FLUCTUATION THEOREM, NONEQUILIBRIUM STEADY STATES AND MACLENNAN- ZUBAREV ENSEMBLES OF A CLASS OF LARGE QUANTUM SYSTEMS

SHUICHI TASAKI

Advanced Institute for Complex Systems and Department of Applied Physics, School of Science and Engineerings, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, JAPAN
E-mail: stasaki@waseda.jp

TAKU MATSUI

Graduate School of Mathematics, Kyushu University, 1-10-6 Hakozaki, Fukuoka 812-8581, JAPAN
E-mail: matsui@math.kyushu-u.ac.jp

For an infinitely extended system consisting of a finite subsystem and several reservoirs, the time evolution of states is studied. Initially, the reservoirs are prepared to be in equilibrium with different temperatures and chemical potentials. If the time evolution is L^1-asymptotic abelian, (i) steady states exist, (ii) they and their relative entropy production are independent of the way of division into a subsystem and reservoirs, and (iii) they are stable against local perturbations. The explicit expression of the relative entropy production and a KMS characterization of the steady states are given. And a rigorous definition of MacLennan-Zubarev ensembles is proposed. A noncommutative analog to the fluctuation theorem is derived provided that the evolution and an initial state are time reversal symmetric.

1 Introduction

The understanding of irreversible phenomena including nonequilibrium steady states is a longstanding problem of statistical mechanics. Various theories have been developed so far[1]. One of promising approaches deals with infinitely extended dynamical systems[2,3,4]. Not only equilibrium properties, but also nonequilibrium properties has been rigorously investigated. The latter include analytical studies of nonequilibrium steady states, e.g., of harmonic crystals[5,6], a one-dimensional gas[7], unharmonic chains[8], an isotropic XY-chain[9], a one-dimensional quantum conductor[10] and an interacting fermion-spin system[11].

Entropy production has been rigorously studied as well (see [11-17] , and the references therein). Based on the idea of Ichiyanagi[18], Ojima, Hasegawa and Ichiyanagi[12] derived a formula relating the relative entropy to the thermodynamic entropy production for an infinitely extended driven system:

$$Ep(t) = \frac{d}{dt} S\left(\omega|\omega_t\right) \ , \tag{1}$$

where ω_t is the state at time t, ω is the initial equilibrium state and $S\left(\omega|\omega_t\right)$ is the C* generalization of the relative entropy[19−22,2 a] . Ojima[13] generalized this formula to include initial states ω where reservoirs are in different equilibria. Convergence of the entropy production to the steady-state value was investigated as well. Recently, Jakšić-Pillet[15] and Ruelle[14] rediscovered and extended his results. Also Jakšić and Pillet obtained a condition for strict positivity of the entropy production[11] (see also [16]).

On the other hand, recent progress in dynamical systems approach to classical nonequilibrium statistical mechanics reveals a new symmetry of entropy production fluctuations, known as the fluctuation theorem. It was found numerically by Evans, Cohen and Morris[23] and shown rigorously for thermostated systems by Gallavotti and Cohen[24]. Roughly speaking, this theorem asserts that the probability of observing the entropy production to be $a(>0)$ during a time interval t is $\exp(at)$ times larger than the probability of observing it to be $-a$ asymptotically in the limit of large t. It was then extended to transient states[25], to stochastically driven systems[26,27,28] and to open conservative systems[29,31]. The related topics have been extensively investigated (see e.g., references in [29,30]). However, its quantum generalization has not been well studied.

In this article, the time evolution of states is investigated for a C* algebraic system consisting of several (infinitely extended) heat reservoirs and a finite subsystem with L^1 asymptotic abelian property, which means that the time evolution *-automorphism τ_t satisfies

$$\int_{-\infty}^{+\infty} dt \|[\tau_t(A), B]\| < +\infty \tag{2}$$

for enoughly many dynamical variables A and B. Note that this is one of mixing conditions. Along the line of thoughts by Spohn and Lebowitz[5], we follow the evolution of states starting from initial states where heat reservoirs are in equilibrium with different temperatures and chemical potentials. Then, nonequilibrium steady states are derived as $t \to \pm\infty$ limits in the weak sense. Weak convergence of the states is guaranteed by the L^1 asymptotic abelian property. When a few conditions are satisfied in addition, the steady states are shown to be KMS (Kubo-Martin-Schwinger) states with respect to certain

[a]Throughout this article, we follow Araki's definition of relative entropy $S\left(\omega|\omega_t\right)$[19]. It is slightly different from the one, $S_{BR}\left(\omega_t|\omega\right)$, e.g., used in [2]: : $S_{BR}\left(\omega_t|\omega\right) = -S\left(\omega|\omega_t\right)$.

*- automorphism. More interestingly, the steady states correspond to the ones proposed by MacLennan[32] and Zubarev[33].

In addition, a quantum analog to the fluctuation theorem is derived for the relative entropy production. As will be explained later, the relative entropy is the average of the logarithm of the so-called relative modular operator, which acts on states but cannot be reduced to left nor right multiplications (such operators are sometimes called superoperators[34]). Hence, this superoperator may be regarded as a relative entropy operator although it is not a standard dynamical variable. We then study fluctuations of the logarithm of the relative modular operator and show that their distribution has a symmetry claimed by the fluctuation theorem. Note that Prigogine and his coworkers[34] have been continuously investigating a realization of entropy as a superoperator, i.e., an operator acting on density matrices but not represented as standard dynamical variables. Also Ojima, Hasegawa and Ichiyanagi[12] studied a free energy operator represented by the relative modular operator.

As previously mentioned, we mainly consider quantum dynamical systems with L^1 asymptotic abelian property. This condition is vaild for free Bose and Fermi Gasses in dimensions greater than or equal to three[2], certain coupled quantum oscillators[35]. It is known that the condition is not valid for the one dimensional XY model, and for some interacting fermions[36]. Thus in view of mathematical rigour, our analysis is restricted to special class of quantum systems. However recent results of spin fermion models due to Jakšić and Pillet in [11] suggest that what we describe here is physically generic. Moreoever, by sticking to the condition of L^1 asymptotic abelian property, we may exhibit an overview of nonequilibrium steady states in a concise manner.

