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On the Characterization of the Stationary State of a Class of Dynamical Semigroups

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We consider a representation of the entropy production for a completely positive, trace-preserving dynamical semigroup satisfying detailed balance with respect to its faithful stationary state defined on a W^*-algebra $\mathscr{B}(\mathscr{H})$: it is expressed as a positive Hermitian form on $\mathscr{B}(\mathscr{H})$, which is analogous to the quantum correlation functions used in the Kubo theory. By considering this Hermitian form as a variation function of a vector in $\mathscr{B}(\mathscr{H})$, an exact characterization of the stationary states of semigroups in a certain class is obtained. On this basis, the problem of characterizing the stationary states discussed by Spohn and Lebowitz for many-reservoir open systems is solved without the restriction to situations near thermal equilibrium.

KEY WORDS: Quantum dynamical semigroups; detailed balance; entropy production; stationary states; variational principle.

1. INTRODUCTION

Spohn introduced the notion of entropy production into quantum dynamical semigroups,[1] and by using its positive and convex properties attempted to characterize the stationary state of the semigroup[2,3] in analogy to the thermodynamic principle of minimal entropy production—a revised problem of what Lebowitz considered many years ago for the model of open systems weakly in contact with several thermal reservoirs.[2,4] Spohn's result is limited to the linear theory of irreversible processes: he takes into account linear terms in the expansion of the entropy production in the temperature differences.[2,3] This paper aims to obtain a rigorous result on the characterization by a variational principle which is not restricted to the linear version. The variational principle here is of a different type from that of Spohn, but our result is in line with the existing thermodynamic argument that stationary states are determined by the principle of minimal entropy production.

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For the sake of simplicity, we confine ourselves to a finite quantum system, viz. a W^*-algebra $\mathscr{B}(\mathscr{H})$ with $\dim \mathscr{H} < \infty$ (so-called N-level system[5,8]), on which a one-parameter family of identity-preserving, completely positive maps $\{\Lambda_t;\, 0 \leqslant t < \infty\}$ (a dynamical semigroup) is defined. Let its infinitesimal generator L be of the form

$$L = \sum_{k=1}^{r} L_k \tag{1}$$

where each L_k is assumed (without loss of generality) to be a dissipative generator on $\mathscr{B}(\mathscr{H})$ satisfying the condition of detailed balance[5] with respect to a faithful state ω_k. Further, assume that Λ_t commutes with the modular automorphism of ω_k for all $k = 1,\ldots, r$. By an argument in Ref. 6, it follows then that there exists a state (in the commutant $\{\omega_1,\ldots, \omega_r\}'$ of all ω_k) stationary under the dynamical semigroup $\{\Lambda_t\}$. Our main result is a variational characterization of such a stationary state. Namely, a faithful state ω in $\{\omega_1,\ldots, \omega_r\}'$ is stationary under Λ_t if and only if ω satisfies

$$\begin{gathered}\log \omega = X_{\min}(\omega)\\ X_{\min}(\omega) \text{ a vector in } \mathscr{B}(\mathscr{H}) \text{ such that}\\ \min_{X \in \mathscr{B}^s(\mathscr{H})} a(\omega, X) = a(\omega, X_{\min}(\omega))\end{gathered} \tag{2}$$

[The commutativity of faithful states is defined in terms of that of their modular automorphisms. $\mathscr{B}^s(\mathscr{H})$ denotes the subspace of all self-adjoint elements.] The function $a(\omega, X)$ is constructed by using a special structure (1) of L:

$$a(\rho, X) = \sum_{k=1}^{r} q_k(\rho;\, X - \log \omega_k,\, X - \log \omega_k) \tag{3}$$

where $q_k(\rho; X, Y)$ is a positive Hermitian form on $\mathscr{B}(\mathscr{H})$ such that $q_k(\rho; X, X)$ at $X = \log \rho - \log \omega_k$, $\rho \in \{\omega_k\}'$, coincides with the entropy production (cf. Ref. 1)

$$\sigma(\rho|\omega_k) = \operatorname{Tr} \rho\, L_k(\log \omega_k - \log \rho) \tag{4}$$

More explicitly,

$$\begin{aligned} q_k(\rho; X, Y) = \frac{1}{2} \int_0^1 \sum_\nu \{&\langle(\rho\omega_k^{-1})^\theta [V_\nu^{(k)}, X](\rho\omega_k^{-1})^{1-\theta}, [V_\nu^{(k)}, Y]\rangle_{\omega_k}\\ &+ \langle(\rho\omega_k^{-1})^\theta [V_\nu^{(k)}, Y^*](\rho\omega_k^{-1})^{1-\theta}, [V_\nu^{(k)}, X^*]\rangle_{\omega_k}\}\, d\theta \end{aligned} \tag{5}$$

where $\{V_\nu^{(k)}\}$ are quantities appearing in Alicki's decomposition of L_k (Ref. 7; see also Ref. 5):

$$L_k X = \frac{1}{2}\sum_\nu ([V_\nu^{(k)*}, X]V_\nu^{(k)} + V_\nu^{(k)*}[X, V_\nu^{(k)}]) \tag{6}$$

(The index ν represents a pair of indices i, j each denoting a CON in $\mathscr{H}$.)

