Entropy production

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Entropy, as defined by Clausius, is the true cornerstone of equilibrium thermodynamics. Its statistical interpretation by Boltzmann is the key to our microscopic understanding of equilibrium. Since then many other concepts of entropy have appeared in physics and mathematics but none of them has significantly contributed to our understanding of nonequilibrium. However, a notion of entropy production (rate) has emerged from recent developments in classical and quantum statistical mechanics of nonequilibrium steady states. Taking this notion seriously, it does not seems possible to define the entropy of a nonequilibrium steady states [R3]. As argued in [G], if such an entropy exists then it is most likely to take the value $-\infty$ because a system in such a state loses entropy at a constant rate.

The purpose of this article is to introduce the notion of entropy production for nonequilibrium steady states of a small quantum system in contact with thermal reservoirs. We shall make free use of the concepts and notation of [NESS in quantum statistical mechanics].

1 Relative entropy

If ρ, ρ' are density matrices their relative entropy is defined, in analogy with the relative entropy of two probability measures, by

$$\mathrm{Ent}(\rho'|\rho) = \mathrm{tr}(\rho'(\log\rho - \log\rho')).$$

It has been generalized by Araki to arbitrary states on a von Neumann algebra [A1, A2]. To describe the general definition we need to introduce the notion of relative modular operator.

Let $\mathfrak{M}$ be a von Neumann algebra acting on the Hilbert space $\mathcal{H}$ and $\Psi, \Phi \in \mathcal{H}$ two unit vectors. Denote by s_Ψ the support of the state $\psi(A) = (\Psi|A\Psi)$, i.e., the orthogonal projection on the closure of $\mathfrak{M}'\Psi$ (see [Tomita-Takesaki theory]). Since $A, B \in \mathfrak{M}$ and $A\Psi = B\Psi$ implies $As_\Psi = Bs_\Psi$, formula

$$A\Psi \oplus \Omega \mapsto s_\Psi A^*\Phi,$$

defines a closable antilinear operator on the dense subspace $\mathfrak{M}\Psi \oplus (\mathfrak{M}\Psi)^\perp \subset \mathcal{H}$. Denote by $S_{\Phi|\Psi}$ its closure. The self-adjoint operator $\Delta_{\Phi|\Psi} = S^*_{\Phi|\Psi}S_{\Phi|\Psi}$ is called relative modular operator of the pair Φ, Ψ.

Definition 1 *Let ω be a modular state on the C^*-algebra $\mathcal{O}$. Denote by $(\mathcal{H}, \pi, \Psi_\omega)$ the induced GNS representation and by $\mathcal{H}_+$ its natural cone. For any ω-normal state ν on $\mathcal{O}$ let Φ_ν be its unique vector representative in $\mathcal{H}_+$ (Theorem 13 in [Tomita-Takesaki theory]). The entropy of a state ν relative to ω is defined by*

$$\mathrm{Ent}(\nu|\omega) = \begin{cases} (\Psi_\nu|\log\Delta_{\Psi_\omega|\Psi_\nu}\Psi_\nu), & \textit{if } \nu \textit{ is } \omega\textit{-normal},\\ -\infty & \textit{otherwise}.\end{cases}$$

Remark. 1. We have restricted the above definition to modular ω for simplicity. To obtain a completely general definition it suffices to pass to a standard representation of the enveloping von Neumann algebra $\mathcal{O}_\omega$ if $s_\nu \leq s_\omega$ and to set $\mathrm{Ent}(\nu|\omega) = -\infty$ otherwise.

2. We use the notation $\mathrm{Ent}(\,\cdot\,|\,\cdot\,)$ of [BR2], [OP] which differs by sign and ordering of the arguments from the original notation in [A1, A2].

The most important properties of relative entropy for our purposes are

1. $\mathrm{Ent}(\nu|\omega) \leq 0$ with equality if and only if $\nu = \omega$.
2. For any $C \in \mathbb{R}$ the set of states $\{\nu \,|\, \mathrm{Ent}(\nu|\omega) \geq C\}$ is a weak-$*$ compact subset of the folium $\mathcal{N}_\omega$.
3. $\mathrm{Ent}(\nu \circ \tau|\omega \circ \tau) = \mathrm{Ent}(\nu|\omega)$ for any $*$-automorphism τ.

The reader should consult [OP] for a more exhaustive list and detailed discussions.

2 The entropy balance equation

The change in relative entropy due to the action of an inner $*$-automorphism is given by the following result (see [JP1]).