The rest of this paper is arranged as follows. Sec. 2 is devoted to the description of a C* algebra corresponding to the system. We specify precisely the decomposition of the system into several heat reservoirs and a finite subsystem. Corresponding to each decomposition, initial states are prepared as KMS states, where heat reservoirs are in equilibrium with different temperatures and chemical potentials. Then, the L^1-asymptotic abelian property and other assumptions on dynamics are explained. In Sec. 3, the convergence of states at time t to steady states as $t \to \pm\infty$ is shown. The steady states do not depend on the choice of initial states of the finite subsystem nor on the way of division. The steady states at $t = \pm\infty$ are time reversal of each other. And the steady states are ergodic in a sense that they are stable against local perturbations in *both* directions of time. We remark that the steady states are related to the initial states via Møller morphisms. In Sec. 4, the definition of the relative entropy in C* algebra and the implications of the previous works[12,15] are summarized. And steady-state entropy production is shown to be independent of the way of division of the system into heat reservoirs and a finite subsystem. Then, the fluctuation theorem for the logarithm of the relative modular operator is derived. In Sec. 5, the existence of a system division with invertible Møller morphisms is assumed and we show that the steady states may be characterized as MacLennan-Zubarev nonequilibrium ensembles in a sense that they are KMS states with respect to a *-automorphism, whose generator is represented by a linear combination of Zubarev's local integrals of motion[33] in a certain sense. Sec. 6 is devoted to the summary. Here we give only the results and the proofs will be given elsewhere[39].

2 Large Quantum Systems

2.1 Field algebra

The system $\mathcal{S}$ in question is described by a field algebra $\mathcal{F}$[2,37]. Namely, $\mathcal{F}$ is a C* algebra where the following *-automorphisms are defined:

(i) a strongly continuous one-parameter group of *- automorphisms τ_t ($t \in \mathbf{R}$), which describes time-evolution.

(ii) a strongly continuous L-parameter group of *- automorphisms $\alpha_{\vec{\varphi}}$ ($\vec{\varphi} \in \mathbf{R}^L$) satisfying $\alpha_{\vec{\varphi}_1}\alpha_{\vec{\varphi}_2} = \alpha_{\vec{\varphi}_1+\vec{\varphi}_2}$, which represent the gauge transformation.

(iii) an involutive *-automorphism Θ, which is represented as $\Theta = \alpha_{\vec{\varphi}_0}$ with some $\vec{\varphi}_0 \in \mathbf{R}^L$.

The groups τ_t, $\alpha_{\vec{\varphi}}$ and Θ are interrelated as

$$\Theta\tau_t = \tau_t\Theta, \quad \Theta\alpha_{\vec{\varphi}} = \alpha_{\vec{\varphi}}\Theta, \quad \tau_t\alpha_{\vec{\varphi}} = \alpha_{\vec{\varphi}}\tau_t$$

for all $t \in \mathbf{R}$ and $\vec{\varphi} \in \mathbf{R}^L$. A subalgebra $\mathcal{A} \subset \mathcal{F}$ which is invariant under the action of $\alpha_{\vec{\varphi}}$ ($\vec{\varphi} \in \mathbf{R}^L$) is called the observable algebra, which describes observable physical quantities. The *-automorphism Θ defines the even and odd subalgebras, respectively, $\mathcal{F}_+$ and $\mathcal{F}_-$:

$$\mathcal{F}_\pm = \{A \in \mathcal{F}; \Theta(A) = \pm A\} \ .$$

When the system involves fermions, even and odd subalgebras correspond to dynamical variables which are sums of products of, respectively, even and odd number of fermion creation and/or annihilation operators.

Let $\vec{e}_\lambda \in \mathbf{R}^L$ be the unit vector whose λth element is 1, then, because of (ii), the *-automorphisms $\alpha_{s\vec{e}_\lambda}$ defines a strongly continuous group and its generator will be denoted as g_λ $(\lambda = 1, \cdots L)$

$$g_\lambda(A) = \lim_{s \to 0} \frac{\alpha_{s\vec{e}_\lambda}(A) - A}{s} \qquad \left({}^\forall A \in D(g_\lambda)\right) \tag{3}$$

where $D(g_\lambda)$ is the domain of g_λ and the limit is in norm. And we assume

(iv) $D(\delta) \subset D(g_\lambda)$ $(\lambda = 1, 2, \cdots L)$, where δ is the generator of the time evolution *-automorphism τ_t and $D(\delta)$ is its domain dense in $\mathcal{F}$.

In addition to the gauge symmetry, the system is assumed to possess time reversal symmetry:

(v) There exists an involutive antilinear *-automorphism ι such that

$$\iota \tau_t \iota = \tau_{-t} \ . \tag{4}$$

2.2 Decomposition of the system and initial states

We consider the situation where the system $\mathcal{S}$ can be decomposed into N independent infinitely extended subsystems $\mathcal{S}_j$ $(j = 1, \cdots N)$, which play a role of heat reservoirs, and a finite-degree-of-freedom subsystem $\mathcal{S}_0$ interacting with all the others. More precisely, the algebra $\mathcal{F}$ is represented as a tensor product of N infinite dimensional subalgebras $\mathcal{F}_j$ $(j = 1, \cdots N)$ of $\mathcal{S}_j$, and a finite dimensional subalgebra $\mathcal{F}_0$ of $\mathcal{S}_0$:

$$\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1 \otimes \cdots \otimes \mathcal{F}_N \ , \tag{5}$$

such that the following conditions are satisfied:

(S1) There exists a gauge-invariant time evolution group τ_t^V $(t \in \mathbf{R})$ which is a perturbation to τ_t by a selfadjoint element $-V \in \mathcal{A} \cap D(\delta)$ and which is a product of strongly continuous groups $\tilde{\tau}_t^{(j)}$ $(j = 1, \cdots N)$ independently acting on subalgebras $\mathcal{F}_j$ $(j = 1, \cdots N)$

$$\tau_t^V = \tilde{\tau}_t^{(1)} \cdots \tilde{\tau}_t^{(N)} \ . \tag{6}$$

Namely, $\tilde{\tau}_t^{(j)}$ leaves the other subalgebras $\mathcal{F}_k$ invariant and it commutes with the other groups $\tilde{\tau}_t^{(k)}$:

$$\tilde{\tau}_t^{(j)}(A) = A \qquad ({}^\forall A \in \mathcal{F}_k \ , \quad k \neq j) \tag{7}$$

$$\tilde{\tau}_t^{(j)} \tilde{\tau}_s^{(k)} = \tilde{\tau}_s^{(k)} \tilde{\tau}_t^{(j)} \qquad (t, s \in \mathbf{R} \ \ k \neq j) \tag{8}$$