The above characterization is stated with proof in Section 4 as two main theorems. Sections 2 and 3 are preparation for the proof. The problem of characterizing the stationary state of the Lebowitz model can be solved as a corollary of the theorems, which is discussed in Section 5. We note that, though the variational principle in (2) is somewhat different from the most conventional form, the minimal value $a(\omega, \log\omega)$ coincides with the total entropy production defined in Refs. 2 and 3, which guarantees the original thermodynamic argument of Bergmann and Lebowitz.[4] In fact, a later development of Prigogine's thermodynamics contains a proposal of variation[14] to which the present scheme (2) conforms. It is based on the thermodynamic stability, which we formulate explicitly in Section 6 by using a convex function considered by Lieb.[11]

It has been argued in Refs. 5 and 6 that the remarkable property of detailed balance in the quantum version stems from the nature of ideal thermal reservoirs, viz. the reservoir satisfying the KMS condition. Therefore, the present result holds also when all the reservoirs in the Lebowitz model are of this ideal nature. The best physical example of such a model with the reservoir temperatures far from each other can be seen in the steadily oscillating state of a laser, which we have discussed elsewhere.[17,18,19]

2. CONDITION OF DETAILED BALANCE FOR THE GENERATOR OF A DYNAMICAL SEMIGROUP

The work of Gorini *et al.*[8] (see also Refs. 5 and 6) and that of Lindblad[9] have established the most general form of the generator L of $\{\Lambda_t; 0 \leqslant t < \infty\}$ (a completely positive, identity-preserving dynamical semigroup which is norm continuous) acting on $X \in \mathscr{B}(\mathscr{H})$ and its predual generator L_* of $\{\Lambda_{t*}\}$ (same as above except with "identity-preserving" replaced by "trace-preserving") on $\rho \in \mathscr{T}_+(\mathscr{H})$, where $\mathscr{B}(\mathscr{H})$ is the W^*-algebra of all bounded operators on a separable Hilbert space $\mathscr{H}$ and $\mathscr{T}_+(\mathscr{H})$ is its trace class of positive, self-adjoint elements in $\mathscr{B}(\mathscr{H})$: in case of dim $\mathscr{H} < \infty$ they are given by

$$LX = i[H, X] + \frac{1}{2}\sum_\nu ([V_\nu^*, X]V_\nu + V_\nu^*[X, V_\nu]) \tag{7}$$

and

$$L_*\rho = -i[H, \rho] + \frac{1}{2}\sum_\nu ([V_\nu, \rho V_\nu^*] + [V_\nu\rho, V_\nu^*]) \tag{8}$$

respectively, where $H(=H^*)$, $V_\nu \in \mathscr{B}(\mathscr{H})$ and the summation runs over a finite set of indices ν (throughout the paper, we have only finite summations). The operator $\pm i[H, \cdot]$ is called the Hamiltonian part, and $L - i[H, \cdot]$ (or $L_* + i[H, \cdot]$) the dissipative part, of L (or L_*), denoted by $L^{(h)}$ and $L^{(d)}$ ($L_*^{(h)}$ and $L_*^{(d)}$), respectively.

Let us assume that the semigroup under consideration satisfies detailed balance, that is:

(i) There exists a faithful state ω satisfying $[H, \omega] = 0$ and $L_*\omega = 0$ (equivalent to $L_*^{(h)}\omega = L_*^{(d)}\omega = 0$).

(ii) L commutes with the modular automorphism group $\{\Sigma_\omega^t\}$ ($\Sigma_\omega^t = \omega^{it}\cdot\omega^{-it}$): $L\Sigma_\omega^t = \Sigma_\omega^t L$ for $-\infty < t < \infty$, which, due to $L_*^{(h)}\omega = 0$, reduces to $L^{(d)}\Sigma_\omega^t = \Sigma_\omega^t L^{(d)}$ and $L_*^{(d)}\Sigma_\omega^t = \Sigma_\omega^t L_*^{(d)}$.

Definition. The dynamical semigroup with its generator (or the generator itself) satisfying (i) and (ii) is said to satisfy detailed balance with respect to (wrt) the faithful state ω.

Remark. This definition of details balance follows that of Ref. 5 except that the normality of the generator ($L^{(h)}L^{(d)} = L^{(d)}L^{(h)}$) is not assumed here.

The commutativity between L and the modular automorphism group is equivalent to that between L and the single automorphism Φ_ω defined by

$$\Phi_\omega X \equiv \omega X \omega^{-1}, \qquad X \in \mathscr{B}(\mathscr{H}) \tag{9}$$

Alicki[7] showed that under detailed balance the decomposition of the dissipative part $L^{(d)}$ in (7) [$L_*^{(d)}$ in (8)] in terms of $\{V_\nu\}$ can be made to satisfy

$$\Phi_\omega V_\nu^* = c_\nu V_\nu^*, \qquad \Phi_\omega V_\nu = c_\nu^{-1} V_\nu, \qquad c_\nu \neq 0 \tag{10}$$

i.e., V_ν^* and V_ν are eigenvectors of the automorphism Φ_ω (his condition of nondegeneracy of the spectrum of ω is unnecessary[5]). Hence we assume (10) hereafter.

Motivated by the above, we recapitulate detailed balance in the following form:

Proposition 1. The predual generator L_* satisfies detailed balance wrt a faithful state ω iff:

(i′) $L_*^{(d)} = \sum_\nu L_{\nu*}^{(d)}$, where

$$L_{\nu*}^{(d)}\rho = \tfrac{1}{2}([V_\nu, \rho V_\nu^*] + c_\nu[V_\nu^*, \rho V_\nu]) + \text{Herm. adj.}$$
$$= \tfrac{1}{2}([V_\nu, J_\nu(\rho)] + [V_\nu, J_\nu(\rho)]^*)$$

in which

$$J_\nu(\rho) \equiv \rho V_\nu^* - c_\nu V_\nu^* \rho, \qquad c_\nu > 0; \qquad c_\nu = 1 \quad \text{iff} \quad V_\nu^* = V_\nu$$

(ii′) $[H, \omega] = 0$ and $J_\nu(\omega) = 0$ (hence $L_{\nu *}^{(d)}\omega = 0$) for all ν.

