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# Entropy Production and Nonequilibrium Stationarity in Quantum Dynamical Systems. Physical Meaning of van Hove Limit

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With aid of the so-called dilation method, a concise formula is obtained for the entropy production in the algebraic formulation of quantum dynamical systems. In this framework, the initial ergodic state of an external force system plays a pivotal role in generating dissipativity as a conditional expectation. The physical meaning of van Hove limit is clarified through the scale-changing transformation to control transitions between microscopic and macroscopic levels. It plays a crucial role in realizing the macroscopic stationarity in the presence of microscopic fluctuations as well as in the transition from non-Markovian (groupoid) dynamics to Markovian dissipative processes of state changes. The extension of the formalism to cases with spatial and internal inhomogeneity is indicated in the light of the groupoid dynamical systems and noncommutative integration theory.

**KEY WORDS:** Entropy production; nonequilibrium stationarity; dilation method; van Hove limit; groupoid dynamical system.

## 1. INTRODUCTION

As is well known, Kubo's linear response theory[1] allows one to calculate most effectively transport coefficients, the quantities intimately related to the *dissipative* aspects of the nonequilibrium and irreversible processes. Since it is formulated in the framework of dynamical systems with *reversible* time developments, however, the origin of such dissipativity as expressed by the positivity of the transport coefficients has been rather mysterious.[2,3] Further, the notions of entropy and entropy production have not been formulated in an explicit form there, in spite of their strong

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connection with transport coefficients. The attempt to fill this gap has been undertaken in ref. 4 by trying to give a sensible definition of entropy production satisfying positivity in the framework of nonlinear response theory of quantum dynamical systems. There we encounter two different kinds of time averaging procedures, the initial- and final-time averaging, which are crucial for ensuring the positivity of entropy production as well as the stationarity of the final nonequilibrium state. The aim of the present paper is to clarify the physical nature of these time averaging procedures in their technical guise, and, by doing so, to clarify the structure of nonequilibrium states in their relation to microscopic dynamics.

For this purpose, it is important to note the close relationship between the scale changes of spacetime lengths and such thermodynamic notions as temperature and "adiabatic switching procedures," etc. For instance, since temperature changes in the opposite direction to the time coordinate in the scale change as shown in ref. 5, our macroscopic world with finite temperatures will be observed by the microscopic observers, if any, in the vacuum state at zero temperature. In view of the actual physical world far from an equilibrium with a uniform temperature, it would be a very important step in implementing the "unification program" of physics to find the connections or transitions among (i) microscopic physics at $T=0$ K described in quantum field theory on the vacuum, (ii) local physics of condensed matter in equilibrium with $T\neq 0$ K treated by statistical mechanics, and (iii) the nonequilibrium self-organizing levels with inhomogeneous structures in evolution processes. In what follows, we will be concerned with the problem of finding some route from the paradigm (ii) toward (iii) taking the notion of entropy production as a guiding principle.

In the next section, we briefly recapitulate the result on the entropy production obtained in ref. 4. In Section 3, our time-inhomogeneous system under the influence of time-dependent external force will be embedded into a larger time-independent system together with the external force driven by its own dynamics. This so-called "dilation technique" will be helpful in understanding the physical structures involved in the situation under consideration. For instance, it clarifies in Section 4 the essential role of the scale changing procedure of the van Hove limit. It is important to note that the dissipativity associated with nonvanishing entropy production in nonequilibrium stationary states means the coexistence of two conflicting aspects, the *stationarity* of the state on one hand and the constant *increase* in the entropy of the system on the other hand. What reconciles this conflict is just the *discrimination of two levels*, microscopic and macroscopic, *interconnected* through the time-scale change in van Hove limit. In the final section, Section 5, we discuss the problem of the inhomogeneous substructures inherent in nonequilibrium stationarity from the viewpoint of a *multi-*

*ple-reservoir system.*[6] For the consistent treatment of spacetime nonequilibrium phenomena such as inhomogeneous temperature distributions, thermal diffusions, etc., quantum-field-theoretic extension of the present framework in combination with the continuous version of multiple-reservoir systems seems to be very important. From this viewpoint, possible relevance of the notion of *groupoid dynamical systems*[7,8],2 to the present context is indicated through the reformulation of the obtained results in terms of groupoid notations.

## 2. RESUME ON ENTROPY PRODUCTION IN QUANTUM DYNAMICAL SYSTEMS

### 2.1. Entropy Production in General Framework of Nonlinear Response Theory

Let the observables and dynamics of our object system be described by an algebra $\mathfrak{A}$ (to be specified as a $C^*$-algebra when necessary) and a one-parameter automorphism group $\alpha_t$ on it (assumed to be strongly continuous in the $C^*$-algebra context). In this general setup, the notion of the temperature equilibrium states has been successfully formulated[10,11] in terms of the KMS condition. In view of the zeroth law of thermodynamics expressing the *stability* of the equilibrium states, we adopt here the viewpoint that the temperature *equilibrium* should be represented by an *ergodic* KMS state (nonergodic KMS states will correspond to mixed thermodynamic phases or metastable states).