(S2) The gauge *-automorphism $\alpha_{\vec{\varphi}}$ is a product of strongly continuous groups $\tilde{\alpha}^{(j)}_{\vec{\varphi}}$ $(j = 0, 1, \cdots N)$ independently acting on subalgebras $\mathcal{F}_j$ $(j = 0, 1, \cdots N)$:

$$\alpha_{\vec{\varphi}} = \tilde{\alpha}^{(0)}_{\vec{\varphi}} \tilde{\alpha}^{(1)}_{\vec{\varphi}} \cdots \tilde{\alpha}^{(N)}_{\vec{\varphi}} \ , \tag{9}$$

and they satisfy

$$\tilde{\alpha}^{(j)}_{\vec{\varphi}}(A) = A \qquad ({}^{\forall}A \in \mathcal{F}_k \ , \quad k \neq j) \tag{10}$$

$$\tilde{\alpha}^{(j)}_{\vec{\varphi}_1} \tilde{\alpha}^{(k)}_{\vec{\varphi}_2} = \tilde{\alpha}^{(k)}_{\vec{\varphi}_2} \tilde{\alpha}^{(j)}_{\vec{\varphi}_1} \qquad (\vec{\varphi}_1, \vec{\varphi}_2 \in \mathbf{R}^L \quad k \neq j) \tag{11}$$

The groups $\tilde{\tau}^{(j)}_t$ and $\tilde{\alpha}^{(j)}_{\vec{\varphi}}$ are interrelated as

$$\tilde{\tau}^{(j)}_t \tilde{\alpha}^{(k)}_{\vec{\varphi}} = \tilde{\alpha}^{(k)}_{\vec{\varphi}} \tilde{\tau}^{(j)}_t$$

for all $j, k = 1, \cdots, N$, $t \in \mathbf{R}$ and $\vec{\varphi} \in \mathbf{R}^L$. And an assumption is made for the domains of the generators $\tilde{\delta}_j$ and $\tilde{g}^{(j)}_\lambda$, respectively, of the strongly continuous groups $\tilde{\tau}^{(j)}_t$ and $\tilde{\alpha}^{(j)}_{s\vec{e}_\lambda}$ $(t, s \in \mathbf{R})$:

(S3) $D(\delta) \subset D(\tilde{\delta}_j) \quad D(\delta) \subset D(\tilde{g}^{(j)}_\lambda)$ for all $j = 0, 1, \cdots N$, $\lambda = 1, \cdots L$.

Then, as the condition (S1) implies that the domain of the generator δ^V of τ^V_t is equal to $D(\delta)$: $D(\delta^V) = D(\delta)$, one has

$$\delta(A) = \delta^V(A) + i[V, A] \quad (\text{for } A \in D(\delta)) \tag{12}$$

$$\delta^V(A) = \sum_{j=1}^{N} \tilde{\delta}_j(A) \qquad (\text{for } A \in D(\delta)) \tag{13}$$

Individual time evolutions and gauge transformations are assumed to be time reversal symmetric:

(S4) $\iota \tilde{\tau}^{(j)}_t \iota = \tilde{\tau}^{(j)}_{-t} \ , \quad \iota \tilde{\alpha}^{(j)}_{\vec{\varphi}} \iota = \tilde{\alpha}^{(j)}_{-\vec{\varphi}}$

Note that one may assume $\iota(V) = V$ without loss of generality. Indeed, any V can be decomposed into an even and odd elements with respect to the time reversal operation ι:

$$V = V_e + V_o \tag{14}$$

where $V_e = \frac{1}{2}\{V + \iota(V)\}$ and $V_o = \frac{1}{2}\{V - \iota(V)\}$. On the other hand, when the conditions (v) and (S4) are satisfied, one has

$$[V_o, A] = 0 \ , \qquad (\forall A \in \mathcal{F}) \tag{15}$$

and the odd part V_o does not contribute to τ_t^V.

As in the previous works[5,9–13,15], we are interested in the evolution of initial states where N infinitely extended heat reservoirs are in equilibrium with different temperatures and different chemical potentials and the finite subsystem is in an arbitrary state, which is described by a nonsingular density matrix. As discussed in [13,15], such states are specified as a KMS state:

(S5) Let σ_x^ω ($x \in \mathbf{R}$) be a strongly continuous group defined by

$$\sigma_x^\omega(A) = \prod_{j=1}^{N} \tilde{\tau}^{(j)}_{-\beta_j x} \tilde{\alpha}^{(j)}_{\beta_j \vec{\mu}_j x} \left(e^{iD_S x} A e^{-iD_S x} \right) , \quad (A \in \mathcal{F}) \tag{16}$$

where β_j and $\vec{\mu}_j = (\mu_j^{(1)}, \cdots \mu_j^{(L)})$ are, respectively, the inverse temperature and a set of chemical potentials of the jth heat reservoir. The operator D_S ($\in \mathcal{F}_0 \cap \mathcal{A}$) is selfadjoint and $\exp(D_S)$ represents an initial state of the finite-degree-of-freedom subsystem $\mathcal{S}_0$. Then an initial state ω is a KMS state with temperature -1 with respect to σ_x^ω. Namely, ω is a state such that, for any pair $A, B \in \mathcal{F}$, there exists a function $F_{A,B}(x)$ of x analytic in the stripe $\{x \in \mathbf{C}; 0 > \mathrm{Im} x > -1\}$ and satisfies the KMS boundary condition:

$$F_{A,B}(x) = \omega(A\sigma_x^\omega(B)) \qquad F_{A,B}(x-i) = \omega(\sigma_x^\omega(B)A) \quad (x \in \mathbf{R}) \tag{17}$$

Because of (S3), the domain of the generator $\hat{\delta}_\omega$ of σ_x^ω satisfies $D(\hat{\delta}_\omega) \supset D(\delta)$ and $\hat{\delta}_\omega$ is given by

$$\hat{\delta}_\omega(A) = -\sum_{j=1}^{N} \left\{ \beta_j \left(\tilde{\delta}_j(A) - \mu_\lambda^{(j)} \tilde{g}_\lambda^{(j)}(A) \right) \right\} + i[D_S, A] \ . \quad (A \in D(\delta)) \tag{18}$$

Note that a decomposition without the finite subsystem is possible as well.