If these conditions are fulfilled, the generator can be expressed in the form

$$L_*\rho = -i[H, \rho] + \frac{1}{2}\sum_\nu \{[V_\nu, \omega[\omega^{-1}\rho, V_\nu^*]] + [V_\nu^*, [\rho\omega^{-1}, V_\nu]\omega]\} \quad (11)$$

Proof. First suppose that L_* satisfies the condition of detailed balance formulated as in (i) and (ii). By Alicki's result,[7] reformulated in a stronger form by Kossakowski *et al.* (see the remark at the end of Section 2 of Ref. 5), L_* has the form given by the first equality of (i′) and (ii′) is satisfied. The second equality of (i′) is a straightforward identity.

Conversely, assume (i′) and (ii′). From (ii′) and the second form of $L_{\nu *}^{(d)}$ in (i′), (i) follows immediately. From $J_\nu(\omega) = 0$, it follows that $\Phi_\omega V_\nu^* = c_\nu V_\nu^*$, $\Phi_\omega V_\nu = c_\nu^{-1} V_\nu$ and hence, by the first form of $L_{\nu *}^{(d)}$ in (i′), $L_*^{(d)}\Phi_\omega = \Phi_\omega L_*^{(d)}$. This implies (ii). Finally, (11) is obtained by substituting

$$J_\nu(\rho) = \rho V_\nu^* - (\Phi_\omega V_\nu)\rho = \omega[\omega^{-1}\rho, V_\nu^*]$$

into the second expression for $L_{\nu *}^{(d)}\rho$ in (i′). QED

Remark. Another useful representation of detailed balance concerning the dissipative parts $L^{(d)}$ and $L_*^{(d)}$ is expressed as

$$L_*^{(d)}(X\omega)\omega^{-1} = \omega^{-1}L_*^{(d)}(\omega X) = L^{(d)}X, \qquad X \in \mathscr{B}(\mathscr{H}) \quad (12)$$

as verified by using (10): the two equalities in (12) and $[H, \omega] = 0$ are equivalent to detailed balance (i) and (ii), where the first equality is equivalent to $L_*^{(d)}\Phi_\omega = \Phi_\omega L_*^{(d)}$ (and hence $L_*^{(d)}\Sigma_\omega{}^t = \Sigma_\omega{}^t L^d$) and the second to the fact that $L^{(d)}$ is Hermitian in the Hilbert space $\mathscr{B}_\omega(\mathscr{H})$, a characteristic of $L^{(d)}$ as the dissipative part.[5,7]

3. ENTROPY PRODUCTION UNDER THE CONDITION OF DETAILED BALANCE

Lindblad[10] proved a general inequality associated with relative entropy $S(\rho|\omega)$ defined for any two elements $\rho, \omega \in \mathscr{T}_+(\mathscr{H})$ in $\mathscr{B}(\mathscr{H})$ (and hence for any two normal states ρ, ω): $S(\Lambda\rho|\Lambda\omega) \leqslant S(\rho|\omega)$, where Λ is any completely positive, trace-preserving map, $\mathscr{T}_+(\mathscr{H}) \to \mathscr{T}_+(\mathscr{H})$. Thus for the trace-preserving, completely positive dynamical semigroup with a faithful stationary state

ω considered in Section 2

$$\text{Tr } \Lambda_{t*}\rho[\log(\Lambda_{t*}\rho) - \log \omega] \leqslant \text{Tr } \rho(\log \rho - \log \omega) \tag{13}$$

A formal differentiation with respect to t at $t = 0$ of both sides of (13) suggests that we write

$$\sigma(\rho|\omega) \equiv -\text{Tr } \rho L(\log \rho - \log \omega) \tag{14}$$

$$= -\left[\frac{d}{dt} S(\Lambda_{t*}\rho|\omega)\right]_{t=0} \geqslant 0 \tag{15}$$

and that we call the quantity $\sigma(\rho|\omega)$ the entropy production associated with the (normal) state ρ relative to the (faithful, normal) state ω.

Spohn[3] has shown a rigorous differentiation procedure in the above, assuming an extra condition for ρ and ω that there exist two positive constants α_1 and α_2 such that $\alpha_1\omega < \rho < \alpha_2\omega$ is satisfied. This is certainly valid for finite systems [$\mathscr{B}(\mathscr{H})$ with dim $\mathscr{H} < \infty$] provided both states ρ and ω are faithful. Accordingly, one has (i) $\sigma(\omega|\omega) = 0$, (ii) $\sigma(\rho|\omega)$ is convex with respect to ρ, and (iii) $\sigma(\rho|\omega) \geqslant 0$ provided ω is stationary, i.e., $L_*\omega = 0$. [A simple proof of (ii) and (iii) on the basis of a theorem of Lieb[11] has been provided by Spohn.[1]] Here, with the additional assumption of detailed balance, we show a more explicit and tractable representation of the $\sigma(\rho|\omega)$ in the quantum correlation (or, relaxation) functions (a concept first introduced in the Kubo theory[12]).