Theorem 2 *Let ω be a modular state on the C^*-algebra $\mathcal{O}$. Denote by δ_ω the infinitesimal generator of its modular group. For any unitary $U \in \mathcal{O}$ set $\tau_U(A) = U^*AU$. Then the following holds*

$$\mathrm{Ent}(\nu \circ \tau_U|\omega) = \mathrm{Ent}(\nu|\omega) - \mathrm{i}\,\nu\left(U^*\delta_\omega(U)\right),$$

for any state ν on $\mathcal{O}$ and any unitary $U \in \mathrm{Dom}(\delta_\omega)$.

Using Property 3 of the relative entropy, a direct application of this theorem to local perturbation of a quantum dynamical system (see section 5 in [Quantum dynamical systems]) yields

Corollary 3 *Let $(\mathcal{O}, \tau)$ be a C^*- or W^*-dynamical system equipped with a modular invariant state ω. Denote by δ_ω the generator of the modular group of ω. For any local perturbation τ_V induced by $V = V^* \in \mathrm{Dom}(\delta_\omega)$ one has*

$$\mathrm{Ent}(\nu \circ \tau_V^t|\omega) = \mathrm{Ent}(\nu|\omega) - \int_0^t \nu \circ \tau_V^s(\delta_\omega(V))\,\mathrm{d}s. \tag{1}$$

Remark. In the case of a time dependent local perturbation $V(t)$ such that $t \mapsto V(t)$ and $t \mapsto \delta_\omega(V(t))$ are continuous in the natural topology of $\mathcal{O}$, Theorem 2 yields

$$\mathrm{Ent}(\nu \circ \tau_V^{s\to t}|\omega) = \mathrm{Ent}(\nu|\omega) - \int_s^t \nu \circ \tau_V^{s\to u}(\delta_\omega(V(u)))\,\mathrm{d}s.$$

To our knowledge, this formula was first obtained in [OHI] for a (τ, β)-KMS state ω. In this special case $\delta_\omega = -\beta\delta$ where δ is the infinitesimal generator of τ.

Assume that $\omega_+ \in \Sigma_+(\tau_V, \omega)$, i.e., that ω_+ is a NESS of the perturbed dynamics (see [NESS in quantum statistical mechanics]). Then there exists a net $t_\alpha \to \infty$ such that

$$\omega_+(A) = \lim_\alpha \frac{1}{t_\alpha} \int_0^{t_\alpha} \omega \circ \tau_V^s(A)\,\mathrm{d}s.$$

The entropy balance formula (1) and property 1 yield

$$0 \leq -\lim_\alpha \frac{\mathrm{Ent}(\omega \circ \tau_V^{t_\alpha}|\omega)}{t_\alpha} = \omega_+(\delta_\omega(V)),$$

from which, given the following definition, the next proposition follows.

Definition 4 *1. We define the entropy production observable of the local perturbation V relative to the reference state ω by $\sigma(\omega, V) = \delta_\omega(V)$.*
2. The entropy production rate of a NESS $\omega_+ \in \Sigma_+(\tau_V, \omega)$ is $\mathrm{Ep}(\omega_+) = \omega_+(\sigma(\omega, V))$.

Proposition 5 *The entropy production rate of a NESS is non-negative.*

For quantum spin systems our definition formally agrees with Ruelle's proposal [R1], [R2]. It is also closely related to the definition of entropy production used in [LS].

3 Thermodynamic interpretation

Let us consider the case of a small system $\mathcal{S}$, with a finite dimensional algebra $\mathcal{O}_0$, coupled to several infinitely extended reservoirs $\mathcal{R}_1, \ldots, \mathcal{R}_M$. We will use freely the notation of [NESS in quantum statistical mechanics].

Denote by δ_a the generator of $\tau_a^t = \tau^t|_{\mathcal{O}_a}$ for $0 \leq a \leq M$. Since $\mathcal{O}_0$ is finite dimensional one has $\delta_0 = \mathrm{i}[H_\mathcal{S}, \,\cdot\,]$ for some Hamiltonian $H_\mathcal{S}$. Observables describing the energy fluxes out of the reservoirs can be obtained in the following way. The total energy of the system is the sum of the energy of each reservoir, of the energy $H_\mathcal{S}$ of the small system and of the interaction energy V. Since the total energy is conserved, the rate at which the energy of the reservoirs decreases under the coupled dynamics is

$$\frac{\mathrm{d}}{\mathrm{d}t}\tau_V^t(H_\mathcal{S} + V) = \tau_V^t \left(\sum_{1\leq j\leq M} \delta_j(H_\mathcal{S} + V) + \mathrm{i}[H_\mathcal{S} + V, H_\mathcal{S} + V] \right) = \tau_V^t \left(\sum_{1\leq j\leq M} \delta_j(V) \right).$$

Noting that $\delta_j(V) = \delta_j(V_j) \in \mathcal{O}_0 \otimes \mathcal{O}_j$, we can identify $\Phi_j = \delta_j(V)$ with the energy flux out of reservoir $\mathcal{R}_j$.