We note that the boundaries among subsystems can be changed in an arbitrary way and, in some cases, it is necessary to compare two situations corresponding to different divisions. For this purpose, we introduce a notion of *locally modified* states. Consider a decomposition different from (5):

$$\mathcal{F} = \mathcal{F}_0' \otimes \mathcal{F}_1' \otimes \cdots \otimes \mathcal{F}_N' \ , \tag{19}$$

and a KMS state ω' of temperature -1 with respect to

$$\sigma_x^{\omega'}(A) = \prod_{j=1}^{N} \tilde{\tau}'^{(j)}_{-\beta_j x} \tilde{\alpha}'^{(j)}_{\beta_j \vec{\mu}_j x} \left(e^{iD_S' x} A e^{-iD_S' x} \right) , \quad (A \in \mathcal{F}) \tag{20}$$

where the temperatures β_j and chemical potentials $\vec{\mu}_j$ are the same as those of σ_x^ω. Then the state ω' is said to be a *locally modified* state of ω if the generators $\hat{\delta}_\omega$ and $\hat{\delta}_{\omega'}$ of, respectively, σ_x^ω and $\sigma_x^{\omega'}$ are related as

$$\hat{\delta}_{\omega'}(A) - \hat{\delta}_\omega(A) = i[W, A] \quad \left({}^\forall A \in D(\hat{\delta}_\omega)\right) \tag{21}$$

where $W \in \mathcal{A}$ is selfadjoint and $D(\hat{\delta}_\omega)$ is the domain of $\hat{\delta}_\omega$. Note that, if there exist several KMS states, locally modified states ω and ω' may be globally different. Note that the state ω'', which corresponds to the same division (5), but to a different initial state $\exp(D_S'')$ of the finite subsystem, is a locally modified state of ω because the generators of the defining groups of ω and ω'' differ by a bounded derivation:

$$\hat{\delta}_{\omega''}(A) - \hat{\delta}_\omega(A) = i[D_S'' - D_S, A] \quad \left({}^\forall A \in D(\hat{\delta}_\omega)\right) \tag{22}$$

2.3 Assumptions on initial states and dynamics

The state ω_t at time t starting with the initial state ω is given by

$$\omega_t = \omega \circ \tau_t \ , \tag{23}$$

and its weak limits for $t \to \pm\infty$ are expected to be nonequlibrium steady states. Of course, the limits do not exist in general. As one of sufficient conditions for the existence of the limits, we assume that the evolution is $L^1(\mathcal{G}_L)$-asymptotically abelian:

(A1) $L^1(\mathcal{G}_L)$-asymptotically abelian property:
There exists a norm dense *-subalgebra $\mathcal{G}_L$ such that

$$\int_{-\infty}^{+\infty} dt \|[A, \tau_t(B)]\| < +\infty \quad (A \in \mathcal{G}_L,\ B \in \mathcal{G}_L \cap \mathcal{F}_+) \tag{24}$$

$$\int_{-\infty}^{+\infty} dt \|[A, \tau_t(B)]_+\| < +\infty \quad (A, B \in \mathcal{G}_L \cap \mathcal{F}_-) \tag{25}$$

where $[\cdot,\cdot]_+$ is the anticommutator and $\mathcal{F}_\pm$ are even/odd subalgebras.

Note that there may exist more than two KMS states at low temperatures, for example, if the quantum system undergoes the phase trasition with symmerty breaking, the KMS states should not be unique. However, because a heat reservoir in thermodynamics is fully characterized by its temperature and chemical potentials, we assume that reservoir states are uniquely determined by the KMS condition:

(A2) Uniqueness of initial states:
There is a division of the system: $\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1 \otimes \cdots \otimes \mathcal{F}_N$ into N heat reservoirs and a finite subsystem such that, for each set of temperatures $\{\beta_j\}$, chemical potentials $\{\vec{\mu}_j\}$, and an initial subsystem state e^{D_S}, there exists a unique KMS state ω of σ_x^ω with temperature -1. And the perturbation V in the time evolution *-automorphism τ_t^V belongs to $\mathcal{G}_L$.

Assumption (A2) implies the invariance of the state ω under the perturbed time evolution τ_t^V. Indeed, as seen from (S1), (S2) and (S5), σ_x^ω and τ_t^V commute. Hence, the state $\omega \circ \tau_t^V$ is again a KMS state of σ_x^ω with temperature -1 and, by assumption (A2), it is equal to ω: $\omega \circ \tau_t^V = \omega$.

The $L^1(\mathcal{G}_L)$-abelian property (A1) and $V \in \mathcal{G}_L$ implies the existence of Møller morphisms $\gamma_\pm$ defined by (cf. Prop. 5.4.10 of Ref. [2])

$$\lim_{t\to\pm\infty} {\tau_t^V}^{-1} \tau_t(A) = \gamma_\pm(A) \ . \quad ({}^\forall A \in \mathcal{F}) \tag{26}$$

To prove certain properties, the invertibility of Møller morphisms is necessary and, in stead of (A2), we assume

(A3) Uniqueness of initial states and invertibility of Møller morphisms:
There is a division of the system: $\mathcal{F} = \mathcal{F}_1 \otimes \cdots \otimes \mathcal{F}_N$ into N heat reservoirs such that, for each set of temperatures $\{\beta_j\}$ and chemical potentials $\{\vec{\mu}_j\}$, there exists a unique KMS state ω of σ_x^ω with temperature -1. And the perturbation V in the time evolution *-automorphism τ_t^V belongs to $\mathcal{G}_L$. In addition, the Møller morphisms $\gamma_\pm$ defined in (26) are invertible.

If the perturbed time evolution τ_t^V admits a finite-dimensional invariant subalgebra, Møller morphisms are not invertible. Hence, the decomposition of the system in (A3) should not contain the finite-dimensional subalgebra $\mathcal{F}_0$.