Proposition 2. Let $\mathscr{B}_\omega(\mathscr{H})$ be the Hilbert space of the algebra $\mathscr{B}(\mathscr{H})$ where a scalar product of X and $Y \in \mathscr{B}(\mathscr{H})$ is defined in terms of a faithful state ω by

$$\langle X, Y\rangle_\omega = \text{Tr } \omega X^* Y \tag{16}$$

If a completely positive, trace-preserving dynamical semigroup defined on $\mathscr{B}(\mathscr{H})$ satisfies detailed balance wrt the state ω, then the entropy production $\sigma(\rho|\omega)$ associated with a state $\rho \in \{\omega\}'$ is given by

$$\sigma(\rho|\omega) = \int_0^1 \sum_\nu \langle(\rho\omega^{-1})^\theta[V_\nu, \log \rho\omega^{-1}](\rho\omega^{-1})^{1-\theta}, [V_\nu, \log \rho\omega^{-1}]\rangle_\omega \, d\theta \tag{17}$$

A deduction of this expression can be seen in the following series of lemmas.

Lemma 1. Lindblad's dissipation function[9] is defined by $D(L; X, Y) \equiv L(X^*Y) - (LX^*)Y - X^*(LY)$. If the generator L is represented as in (7), then

$$D(L; X, Y) = D(L^{(d)}; X, Y) = \sum_\nu [V_\nu^*, X^*][Y, V_\nu] \tag{18}$$

Lemma 2. In the Hilbert space $\mathscr{B}_\omega(\mathscr{H})$ the dissipative part of L, $L^{(d)}$, is a Hermitian operator under detailed balance wrt ω for which

$$\langle X, L^{(d)}Y\rangle_\omega = \langle L^{(d)}X, Y\rangle_\omega = -\tfrac{1}{2}\operatorname{Tr}\omega D(L; X, Y)$$
$$= -\frac{1}{2}\sum_\nu \{\langle [V_\nu, X], [V_\nu, Y]\rangle_\omega + c_\nu \langle [V_\nu{}^*, X], [V_\nu{}^*, Y]\rangle_\omega\} \tag{19}$$

Here the summation over ν in (18) is rearranged such that the two terms $[V_\nu{}^*, X^*][Y, V_\nu]$ and $c_\nu[V_\nu, X^*][Y, V_\nu{}^*]$ are combined into a single term in accordance with Proposition 1.

Remark. Alicki[7] showed that the Hilbert space adjoint L^+ of a linear (bounded) operator L with respect to scalar product (16) in $\mathscr{B}_\omega(\mathscr{H})$ $(\langle L^+X, Y\rangle_\omega = \langle X, LY\rangle_\omega)$ is related to the predual L_* in $\mathscr{B}(\mathscr{H})$ through $L^+X = L_*(X\omega)\omega^{-1}$ if $(LX)^* = LX^*$ is satisfied [this is true for L given in (7) and for L_* in (8)]. Therefore, the condition of detailed balance represented in (12) for the dissipative part $L^{(d)}$ is equivalent to

$$(L^{(d)+}X)^* = L^{(d)+}X^* = L^{(d)}X^*, \qquad X \in \mathscr{B}(\mathscr{H}) \tag{12'}$$

Lemma 3. The intertwining formula between a $V \in \mathscr{B}(\mathscr{H})$ and an invertible $\rho \in \mathscr{T}_+(\mathscr{H})$ is given by

$$[V, \rho] = \int_0^1 \rho^{1-\theta}[V, \log\rho]\rho^\theta\, d\theta \tag{20}$$

$$= \int_0^1 \rho^\theta[V, \log\rho]\rho^{1-\theta}\, d\theta \tag{20'}$$

Formula (20) is the integration with respect to θ, $0 \leqslant \theta \leqslant 1$, of the identity

$$\frac{d}{d\theta}(\rho^{1-\theta}V\rho^\theta) = \rho^{1-\theta}[V, \log\rho]\rho^\theta$$

and (20′) can be obtained by a change of the variable of integration, $\theta \to 1-\theta$.

On the basis of the above, one proceeds to calculate the entropy production $\sigma(\rho|\omega)$, noting that the Hamiltonian part does not contribute to $\sigma(\rho|\omega)$ $([\rho, \log\rho] = 0$ and $[H, \omega] = 0)$:

$$\sigma(\rho|\omega) = -\operatorname{Tr}\rho L^{(d)}(\log\rho - \log\omega) = -\operatorname{Tr}\omega\omega^{-1}\rho L^{(d)}(\log\rho - \log\omega)$$
$$= \frac{1}{2}\sum_\nu \{\langle [V_\nu, \rho\omega^{-1}], [V_\nu, \log\rho - \log\omega]\rangle_\omega$$
$$+ c_\nu\langle [V_\nu{}^*, \rho\omega^{-1}], [V_\nu{}^*, \log\rho - \log\omega]\rangle_\omega\}$$

by taking into account the second term $c_\nu\langle[V_\nu^*, X], [V_\nu^*, Y]\rangle_\omega$ associated with the term $\langle[V_\nu, X], [V_\nu, Y]\rangle_\omega$ in the sum (19). Note that

$$c_\nu[V_\nu^*, \rho\omega^{-1}] = [\Phi_\omega V_\nu^*, \Phi_\omega \omega^{-1}\rho] = \Phi_\omega[V_\nu^*, \omega^{-1}\rho]$$

$$= (\Phi_\omega^{-1}[\rho\omega^{-1}, V_\nu])^* = (\omega^{-1}[\rho\omega^{-1}, V_\nu]\omega)^*$$

by virtue of which

$$\sigma(\rho|\omega) = \frac{1}{2}\sum_\nu \{\langle[V_\nu, \rho\omega^{-1}], [V_\nu, \log\rho - \log\omega]\rangle_\omega + \langle[V_\nu, \log\rho - \log\omega], [V_\nu, \rho\omega^{-1}]\rangle_\omega\} \tag{21}$$