Then, any other states *outside* this category would be interpreted as the nonequilibrium ones from this standpoint. Obviously, such an "abstract definition" in a negative expression cannot convey any positive messages about the dynamic aspects of nonequilibrium in the actual physical world. In order to avoid this kind of *a priori* definition, we consider here the "adiabatic switching procedure" to creat a nonequilibrium state from a temperature equilibrium state $\omega_\beta$ prepared at "infinite past $t_0 \to -\infty$" by perturbing the system with external force $\mathbb{X}(t) \equiv (X_1(t),..., X_n(t))$. If $\mathbb{X}(t)$ couples to the system variable $\mathbb{A} \equiv (A_1,..., A_n)$, $A_i \in \mathfrak{A}$, through a coupling Hamiltonian $H_I(t)$ given by

$$H_I(t) = -\mathbb{A} \cdot \mathbb{X}(t) \equiv -\sum_i A_i X_i(t) \tag{2.1}$$

[2] See ref. 9 for a recent overview.

the time-dependent perturbed dynamics of the system is described by a family of automorphisms $\alpha_{s,t;\mathbb{X}}$ on $\mathfrak{A}$ characterized by the equation

$$\frac{d}{dt}\alpha_{s,t;\mathbb{X}}(B) = \alpha_{s,t;\mathbb{X}}(\delta(B) + [iH_I(t), B]) \tag{2.2}$$

together with the initial condition $\alpha_{s,t=s} = \mathrm{Id}_{\mathfrak{A}}$. Here $\delta$ is the infinitesimal generator of the unperturbed dynamics $\alpha_t$,

$$\frac{d}{dt}\alpha_t(B) = \alpha_t \circ \delta(B) \tag{2.3}$$

defined on some dense subset of observables $B$ in $\mathfrak{A}$. The solution of this equation can be expressed for an arbitrary observable $B \in \mathfrak{A}$ as

$$\alpha_{s,t;\mathbb{X}}(B) = \alpha_{-s}[U(t, s; \mathbb{X})^* \alpha_t(B)\, U(t, s; \mathbb{X})] \tag{2.4}$$

in terms of the "propagator" $U(t, s; \mathbb{X})$ in the interaction picture:

$$U(t, s; \mathbb{X}) = T \exp\left\{ i \int_s^t d\tau\, \alpha_\tau(\mathbb{A}) \cdot \mathbb{X}(\tau) \right\} \tag{2.5}$$

On the basis of the formula due to Ichiyanagi[12] relating the external force to the relative entropy[13] between the initial state $\varphi_{t=t_0} \equiv \omega_\beta$ and the state $\varphi_t \equiv \omega_\beta \circ \alpha_{t_0,t}$ at present time $t$,

$$S(\varphi_t \,|\, \varphi_{t_0} = \omega_\beta) = \beta \int_{t_0}^t ds\, \varphi_s(\delta(\mathbb{A})) \cdot \mathbb{X}(s) \tag{2.6}$$

"microscopic" entropy production $P(t, t_0; \mathbb{X})$,[12] and *mean* entropy production $\bar{P}$,[4] are defined, respectively, by

$$\begin{aligned} P(t, t_0; \mathbb{X}) &\equiv \frac{d}{dt} S(\varphi_t \,|\, \omega_\beta) \\ &= \beta \varphi_t(\delta(\mathbb{A})) \cdot \mathbb{X}(t) \\ &\equiv \beta \langle \mathbb{J} \rangle(t) \cdot \mathbb{X}(t) \end{aligned} \tag{2.7}$$

$$\begin{aligned} \bar{P} &\equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \lim_{T_0\to\infty} \frac{1}{T_0} \int_{-T_0}^0 dt_0\, P(t + t_0, t_0; \mathbb{X}) \\ &= \lim_{T\to\infty} \frac{1}{T} \lim_{T_0\to\infty} \frac{1}{T_0} \int_{-T_0}^0 dt_0\, S(\varphi_{T+t_0} \,|\, \varphi_{t_0} = \omega_\beta) \geqslant 0 \end{aligned} \tag{2.8}$$

The operator $\mathbb{J}$ in (2.7) is the current operator conjugate to the external force $\mathbb{X}(t)$ defined by

$$\mathbb{J} = \delta(\mathbb{A}) \tag{2.9}$$

Although the relative entropy $S(\varphi_t \mid \omega_\beta)$ is always nonnegative,[13] the "microscopic" entropy production $P(t, t_0; \mathbb{X})$ in (2.7) may become temporarily negative and the first limit, initial time average, is essential for the positivity of the mean entropy production $\bar{P}$, (2.8). The latter limit is important for attaining the stationarity of the final state. Owing to their technical nature, the physical meaning of these limits may not be clear at this stage. We will see in the following their crucial roles in the transitions from the regimes of reversible dynamical systems to the regimes characterized by the nonequilibrium stationary structures and their evolution processes in the real physical world.