3 Steady states

3.1 Properties of steady states

Theorem 1: Existence of steady states

When the evolution τ_t satisfies (A1) the $L^1(\mathcal{G}_L)$-asymptotic abelian property, the weak limits

$$\lim_{t\to\pm\infty} \omega \circ \tau_t(A) \equiv \omega_{\pm\infty}(A) \quad ({}^\forall A \in \mathcal{F}) \tag{27}$$

exist for each initial state ω explained in (S5). The states $\omega_{\pm\infty}$ are τ_t-invariant[17].

In view of thermodynamics, steady states are expected to depend only on the global boundary conditions such as the temperatures and chemical potentials of the reservoirs. Indeed, we have

Theorem 2: Independence of steady states on division and D_S

When τ_t is (A1) $L^1(\mathcal{G}_L)$-asymptotically abelian and (A2) the KMS state for σ_x^ω is unique, for any locally modified state ω' of ω, one has

$$\lim_{t\to\pm\infty} \omega' \circ \tau_t(A) = \lim_{t\to\pm\infty} \omega \circ \tau_t(A) = \omega_{\pm\infty}(A) \quad ({}^\forall A \in \mathcal{F}) \ . \tag{28}$$

This implies that the steady states $\omega_{\pm\infty}$ are determined only by the temperatures and chemical poteitials of the heat reservoirs, but does not depend on the way of division into subsystems nor on the initial state of the finite-degree-of-freedom subsystem.

For Spin Fermion models, the same result is obtained by Jakšić, and Pillet in [11].

As an immediate consequence of Theorem 2, one has

Proposition 3: Time reversal property of the steady states

Under the assumption of Theorem 2, the two steady states are time reversal with each other:

$$\omega_{\pm\infty} = \iota^* \omega_{\mp\infty} \tag{29}$$

where the time reversal operation ι^* on a state ω is defined by

$$\iota^* \omega(A) \equiv \omega\left(\iota(A^*)\right) \ . \tag{30}$$

Under stronger assumptions, steady states have certain ergodicity.

Theorem 4: Stability of steady states against local disturbance

When τ_t is (A1) $L^1(\mathcal{G}_L)$-asymptotically abelian, (A3) the KMS state for σ_x^ω is unique and the Møller morphisms $\gamma_\pm$ are invertible, the steady states $\omega_{+\infty}$ are stable against local pertubation in the sense

$$\lim_{t\to\pm\infty} \frac{\omega_{+\infty}\left(B^* \tau_t(A) B\right)}{\omega_{+\infty}(B^* B)} = \omega_{+\infty}(A) \ . \ ({}^\forall A, B \in \mathcal{F}) \tag{31}$$

The same is true for the state $\omega_{-\infty}$. This corresponds to the 'return to equilibrium' property of equilibrium states[2] and implies certain ergodicity of the steady states.

4 Relative entropy, its production and fluctuation theorem

4.1 Relative entropy of states over C algebra*

For a finite dimensional C* algebra, the relative entropy $S(\rho_2|\rho_1)$ of two states represented by density matrices ρ_1 and ρ_2 is given by

$$S(\rho_2|\rho_1) = \mathrm{Tr}\left\{\rho_1 \left(\log\rho_1 - \log\rho_2\right)\right\} \ , \tag{32}$$

where Tr stands for the trace. A generalization to states over a C* algebra is carried out with the aid of GNS (Gelfand-Naimark-Segal) representation and Tomita-Takesaki theory of von Neumann algebras. We summarize the outline following [12].

For a given C* algebra $\mathcal{A}$, there exist a Hilbert space $\mathcal{K}$, a vector $\Omega \in \mathcal{K}$ and a *-morphism $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{K})$ from $\mathcal{A}$ to a set $\mathcal{B}(\mathcal{K})$ of all bounded linear operators on $\mathcal{K}$, such that (i) $\omega(A) = (\Omega, \pi(A)\ \Omega)$ ($^\forall A \in \mathcal{A}$) and (ii) the set $\{\pi(A)\Omega | A \in \mathcal{A}\}$ is dense in $\mathcal{K}$ (cyclicity of the state Ω). The triple $(\mathcal{K}, \Omega, \pi)$ is called the GNS representation. A set of all $B \in \mathcal{B}(\mathcal{K})$ which commute with every element of $\pi(\mathcal{A})$ is denoted as $\pi(\mathcal{A})'$ (commutant of $\pi(\mathcal{A})$). $\pi(\mathcal{A})'$ is again an algebra. Let $\mathcal{M}$ be a double commutant of $\pi(\mathcal{A})$: $\mathcal{M} = \pi(\mathcal{A})''$, then $\mathcal{M}'' = \mathcal{M}$. An algebra like $\mathcal{M}$ is called a von Neumann algebra.

Given a von Neumann algebra $\mathcal{M} \subset \mathcal{B}(\mathcal{K})$, a vector $\Omega \in \mathcal{K}$ is called separating if $A\Omega = 0$ for $A \in \mathcal{M}$ implies $A = 0$. If a vector Ω is separating and cyclic with respect to $\mathcal{M}$, there exist antilinear operators S and F satisfying

$$SA\Omega = A^*\Omega \quad (^\forall A \in \mathcal{M}) \ , \qquad FA'\Omega = A'^*\Omega \quad (^\forall A' \in \mathcal{M}') \ . \tag{33}$$

The closure $\bar{S}$ of S admits a polar decomposition:

$$\bar{S} = J\Delta^{1/2} \tag{34}$$

where $\Delta = S^*\bar{S}$ is positive and self-adjoint, and J is an antilinear involution. Moreover, they satisfy $J\mathcal{M}J = \mathcal{M}'$ and $\Delta^{it}\mathcal{M}\Delta^{-it} = \mathcal{M}$. This is the outline of Tomita-Takesaki theory.