Assume that $\rho \in \{\omega\}'$, so that $[\rho, \omega] = 0$, and that ρ is faithful. The intertwining formulas (20) and (20′) then yield

$$\langle[V_\nu, \rho\omega^{-1}], [V_\nu, \log\rho - \log\omega]\rangle_\omega$$
$$= \int_0^1 \langle(\rho\omega^{-1})^\theta[V_\nu, \log\rho\omega^{-1}](\rho\omega^{-1})^{1-\theta}, [V_\nu, \log\rho\omega^{-1}]\rangle_\omega\, d\theta$$

$$\langle[V_\nu, \log\rho - \log\omega], [V_\nu, \rho\omega^{-1}]\rangle_\omega$$
$$= \int_0^1 \langle[V_\nu, \log\rho\omega^{-1}], (\rho\omega^{-1})^\theta[V_\nu, \log\rho\omega^{-1}](\rho\omega^{-1})^{1-\theta}\rangle_\omega\, d\theta$$
$$= \int_0^1 \langle(\rho\omega^{-1})^\theta[V_\nu, \log\rho\omega^{-1}](\rho\omega^{-1})^{1-\theta}, [V_\nu, \log\rho\omega^{-1}]\rangle_\omega\, d\theta$$

showing that both expressions are identical. Hence the expression (17) follows.

In the above connection we summarize the property of a sesquilinear form of X and Y defined for a fixed faithful state $\rho \in \{\omega\}'$ by

$$q(\rho; X, Y) \equiv \frac{1}{2}\int_0^1 \sum_\nu \{\langle(\rho\omega^{-1})^\theta[V_\nu, X](\rho\omega^{-1})^{1-\theta}, [V_\nu, Y]\rangle_\omega + \langle(\rho\omega^{-1})^\theta[V_\nu, Y^*](\rho\omega^{-1})^{1-\theta}, [V_\nu, X^*]\rangle_\omega\}\, d\theta \tag{22}$$

Lemma 4. Let $q(\rho; X, Y)$ be a sesquilinear form $\mathscr{B}(\mathscr{H}) \times \mathscr{B}(\mathscr{H}) \mapsto \mathbb{C}$ given in (22). Then it is Hermitian and positive. It is symmetric for the subspace of all self-adjoint elements $\mathscr{B}^s(\mathscr{H}) = \{X \in \mathscr{B}(\mathscr{H});\, X = X^*\}$:

(i) $\overline{q(\rho; Y, X)} = q(\rho; X, Y), \qquad X, Y \in \mathscr{B}(\mathscr{H})$

(ii) $q(\rho; Y, X) = q(\rho; X, Y), \qquad X, Y \in \mathscr{B}^s(\mathscr{H})$

(iii) $q(\rho; X, X) \geqslant 0 \qquad X \in \mathscr{B}(\mathscr{H})$

The entropy production $\sigma(\rho|\omega)$ under detailed balance (17) is given by

$$\sigma(\rho|\omega) = q(\rho; X - \log\omega, X - \log\omega)_{X=\log\rho} \tag{23}$$

Remark. The symmetry (ii) stems from the presence of the second term associated with the first in the integrand in (22) due to detailed balance, and is independent of (i). Both symmetries are combined to conclude that $q(\rho; X, Y)$ is real for any real elements X and Y.

4. CHARACTERIZATION OF THE STATIONARY STATE OF A DYNAMICAL SEMIGROUP IN A WIDER CLASS

Theorem 1. Let L be the generator of a completely positive, identity-preserving dynamical semigroup defined on $\mathscr{B}(\mathscr{H})$, $\dim \mathscr{H} < \infty$, decomposed into a sum $L = \sum_{k=1}^{r} L_k$ such that each L_k, with vanishing Hamiltonian part, satisfies detailed balance wrt a faithful stationary state ω_k. Let all the modular automorphism groups of ω_k, $k = 1,..., r$, be assumed to commute with the semigroup. Then, there exists at least one stationary state of the semigroup in the commutant $\{\omega_1,..., \omega_r\}'$. A faithful state $\omega \in \{\omega_1,..., \omega_r\}'$ is stationary under the semigroup map, iff

$$\log \omega \in \mathscr{H}_{\min}(\omega) \equiv \left\{X_m;\ \min_{X \in \mathscr{B}^s(\kappa)} a(\omega, X) = a(\omega, X_m)\right\} \tag{24}$$

where $a(\rho, X)$ is defined for a fixed faithful state $\rho \in \{\omega_1,..., \omega_r\}'$ and an $X \in \mathscr{B}(\mathscr{H})$ by

$$a(\rho, X) \equiv \sum_{k=1}^{r} q_k(\rho; X - \log \omega_k, X - \log \omega_k) \tag{25}$$

in which $q_k(\rho; X, Y)$ is given by (22) with $V_\nu = V_\nu^{(k)}$, $\omega = \omega_k$, and hence

$$a(\rho, \log \rho) = \sum_{k=1}^{r} \sigma(\rho|\omega_k) \tag{26}$$

Proof. Suppose that a semigroup $\{\Lambda_t; 0 \leqslant t < \infty\}$ satisfies the hypothesis of the theorem, i.e. (besides the dynamical structure and finiteness),

$$\Sigma_{\omega^k}^t \Lambda_t = \Lambda_t \Sigma_{\omega^k}^t, \qquad k = 1,..., r$$

where $\Sigma_{\omega^k}^t = \omega_k^{it} \cdot \omega_k^{-it}$ (the modular automorphism of ω_k) and $L_{k*}\omega_k = 0$. It then follows that the commutant $\{\omega_1,..., \omega_r\}'$ is stable under the semigroup maps Λ_t and Λ_{t*}, i.e.,

$$\Lambda_t, \Lambda_{t*}\{\omega_1,..., \omega_r\}' \subset \{\omega_1,..., \omega_r\}'$$

Since $\{\omega_1,..., \omega_r\}'$ is compact and Λ_t is contractive, the Markov–Kakutani fixed-point theorem[13] ensures the existence of a stationary state in $\{\omega_1,..., \omega_r\}'$. (A sufficient condition of its uniqueness and faithfulness, viz. $\{V_\nu\}' = \mathbb{C}1$, has been pointed out.[3] Let us now proceed to the variational principle of the theorem.