Suppose now that each reservoir $\mathcal{R}_j$ is initially at thermal equilibrium at inverse temperature β_j, the system $\mathcal{S}$ being in an arbitrary τ_0-invariant faithful state. From the observation in the paragraph following Theorem 2 in [NESS in quantum statistical mechanics], we conclude that the generator of the modular group of the initial state ω takes the form

$$\delta_\omega = -\sum_{1\leq j\leq M} \beta_j \delta_j + \mathrm{i}[K, \,\cdot\,],$$

for some $K \in \mathcal{O}_0$ such that $\delta_a(K) = 0$ for $0 \leq a \leq M$. It follows that the entropy production observable is

$$\sigma(\omega, V) = -\sum_{1\leq j\leq M} \beta_j \delta_j(V) + \mathrm{i}[K, V] = -\sum_{1\leq j\leq M} \beta_j \Phi_j - \delta_V(K),$$

where $\delta_V = \sum_a \delta_a + \mathrm{i}[V, \,\cdot\,]$ is the generator of τ_V. It is important to realize that the second term in the right hand side of this identity is a total derivative. Consequently, its contribution to entropy production remains uniformly bounded in time

$$\int_0^t \tau_V^s(\sigma(\omega, V))\,\mathrm{d}s = -\sum_{1\leq j\leq M} \beta_j \int_0^t \tau_V^s(\Phi_j)\,\mathrm{d}s + \left(\tau_V^t(K) - K\right).$$

In particular, since $\omega_+ \in \Sigma_+(\tau_V, \omega)$ is τ_V-invariant, this boundary term does not contribute to the entropy production rate of the NESS, and we can write

$$\mathrm{Ep}(\omega_+) = -\sum_{1\leq j\leq M} \beta_j\, \omega_+(\Phi_j),$$

which is the familiar phenomenological expression (Equ. (1) in [Nonequilibrium steady states]).

A similar interpretation is possible in the case of time dependent perturbations, see [OHI].

For classical, thermostated systems used in the construction of microcanonical NESS, entropy production is usually defined as the local rate of phase space contraction α (see [G], [NESS in classical statistical mechanics]). If ϕ^t denotes the phase space flow and μ the reference measure (typically, this is just Lebesgue), then

$$\mu_t(f) = \mu(f \circ \phi^t) = \mu(f \, \mathrm{e}^{\int_0^t \alpha \circ \phi^{-s} \, \mathrm{d}s}).$$

A simple calculation shows that, if ν is absolutely continuous with respect to μ, then

$$\mathrm{Ent}(\nu_t|\mu) = \mathrm{Ent}(\nu|\mu) - \int_0^t \nu(\alpha \circ \phi^s) \, \mathrm{d}s.$$

Comparison with Equ. (1) shows perfect agreement with Definition 4 (see [P] for a completely parallel treatment of the classical and quantum cases).

4 Strict positivity of entropy production

We have seen that $\mathrm{Ep}(\omega_+) \geq 0$ for a NESS ω_+. One expects more, namely $\mathrm{Ep}(\omega_+) > 0$. Strict positivity of entropy production is a delicate dynamical problem. It is related to the singularity of the NESS with respect to the reference state, as indicated by the following result ([JP3]).

Theorem 6 *If $\omega_+ \in \Sigma_+(\tau_V, \omega)$ is ω-normal, then $\mathrm{Ep}(\omega_+) = 0$. Moreover, if*

$$\sup_{t>0} \left| \int_0^t \{\omega \circ \tau_V^s(\sigma(\omega, V)) - \omega_+(\sigma(\omega, V))\} \, \mathrm{d}s \right| < \infty,$$

then $\mathrm{Ep}(\omega_+) = 0$ implies that ω_+ is ω-normal.

Strict positivity of entropy production has been proved in a number of models. We refer to the original articles [LS], [JP2], [FMU], [AS]. Its genericity has been studied in [JP4].

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