The set

$$\mathcal{P} \equiv \overline{\{AJAJ\Omega | A \in \mathcal{M}\}} \subset \mathcal{K} \ , \tag{35}$$

is called the natural positive cone, where the bar stands for the closure. For two vectors $\Psi, \Omega \in \mathcal{P}$ which are both cyclic and separating, one defines an operator $S_{\Psi,\Omega}$ by

$$S_{\Psi,\Omega}A\Omega = A^*\Psi \ . \quad (A \in \mathcal{M}) \tag{36}$$

Araki[19] defined the relative entropy of Ψ and Ω by

$$S(\Omega|\Psi) = (\Psi, \ln\Delta_{\Psi,\Omega}\Psi) \ , \tag{37}$$

where $\Delta_{\Psi,\Omega} \equiv S^*_{\Psi,\Omega}\bar{S}_{\Psi,\Omega}$ is called the relative modular operator with $\bar{S}_{\Psi,\Omega}$ the closure of $S_{\Psi,\Omega}$. For any faithful states ω_1 and ω_2 on a C* algebra, when both of them are represented by separating and cyclic vectors, Ψ and Ω respectively, belonging to the same natural positive cone in a GNS representation, their relative entropy $S(\omega_2|\omega_1)$ is defined by

$$S(\omega_2|\omega_1) = S(\Omega|\Psi) \ . \tag{38}$$

In the next subsection, we investigate the temporal change of the relative entropy $S(\omega|\omega_t)$ between the initial and present states.

4.2 Relative entropy and its change

Explicit expression of the relative entropy production was obtained by Ojima et al.[12,13] and Jakšić and Pillet[15,11].

Theorem 5: Relative entropy [Ojima et al.[12,13] and Jakšic and Pillet[15,11]]

The relative entropy $S(\omega|\omega_t)$ between the initial and present states is given by

$$S(\omega|\omega_t) = \sum_{j=1}^{N} \beta_j \int_0^t \omega_s(J_j^q)ds - \omega_t(D_S) + \omega(D_S) \tag{39}$$

where $\omega_s \equiv \omega \circ \tau_s$ and J_j^q corresponds to the heat flow to the jth reservoir:

$$J_j^q \equiv -\tilde{\delta}_j(V) + \sum_{\lambda=1}^{L} \mu_\lambda^{(j)} \tilde{g}_\lambda^{(j)}(V) \ . \tag{40}$$

Moreover if (A1) the time evolution τ_t is asymptotically abelian, (i) the relative entropy production $Ep(\omega_t) \equiv \frac{d}{dt}S(\omega|\omega_t)$ at time t converges to the steady state values in the limit of $t \to \pm\infty$:

$$\lim_{t\to\pm\infty} Ep(\omega_t) = Ep(\omega_{\pm\infty}) \equiv \sum_{j=1}^{N} \beta_j \omega_{\pm\infty}(J_j^q) \ , \tag{41}$$

(ii) they do not depend on the initial states of finite dimensional subsystem, (iii) $Ep(\omega_{+\infty}) \geq 0$ and $Ep(\omega_{-\infty}) \leq 0$. Note that the positivity of $Ep(\omega_{+\infty})$ is consistent with thermodynamics.

NB 5.1 For finite-degree-of-freedom systems, the generators $\tilde{\delta}_j$ and $\tilde{g}_\lambda^{(j)}$ are given by local Hamiltonians H_j and number operators $N_j^{(\lambda)}$ as commutators:

$\tilde{\delta}_j(A) = i[H_j, A]$ and $\tilde{g}_\lambda^{(j)}(A) = i[N_j^{(\lambda)}, A]$, where H_j and $N_j^{(\lambda)}$ commute with each other. And the total Hamiltonian H is $H = \sum_{j=1}^N H_j + V$. Therefore, because of $-[H_j, V] = [H, H_j]$ and $-[N_j^{(\lambda)}, V] = [H, N_j^{(\lambda)}]$,

$$J_j^q = -i[H_j, V] + \sum_{\lambda=1}^{L} \mu_\lambda^{(j)} i[N_j^{(\lambda)}, V] = \frac{d}{dt}\tau_t(H_j) - \sum_{\lambda=1}^{L} \mu_\lambda^{(j)} \frac{d}{dt}\tau_t\left(N_j^{(\lambda)}\right) ,$$

which, indeed, represents nonsystematic energy flow to the jth reservoir.

NB 5.2 Since D_S corresponds to the logarithm of density matrix describing the initial state of the finite system, it is interesting to rewrite (39) as

$$-\frac{d}{dt}\omega_t(D_S) = -\sum_{j=1}^{N} \beta_j \omega_t(J_j^q) + \frac{d}{dt} S(\omega|\omega_t) \tag{42}$$

which may read as follows: The entropy change of the finite subsystem $-\omega_t(D_S)$ is the sum of entropy flow from the resevoirs and the entropy production $\frac{d}{dt}S(\omega|\omega_t) \equiv Ep(\omega_t)$. However, as discussed elsewhere[38], such an interpretation is not correct in general, but $Ep(\omega_t)$ can be identified with thermodynamic entropy production only for very large $|t|$.

Under stronger assumptions, one can show the independence of the limits on the way of division.

Theorem 6: Division independence of $Ep(\omega_{\pm\infty})$

Let ω' be a locally modified state of ω by W. Then, if τ_t is (A1) $L^1(\mathcal{G}_L)$-asymptotically abelian, (A2) the KMS state for σ_x^ω is unique and $D_S, D_S', W \in D(\delta)$, one has

$$\lim_{t\to\pm\infty} Ep(\omega' \circ \tau_t) = \lim_{t\to\pm\infty} Ep(\omega \circ \tau_t) , \tag{43}$$

or $Ep(\omega_{\pm\infty})$ is independent of the way of division of the system.

4.3 Fluctuation theorem

In view of (37) and (38), the logarithm of the relative modular operator between the present and initial states divided by the duration t can be regarded as the mean entropy production operator $\hat{\Pi}_t$:

$$\hat{\Pi}_t \equiv \frac{1}{t} \ln \Delta_{\Omega_t,\Omega} \tag{44}$$

where Ω_t and Ω are vector representions of ω_t and ω, respectively, in a GNS representation. Since $\Delta_{\Omega_t,\Omega}$ is positive, $\hat{\Pi}_t$ is selfadjoint and admits a spectral decomposition:

$$\hat{\Pi}_t = \int_{-\infty}^{+\infty} \lambda dP_t(\lambda) \tag{45}$$

where $P_t(\lambda)$ is a spectral family of $\hat{\Pi}_t$. Then the expectation value of $P_t([a,b]) \equiv P_t(b) - P_t(a-0)$:

$$(\Omega_t, P_t([a,b])\,\Omega_t) \equiv \Pr([a,b];\omega_t) \tag{46}$$

may be regarded as the probability of finding the values of the mean relative entropy production within an interval $[a,b]$ at the state ω_t. As seen in the proof of Theorem 7, the probability is uniquely determined by the initial state and the time evolution automorphism. As a result of the time reversal symmtery, the probability distribution $\Pr([a,b];\omega_t)$ enjoys a simple symmetry property analogous to the Gallavotti-Cohen fluctuation theorem[23−31].