Since the variation function $a(\rho, X)$ with a fixed ρ (a faithful state belonging to $\{\omega_1, \ldots, \omega_r\}'$) is a positive, inhomogeneous quadratic form of $X \in \mathscr{B}(\mathscr{H})$ by the definition of $q(\rho; X, Y)$ in (22), it can be represented as

$$\tfrac{1}{2}a(\rho, X) = \tfrac{1}{2}(X, A\rho X) - \mathrm{Re}(F_\rho, X) + \mathrm{const}$$

where the scalar product (X, Y) is defined by Tr $X^* Y$, and the operator A_ρ and the vector F_ρ, both depending on ρ, are of the form

$$A_\rho = \sum_{k=1}^{r} A_{k\rho}, \qquad F_\rho = \sum_{k=1}^{r} A_{k\rho} \log \omega_k \tag{27}$$

By virtue of the symmetries (i) and (ii) in Lemma 4, $(X, A_\rho Y)$ is real for self-adjoint elements $X, Y \in \mathscr{B}^s(\mathscr{H})$ and $A_{k\rho}$ is symmetric, i.e., $(X, A_{k\rho} Y) = (A_{k\rho} X, Y)$ holds for all k.

The problem of minimizing a bounded function of a vector X associated with a positive, symmetric bilinear form in a real vector space is elementary for the finite-dimensional case:

$$\tfrac{1}{2}(X, AX) - (F, X) = \min \qquad \text{iff} \quad AX = F$$

Remark. The condition of strict positivity (or nonsingularity) of the positive, symmetric linear operator A [i.e., $N(A) \equiv \{X; AX = 0\} = \{0\}$] is not assumed in the above statement: more specifically, the finite minimum of the form $\tfrac{1}{2}(X, AX) - (F, X)$ is attained by an X iff X satisfies the solvable linear equation $AX = F$ with $F \in N(A)^\perp$, where $N(A)^\perp$ denotes the orthogonal complement of the null space $N(A)$ in the vector space.

Therefore, in order to verify the equivalence between condition (24) and the stationariness condition for ω, it is necessary and sufficient to show that[2]

$$(A\omega X)_{X=\log \omega} = F_\omega \qquad \text{iff} \quad L_* \omega = \sum_{k=1}^{r} L_{k*} \omega = 0$$

Consider the first equality, into which the relations in (27) are inserted:

$$\sum_{k=1}^{r} A_{k\omega}(\log \omega - \log \omega_k) = 0$$

But this is shown to be precisely identical with the second equality, if we compare the following two relations:

$$q_k(\rho; X, Y) = \mathrm{Tr}(A_{k\rho} X) Y \qquad \text{for all} \quad X, Y \in \mathscr{B}^s(\mathscr{H})$$

$$q_k(\rho; X, Y)_{X=\log \rho - \log \omega_k} = -\mathrm{Tr}(L_{k*}\rho) Y \qquad \text{for all} \quad Y \in \mathscr{B}^s(\mathscr{H})$$

[2] In connection with the above remark, it is of interest to show that the operator A_ρ and the vector F_ρ given by (27) satisfy in fact the solvability condition $F_\rho \in N(A_\rho)^\perp$. It can be seen from $N(A_\rho) = \bigcap_{k=1}^{r} N(A_{k\rho})$ and hence $N(A_\rho)^\perp = N(A_{1\rho})^\perp + \cdots + N(A_{r\rho})^\perp$, which is ensured by the fact that A_ρ is the sum of the positive, symmetric operators $A_{1\rho}, \ldots, A_{r\rho}$.

The latter relation can be obtained by rewriting (22), applied to each $k = 1,\ldots, r$, as

$$q_k(\rho; X, Y) = \frac{1}{2} \int_0^1 \sum_\nu \operatorname{Tr}\{[V_\nu^{(k)}, \omega_k(\omega_k^{-1}\rho)^{1-\theta}[X, V_\nu^{(k)*}](\omega_k^{-1}\rho)^\theta] + [V_\nu^{(k)*}, (\omega_k^{-1}\rho)^\theta[X, V_\nu^{(k)}](\omega_k^{-1}\rho)^{1-\theta}\omega_k]\} Y\, d\theta$$

and by using the representation of L_{k*} in (11) and the intertwining formulas (20) and (20′) with ρ replaced by $\rho\omega_k^{-1}$, $\rho \in \{\omega_k\}'$. QED

Remark. From the above analysis it can be observed that the identity

$$\sum_{k=1}^{r} q_k(\rho; X - \log \omega_k, Y)_{X-\log\rho} = -\sum_{k=1}^{r} \operatorname{Tr}(L_{k*}\rho)Y, \qquad \forall Y \in \mathscr{B}^s(\mathscr{H})$$

holds, and that by virtue of this identity a convenient presentation of the variational principle of Theorem 1 may be expressed as

$$\begin{aligned} \delta_X \tfrac{1}{2} a(\rho, X)_{X=\log\rho} &= \sum_{k=1}^{r} q_k(\rho; \log \rho - \log \omega_k, \delta X) \\ &= -\operatorname{Tr}(L_*\rho)\, \delta X \\ &= 0, \qquad \delta X = X - \log \rho \in \mathscr{B}^s(\mathscr{H}) \end{aligned} \tag{28}$$

to first-order increment δX, and $\delta^{(2)} \tfrac{1}{2} a(\rho, X) \geqslant 0$. Since the first-order variation is real for real δX, its vanishing for arbitrary $\delta X \in \mathscr{B}^s(\kappa)$ implies that $L_*\rho = 0$.

