2} \tau_V^t(A)\Omega_{\omega}, \end{aligned}$$

where we used (2.7). Since $\mathfrak{M}\Omega_{\omega}$ is a core for $\Delta_{\eta|\omega}^{1/2}$ and $e^{-itL_V} \mathfrak{M}\Omega_{\omega} = \mathfrak{M}\Omega_{\omega \circ \tau_V^t}$ is a core for $\Delta_{\eta \circ \tau_V^t|\omega \circ \tau_V^t}^{1/2}$, we derive the relation

$$\Delta_{\eta \circ \tau_V^t|\omega \circ \tau_V^t} = e^{-itL_V} \Delta_{\eta|\omega} e^{itL_V}. \quad (2.13)$$

We now deal with $\Delta_{\omega|\omega \circ \tau_V^t}$. First, for any $A \in \mathfrak{M}$,

$$J\Delta_{\omega|\omega \circ \tau_V^t}^{1/2} A\Omega_{\omega \circ \tau_V^t} = A^* \Omega_{\omega}.$$

Equations (2.8), (2.11) and (2.4) yield that

$$\Omega_{\omega \circ \tau_V^t} = U^*(t)j(U^*(t))\Omega_{\omega},$$

and since $j(U^*(t)) \in \mathfrak{M}'$, we derive

$$\begin{aligned} J\Delta_{\omega|\omega \circ \tau_V^t}^{1/2} j(U^*(t))AU^*(t)\Omega_{\omega} &= A^* \Omega_{\omega} \\ &= U^*(t)(AU^*(t))^* \Omega_{\omega} \\ &= U^*(t)J\Delta_{\omega}^{1/2} AU^*(t)\Omega_{\omega} \\ &= Jj(U^*(t))\Delta_{\omega}^{1/2} AU^*(t)\Omega_{\omega}. \end{aligned}$$

Since $\mathfrak{M}\Omega_\omega$ is a core of $\Delta_\omega^{1/2}$ and $j(U^*(t))\mathfrak{M}\Omega_\omega = \mathfrak{M}\Omega_{\omega \circ \tau_V^t}$ is a core of $\Delta_{\omega|\omega \circ \tau_V^t}^{1/2}$ we conclude that

$$\Delta_{\omega|\omega \circ \tau_V^t} = j(U^*(t))\Delta_\omega j(U(t)). \quad (2.14)$$

Going back to (2.12), we derive from Equations (2.13) and (2.14)

$$\begin{aligned} [D\omega : D\eta \circ \tau_V^t]^s &= j(U^*(t))\Delta_\omega^{is} j(U(t))e^{-itL_V} \Delta_{\eta|\omega}^{-is} e^{itL_V} \\ &= j(U^*(t))\Delta_\omega^{is} U^*(t)e^{-itL} \Delta_{\eta|\omega}^{-is} e^{itL_V} \\ &= j(U^*(t))\sigma_\omega^s(U^*(t))e^{-itL} \Delta_\omega^{is} \Delta_{\eta|\omega}^{-is} e^{itL_V}, \end{aligned}$$

where we used (2.11) and (2.5). Since $\sigma_\omega^s(U^*(t)) \in \mathfrak{M}$, it commutes with $j(U^*(t))$ and another application of (2.11) (together with Relation (2.12) at $t = 0$) gives

$$[D\omega : D\eta \circ \tau_V^t]^s = \sigma_\omega^s(U^*(t))U(t)\tau_V^{-t}([D\omega : D\eta]^s). \quad (2.15)$$

We can therefore write

$$\eta \circ \tau_V^t([D\omega : D\eta \circ \tau_V^t]^s) = (e^{itL_V} U^*(t)\sigma_\omega^s(U(t))e^{-itL_V} \Omega_\eta, [D\omega : D\eta]^s \Omega_\eta). \quad (2.16)$$

Since $U(t) \in \mathcal{D}(\delta_\omega)$, the estimate

$$e^{itL_V} U^*(t)\sigma_\omega^s(U(t))e^{-itL_V} \Omega_\eta = \Omega_\eta + se^{itL_V} U^*(t)\delta_\omega(U(t))e^{-itL_V} \Omega_\eta + o(s),$$

holds in the norm of \mathcal{H}_ω as $s \downarrow 0$. Furthermore, Equation (2.10) is easily rewritten as

$$e^{itL_V} U^*(t)\delta_\omega(U(t))e^{-itL_V} = i \int_0^t \pi_\omega(\tau_V^u(\sigma_V)) du.$$

Equation (2.16) leads to the estimate

$$\begin{aligned} \eta \circ \tau_V^t([D\omega : D\eta \circ \tau_V^t]^s) &= \eta([D\omega : D\eta]^s) \\ &\quad - is \int_0^t (\Omega_\eta, \pi_\omega(\tau_V^u(\sigma_V))[D\omega : D\eta]^s \Omega_\eta) du + o(s), \end{aligned} \quad (2.17)$$

as $s \downarrow 0$. Since the cocycle $[D\omega : D\eta]^s$ is strongly continuous, insertion in Equation (2.9) gives the result. \square

Proof of Proposition 1.3. For any self-adjoint $P \in \mathfrak{M}$ we define a group of automorphisms of \mathfrak{M} by

$$\sigma_P^t(A) = e^{it(\mathcal{L}_\omega + P)} A e^{-it(\mathcal{L}_\omega + P)}.$$

Araki's perturbation theory yields that there is a state $\omega_P \in \mathcal{N}_\omega$ which is a $(\sigma_P, -1)$ -KMS state. Let \mathcal{N}'_ω be the set of all states obtained in this manner. It is well-known that \mathcal{N}'_ω is dense in \mathcal{N}_ω (see, e.g., [R]). By the result of Araki (see Proposition 6.2.32 in [BR2]),

$$\text{Ent}(\eta \circ \tau_V^t | \omega_P) = \text{Ent}(\eta \circ \tau_V^t | \omega) + \eta(\tau_V^t(P)) - \log \|e^{(\mathcal{L}_\omega + P)/2} \Omega_\omega\|^2.$$

The statement follows from this relation, the obvious estimate $|\eta(\tau_V^t(P))| \leq \|P\|$ and the fact that $0 < \|e^{(\mathcal{L}_\omega + P)/2} \Omega_\omega\| < \infty$. \square

Proof of Proposition 1.4. Since $\eta \circ \tau_V^t = \eta$, Relation (2.17) yields that for all $s > 0$,

$$\int_0^t (\Omega_\eta, \pi_\omega(\tau_V^u(\sigma_V)) [D\omega : D\eta]^s \Omega_\eta) du = o(1).$$

Taking $s \downarrow 0$ we get that for all t ,

$$\int_0^t \eta(\sigma_V) du = t\eta(\sigma_V) = 0,$$

and so $\text{Ep}_V(\eta) = 0$. \square

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