Theorem 7: Fluctuation theorem

Let $\Pr([a,b];\omega_t)$ $(t > 0)$ be the probability of finding the values of the mean relative entropy production within the interval $[a,b]$ as defined above. Then, if the initial state ω is time reversal symmetric, the probability satisfies an inequality

$$a \le \frac{1}{t}\log\frac{\Pr([a,b];\omega_t)}{\Pr([-b,-a];\omega_t)} \le b \tag{47}$$

for $0 \le a \le b$.

NB 7.1 If the probality measure $\Pr((a,b];\omega_t)$ is absolutely continuous with respect to a reference measure ν_R with a density function $p(\lambda;\omega_t)$:

$$\Pr((a,b];\omega_t) = \int_a^b p(\lambda;\omega_t)d\nu_R(\lambda)\ ,$$

Theorem 7 implies

$$\frac{p(a;\omega_t)}{p(-a;\omega_t)} = e^{at}\ .$$

This is a noncommutative extenion of the transient fluctuation theorem of Evans-Searles[25] and of the detailed fluctuation theorem of Jarzynski[29]. Also if $\lambda = a$ is a discrete point, one has

$$\frac{\Pr(\{a\};\omega_t)}{\Pr(\{-a\};\omega_t)} = e^{at}\ .$$

For a particular value $a = Ep(\omega_{+\infty})$, Theorem 7 implies that the probability of finding the mean relative entropy production at the steady-state average $Ep(\omega_{+\infty})$ is exponentially larger than the probability of finding it at the opposite value $-Ep(\omega_{+\infty})$.

4.4 Outline of the proof of Theorem 7

Because ω is τ_t^V-invariant, one has

$$\omega \circ \tau_t(A) = \omega_0(Y_t A Y_t^*) \tag{48}$$

where a unitary element Y_t is defined as a norm convergent series:

$$Y_t = \mathbf{1} + \sum_{n=1}^{+\infty} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \tau_{-t_n}(V) \cdots \tau_{-t_2}(V) \tau_{-t_1}(V) \; . \tag{49}$$

In order to give a simple explanation, Y_t is assumed to be σ_x^ω-analytic. Let Ω and Ω_t be the vector representations of ω and ω_t, respectively, and let $\Delta_{\Omega_t,\Omega}$ be the relative modular operator, then the characteristic function for the mean entropy production operator $\hat{\Pi}_t$ is given by

$$\Phi(\xi) \equiv \left(\Omega_t, \exp(i\hat{\Pi}_t \xi)\Omega_t\right) = \left(\Omega_t, \Delta_{\Omega_t,\Omega}^{i\xi/t}\Omega_t\right) = \omega\left(Y_t \sigma_{-\xi/t}^\omega (Y_t^*)\right) \; .$$

On the other hand, if ω is time reversal symmetric, the time reversal symmetry of σ_x^ω and the KMS boundary condition give

$$\Phi(-\xi) = \omega\left(\sigma_{-\xi/t}^\omega (Y_t^*)\, Y_t\right) = \omega\left(Y_t \sigma_{-\xi/t-i}^\omega (Y_t^*)\right) = \Phi(\xi + it) \; . \tag{50}$$

In terms of the cumulative distribution function $F(\lambda) \equiv \Pr\left((-\infty, \lambda]; \omega_t\right)$, this reads as

$$-\int_{-\infty}^{+\infty} e^{i\xi\lambda} dF(-\lambda) = \int_{-\infty}^{+\infty} e^{i\xi\lambda} e^{-\lambda t} dF(\lambda) \; ,$$

which gives

$$\int_{a-0}^{b+0} dF(\lambda) = \int_{-b-0}^{-a+0} e^{-\lambda t} dF(\lambda) \; .$$

The desired result immediately follows from this.

5 Characterization of steady states

5.1 KMS Characterization of states

Under the setting (S1)-(S5), the evolving state ω_t is characterized as a KMS state.

Theorem 8: KMS characterization of evolving states

The state ω_t at time t is a KMS state at temperature -1 with respect to the strongly continuous *-automorphism

$$\sigma_x^{\omega_t} \equiv \gamma_t^{-1} \sigma_x^{\omega} \gamma_t \ , \tag{51}$$

where $\gamma_t = \tau_t^{V\,-1} \tau_t$, and its generator is given by

$$\hat{\delta}_\omega^{(t)}(A) = \hat{\delta}_\omega(A) + i \int_{-t}^{0} ds \left[\tau_s \left(\hat{\delta}_\omega(V) \right), A \right] \tag{52}$$

for all $A \in D(\hat{\delta}_\omega^{(t)}) = D(\hat{\delta}_\omega)$.

When the Møller morphisms $\gamma_\pm$ exist and are invertible, the steady states $\omega_{\pm\infty}$ are characterized as KMS states:

Theorem 9: KMS characterization of steady states

When (A1) the time evolution *-automorphism τ_t is $L^1(\mathcal{G}_L)$- asymptotically abelian and (A3) the Møller morphisims $\gamma_\pm$ are invertible, the steady states $\omega_{\pm\infty}$ are KMS states at temperature -1 with respect to the strong continuous *-automorphism

$$\sigma_x^{\omega_\pm} \equiv \gamma_\pm^{-1} \sigma_x^{\omega} \gamma_\pm \ . \tag{53}$$

Furthermore, if $\hat{\delta}_\omega(V) \in \mathcal{G}_L$, its generator $\hat{\delta}_\omega^\pm$ satisfies

$$\hat{\delta}_\omega^\pm(A) = \hat{\delta}_\omega(A) + i \int_{\mp\infty}^{0} ds \left[\tau_s \left(\hat{\delta}_\omega(V) \right), A \right] \ , \tag{54}$$

for all $A \in D(\hat{\delta}_\omega) \cap \mathcal{G}_L$.