The variational calculus of the form (28) enables one to extend Theorem 1 to a more general class of dynamical semigroups, viz. to those whose generator has a nonvanishing Hamiltonian part and also a dissipative part that satisfies the same condition as in the theorem:

Theorem 2. Let $L = L^{(h)} + L^{(d)}$ be the generator of a completely positive, identity-preserving dynamical semigroup defined on $\mathscr{B}(\mathscr{H})$, $\dim \mathscr{H} < \infty$, with $L^{(h)} = i[H, \cdot]$ and $L^{(d)}$ of the same decomposed form as in Theorem 1. Let all the modular automorphism groups of ω_k, $k = 1,\ldots, r$, be assumed to commute with the semigroup. A faithful state $\omega \in \{\omega_1,\ldots, \omega_r\}'$ is stationary under the semigroup map iff

$$\log \omega \in \mathscr{H}_{\min}(\omega) \equiv \left\{ X_m;\ \min_{X \in \mathscr{B}^s(\mathscr{H})} (\operatorname{Tr} 2i[H, \omega]X + a(\omega, X)) = a(\omega, X_m) \right\} \tag{29}$$

where $a(\rho, X)$ is the same function as defined in Theorem 1.

Proof. The minimization of $\operatorname{Tr} 2i[H, \omega]X + a(\omega, X)$ on the right-hand side of (29) and its identification with $a(\omega, X_m)$ at $X_m = \log \omega$ is performed according to the variational calculus (28):

$$\delta_X(\mathrm{Tr}\, i[H,\omega]X + \tfrac{1}{2}a(\omega, X))_{X=\log\omega} = \mathrm{Tr}(i[H,\omega] - L_*^{(d)}\omega)\,\delta X$$
$$= 0, \qquad \delta X = X - \log\omega \in \mathscr{B}^s(\kappa)$$

which is satisfied iff $-i[H,\omega] + L_*^{(d)}\omega = L_*\omega = 0$, and

$$\delta_X^{(2)}(\mathrm{Tr}\, i[H,\omega]X + \tfrac{1}{2}a(\omega, X)) = \delta^{(2)}\tfrac{1}{2}a(\omega, X) \geqslant 0 \quad \text{QED}$$

5. APPLICATION TO LEBOWITZ-TYPE OPEN SYSTEMS WITH SEVERAL THERMAL RESERVOIRS

From a mathematical point of view, the Lebowitz model[2,4] can be looked upon as a special example of our Theorem. Namely, every ω_k, the stationary state of the dissipative generator L_k, $k = 1,\ldots, r$, is given by the canonical equilibrium state with temperature β_k^{-1} and a common Hamiltonian $H \in \mathscr{B}^s(\mathscr{H})$, i.e.,

$$\omega^k = Z_k^{-1} e^{-\beta_k H}, \qquad Z_k = \mathrm{Tr}\, e^{-\beta_k H}$$

Clearly, all the automorphism groups $\{\Sigma_{\omega k}^t\}$, $k = 1,\ldots, r$, coincide and the commutant $\{\omega_1,\ldots,\omega_r\}'$ reduces to $\{H\}'$. The Hamiltonian H that arises in the Hamiltonian part $L^{(h)} = i[\bar{H}, \cdot]$ may be different from H but still $\bar{H} \in \{H\}'$ (this is actually the case in the explicit construction of the generator by the weak coupling limit theory, where the original Hamiltonian H admits a shift ΔH, $[\Delta H, H] = 0$[1,2,6]). Thus our Theorem 2 may apply (actually it reduces to Theorem 1).

Corollary. Let $L = i[\bar{H}, \cdot] + \sum_{k=1}^r L_k$ be the generator of a dynamical semigroup which represents the Lebowitz model, where L_k, a dissipative generator in Theorem 1, satisfies detailed balance wrt $\omega_k = Z_k^{-1} e^{-\beta_k H}$, $k = 1,\ldots, r$. The stationary state ω of the semigroup (which is stationary of both generators $L^{(h)}$ and $L^{(d)}$, though L may not be normal) is characterized by

$$\log\omega \in \left\{X_m;\ \min_{X\in\mathscr{B}^s(\mathscr{H})} a(\omega, X) = a(\omega, X_m)\right\}, \qquad a(\omega, \log\omega) = \sum \beta_k \frac{dQ_k}{dt} \tag{30}$$

where $dQ_k/dt = -\mathrm{Tr}\,\omega(L_k H)$ represents the heat flow from the system into the kth reservoir: the minimal value is identified with the thermodynamic entropy production.

6. THERMODYNAMIC STABILITY AGAINST FLUCTUATIONS

The positive quadratic form $q(\rho; X, X)$ defined by the expression (22) can be identified with the coefficient of λ^2 of the power series expansion in λ

of the function

$$Z(\rho, X; \lambda) = \operatorname{Tr} \exp[\log \rho\omega^{-1} + \lambda S(X)], \qquad \rho \in \{\omega\}'$$

where

$$S(X) = \sum_{\nu} \{[V_\nu, X]\omega^{1/2} + ([V_\nu, X]\omega^{1/2})^*\}$$

$\{V_\nu\}$ satisfying condition (10). The function $Z(\rho, X; \lambda)$ is convex with respect to $X \in \mathscr{B}(\mathscr{H})$. Also, it is concave with respect to faithful states $\rho \in \mathscr{T}_+(\mathscr{H})$ according to a theorem of Lieb's.[11] Hence $q(\rho; X, X)$ has the same properties [the concavity of $q(\rho; X, X)$ wrt ρ is a consequence of the Wigner–Yanase–Dyson conjecture, the validity of which was shown to be equivalent to that of $Z(\rho, X; \lambda)$ by Lieb]. We infer that physically it represents a measure of fluctuations which influence a state ρ driven arbitrarily from the equilibrium state ω. In terms of this, the entropy production associated with ρ relative ω is given by

$$\sigma(\rho|\omega) = \frac{1}{2}\left[\frac{\partial^2}{\partial\lambda^2} Z(\rho, X - \log\omega; \lambda)\right]_{X = \log\rho,\, \lambda = 0}$$

We note that Spohn's variation principle selects those ρ that satisfy

$$\sigma(\rho|\omega) = \min_{\rho' \in \mathscr{T}_+(\mathscr{H}),\ \operatorname{Tr}\rho' = 1} \sigma(\rho'|\omega) = 0$$

The set of the solutions of this variation problem includes the set of all the stationary solutions $L_*\rho = 0$, $\rho \in \mathscr{T}(\mathscr{H})$, with

$$L_* = \frac{1}{2}\sum_{\nu} ([V_\nu, \cdot V_\nu^*] + [V_\nu \cdot, V_\nu^*])$$

but in general the latter set is a proper subset of the former such that

$$\{\rho \in \mathscr{T}_+(\mathscr{H});\ L_*\rho = 0\} \subsetneq \{\rho \in \mathscr{T}_+(\mathscr{H});\ \sigma(\rho|\omega) = 0\}$$

(Corollary 4 of Ref. 1). On the other hand, our variational principle selects precisely every stationary solution of the above L_*: It selects those ρ that satisfy $X_{\min}(\rho) = \log\rho$, where $X_{\min}(\rho)$ is any solution of the minimum problem

$$Z^{(2)}(\rho, X_{\min}(\rho) - \log\omega) = \min_{X \in \mathscr{B}^s(K)} Z^{(2)}(\rho, X - \log\omega) = 0$$

where

$$Z^{(2)}(\rho, X) = \frac{1}{2}\left[\frac{\partial^2}{\partial\lambda^2} Z(\rho, X; \lambda)\right]_{\lambda = 0}$$

The additional condition that such a minimum be at $X = \log\rho$ imposes a requirement on ρ that is the stationariness condition $L_*\rho = 0$.

The variational technique of the second type was proposed by Prigogine under the name of "local potential,"[14] to which our solution of the problem of characterizing the stationary state in a class of quantum dynamical semigroups conforms in its spirit. Its physical motivation, *stability against fluctuations*, was discussed in Ref. 15. We hope to find a more systematic foundation of the variational principle of this kind (cf. Ref. 16).

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REFERENCES

1. H. Spohn, *J. Math. Phys.* **19**:1227 (1978).
2. H. Spohn and J. L. Lebowitz, *Adv. Phys. Chem.* **38**:109 (1978).
3. A. Frigerio and H. Spohn, *Stationary States of Quantum Dynamical Semigroups and Applications* (Lecture Notes at the meeting, Mathematical Problems in the Theory of Quantum Irreversible Processes, Arco Felice, Italy, 1978).
4. P. G. Bergmann and J. L. Lebowitz, *Phys. Rev.* **99**:578 (1955).
5. A. Kossakowski, A. Frigerio, V. Gorini, and M. Verri, *Commun. Math. Phys.* **57**:97 (1977).
6. V. Gorini, A. Frigerio, M. Verri, A. Kossakowski, and E. C. G. Sudarshan, *Rep. Math. Phys.* **13**:149 (1978).
7. R. Alicki, *Rep. Math. Phys.* **10**:249 (1976).
8. V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, *J. Math. Phys.* **17**:821 (1976).
9. G. Lindblad, *Commun. Math. Phys.* **48**:119 (1976).
10. G. Lindblad, *Commun. Math. Phys.* **40**:147 (1975).
11. E. H. Lieb, *Adv. Math.* **11**:267 (1973).
12. R. Kubo, *J. Phys. Soc. Japan* **12**:570 (1957).
13. N. Dunford and J. T. Schwartz, *Linear Operators* (Interscience, New York, 1958, Part I, V.10.6.
14. P. Glansdorff and I. Prigogine, *Thermodynamic Theory of Structure Stability and Fluctuations* (Wiley–Interscience, London, 1971).
15. I. Prigogine and P. Glansdorff, *Physica* **31**:1242 (1965).
16. H. Hasegawa, *Prog. Theor. Phys.* **58**:128 (1977).
17. H. Hasegawa and T. Nakagomi, *Prog. Theor. Phys. Suppl.* **64**:321 (1978).
18. H. Hasegawa and T. Nakagomi, *J. Stat. Phys.* **21**:191 (1979).
19. H. Hasegawa, T. Nakagomi, M. Mabuchi, and K. Kondo, *J. Stat. Phys.* **23**:281 (1980).