NB 9.1 For finite systems, the KMS state ω with respect to the *-automorphism σ_x^ω corresponds to the density matrix

$$\rho_\omega = \frac{1}{Z} \exp \left\{ - \sum_{j=1}^{N} \beta_j \left(H_j - \sum_{\lambda=1}^{L} \mu_\lambda^{(j)} N_j^{(\lambda)} \right) \right\} \ ,$$

where Z is the normalization constant, β_j, H_j, $\mu_\lambda^{(j)}$ and $N_j^{(\lambda)}$ are, respectively, the local temperature, local energy, local chemical potential and local number operator of the jth reservoir. As discussed in NB 5.1,

$$\tau_t\left(\hat{\delta}_\omega(V)\right) = -\sum_{j=1}^{N} \beta_j \frac{d}{dt}\tau_t\left(H_j - \sum_{\lambda=1}^{L} \mu_\lambda^{(j)} N_j^{(\lambda)}\right) = -\sum_{j=1}^{N} \beta_j \tau_t(J_j^q) \ ,$$

where J_j^q is a heat flow to the jth reservoir. Therefore, because of Theorem 8, the density matrix ρ_{ω_t} correponding to ω_t is given by

$$\rho_{\omega_t} = \frac{1}{Z}\exp\left\{-\sum_{j=1}^{N}\beta_j\left[H_j - \sum_{\lambda=1}^{L}\mu_\lambda^{(j)}N_j^{(\lambda)} - \int_{-t}^{0} ds\tau_s(J_j^q)\right]\right\} \ ,$$

Note that one has $\rho_{\omega_t} = \tau_{-t}(\rho_\omega)$ and this is consistent with the Liouville-von Neumann equation for the density matrices.

NB 9.2 For infinite systems, the case when the right-hand side of (54) generates $\sigma_x^{\omega\pm}$ is most interesting. Then, if the integral

$$\widetilde{V}_\pm \equiv \int_{\mp\infty}^{0} ds\tau_s\left(\hat{\delta}_\omega(V)\right) \tag{55}$$

would converge, $\omega_{\pm\infty}$ would be a perturbed KMS state of the initial state ω by a self-adjoint operator $\widetilde{V}_\pm$. Moreover, NB 9.1 suggests that the corresponding density matrices would be

$$\rho_\pm = \frac{1}{Z}\exp\left\{-\sum_{j=1}^{N}\beta_j\left[H_j - \sum_{\lambda=1}^{L}\mu_\lambda^{(j)}N_j^{(\lambda)} - \int_{\mp\infty}^{0} ds\tau_s(J_j^q)\right]\right\} \ . \tag{56}$$

Note that such statistical ensembles for steady states were introduced by MacLennan[32] and Zubarev[33].

However, if the steady state carries nonvanishing entropy production, the integral $\widetilde{V}_\pm$ does not converge since the ω-average of its integrand does not vanish at infinities:

$$\lim_{s\to\pm\infty}\omega\left(\tau_s\left(\hat{\delta}_\omega(V)\right)\right) = Ep(\omega_{\pm\infty}) \neq 0 \ .$$

Thus, the original proposal (56) by MacLennan and Zubarev cannot be justified. Rather, the KMS states with respect to $\sigma_x^{\omega\pm}$ generated by (54) should be regarded as a precise definition of the MacLennan-Zubarev ensembles. Note that the above observation is consistent with the result by Jakšić and Pillet[11], which asserts that the relative entropy production between the steady state and the initial state vanishes if the former is a normal state of the latter.

6 Summary

For an infinitely extended system consisting of a finite subsystem and several reservoirs, we have studied the time evolution of states. Initially, the reservoirs are prepared to be in equilibrium with different temperatures and chemical potentials. If the time evolution is L^1-asymptotic abelian and a few more conditions are satisfied, (i) steady states exist, (ii) they and their relative entropy production are independent of the way of division into subsystem and reservoirs, and (iii) they are stable against local perturbations. The relative entropy production is calculated explicitly and we have given a KMS characterization of the steady states, which provides a rigorous meaning to the MacLennan-Zubarev steady state ensembles. In addition, a noncommutative analog to the fluctuation theorem is derived provided that the evolution and an initial state are time reversal symmetric.

Before closing, we remark that the unidirectional evolution is consistent with the time reversal symmetry of the system. To see this, let us consider the following thought experiment: At $t = 0$, the system is prepared to be in an ι^*-invariant state ω. Until time $t = t_1 (> 0)$, the system evolves according to the *-automorphism τ_t. At $t = t_1$, time reversal operation ι^* is applied. After $t = t_1$, the system evolves according to τ_t again. The state ω_t at time t is given by

$$\omega_t = \begin{cases} \omega \circ \tau_t \ , & (0 \leq t < t_1) \\ \omega \circ \tau_{t-2t_1} \ . & (t_1 \leq t) \end{cases} \tag{57}$$

where we have used $\iota^* \omega = \omega$.

Because of Theorem 1, the initial state ω evolves towards the steady state $\omega_{+\infty}$ and, for large t_1, the state just before the time reversal operation $\omega_{t_1 -} = \omega \circ \tau_{t_1}$ is close to $\omega_{+\infty}$. On the other hand, as $-t_1 < 0$, the state $\omega \circ \tau_{-t_1}$ just after the time reversal operation is close to the other steady state $\omega_{-\infty}$. Afterwards, the state $\omega_t = \omega \circ \tau_{t-2t_1}$ deviates from $\omega_{-\infty}$ and reaches ω at time $t = 2t_1$. Then, the state ω_t again approaches $\omega_{+\infty}$. Thus, the time reversal operation discontinuously changes a state $\omega_{t_1 -} (\sim \omega_{+\infty})$ to a state $\omega_{t_1 +} (\sim \omega_{-\infty})$, but does not invert the evolution. In this way, the unidirectional state evolution is consistent with the time reversal symmetry. A similar view was given by Prigogine et al.[34] for the behavior of entropy under time reversal experiments, where dynamics was considered to increase entropy and the time reversal operation was thought to induce a discontinuous entropy decrease.

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