## 2.2. Initial and Final Long-Time Averages and Almost Periodicity

In order for these two limiting procedures to be meaningful, we need first to give some suitable characterizations to the external force $\mathbb{X}(t)$. In Kubo's linear response theory, for instance, it is customary to choose *periodic* perturbations (with some damping factor). On the other hand, if the external force $\mathbb{X}(t)$ is taken as *random noise*, then our formulation reduces to the standard stochastic process approach. In the former case, it would be difficult to get out of thermodynamic branches due to the stability property of equilibrium states,[11] and the physical origin of dissipativity is liable to be missed in the formal procedure of linear approximation.[3] As for the latter case, dynamics of the system is described from the beginning by an irreversible stochastic process with dissipativity, but the probabilistic law governing the noise is just an input brought into the theory by hand.

If we want to seek the dynamical origin of dissipativity and the natural framework accommodating the nonequilibrium structure belonging to non-thermodynamic branches, what is most crucial is to find some interpolating bridges between these two extreme opposite cases, ⟨periodic regularity⟩ vs. ⟨chaotic randomness⟩. Although the traditional branches of physics have covered both of these extremes, the intermediate regions remain to be cultivated. In this respect, the notion of almost periodicity (e.g., refs. 14 and 15) is very remarkable as it encompasses some of the most important aspects of the "complexity" intervening between the above two opposites without being absorbed into either one. The pertinence of the choice of almost-periodic perturbation adopted in ref. 4 could most suitably be judged from this point of view.

Although the physical essence of the almost-periodic perturbation can be seen in Section 5 from the more general context of groupoid dynamical systems[7] in noncommutative integration theory,[8] we start our discussion, just to fix notations, from the definition of almost periodicity[14] in the special case of a one-dimensional Abelian group $\mathbb{R}$ identified with the time axis.

(i) A continuous function $X(t)$ is said to be *almost periodic* in $t \in \mathbb{R}$ if it can be approximated uniformly by linear combinations of the periodic functions: $X(t) = \sum_k a_k \exp i\omega_k t$ [convergence in the uniform topology with norm $\|X\| \equiv \sup_{t \in \mathbb{R}} |X(t)|$]. By Bochner's theorem,[14] this is equivalent to the condition that the orbit $\{X_\lambda; \lambda \in \mathbb{R}\}$ of $X(t)$ under the time flow $X_\lambda(t) \equiv X(t-\lambda)$ is *precompact* in the uniform topology.

(ii) On the basis of the latter condition, the *hull* $M_X$ of $X(t)$ is defined as the completion of this orbit in the uniform topology

$$M_X \equiv \overline{\{X_\lambda; \lambda \in \mathbb{R}\}} \tag{2.10}$$

and it turns out to be a *compact* Abelian group[3] having a unique normalized *Haar measure* $\mu$. As a probability measure, $\mu$ can be interpreted as a *state* on the commutative algebra $C(M_X)$. The time translation group $\mathbb{R}$ acts on $M_X$ by extending $X \mapsto X_\lambda$ by continuity and each orbit is dense in $M_X$. Thus, denoting the time flows on the hull $M_X$ and on the algebra $C(M_X)$, respectively, by $\lambda_t$ and $\sigma_t$,

$$\lambda_t \xi \equiv \xi_t \qquad \text{for} \quad \xi \in M_X \tag{2.11a}$$

$$(\sigma_t f)(\xi) \equiv f(\xi_{-t}) \qquad \text{for} \quad f \in C(M_X) \tag{2.11b}$$

we obtain an ergodic classical dynamical system $(C(M_X), \sigma_t, \mu)$. Now the time dependence of $X(t)$ can be totally absorbed in this time flow $\sigma_t$, and the remaining degrees of freedom specifying the function $X(t)$ itself are represented by a time-independent function $\hat{X}(\xi)$ on $M_X$ so that there exists a $\xi^{(0)} \in M_X$ satisfying

$$X(t) = \hat{X}(\xi^{(0)}_{-t}) \tag{2.12}$$

In view of the expansion $X(t) = \sum_k a_k \exp i\omega_k t$, a point $\xi$ and the flow $\lambda_t$ on the hull $M_X$ can be identified, respectively, with a sequence $\xi = (\xi_k)$,

[3] The multiplication law in $M_X$ is given by extending the definition $X_s * X_t \equiv X_{s+t}$ on the dense subset to the whole $M_X$ by continuity.

$\xi_k \in \mathbb{T}$, on the torus $\mathbb{T}$, and with $\lambda_t(\xi) \equiv (e^{-i\omega_k t}\xi_k)$. The function $\hat{X}$ then corresponds to the sequence $(a_k)$ of the expansion coefficients of $X(t)$: $\hat{X}(\xi) = \sum_k a_k \xi_k$. Physically, the variable $\xi$ on the hull $M_X$ may be interpreted as the *microscopic fluctuations* of the external force $X(t)$ and its coefficients $(a_k)$ as the time-independent "shape" of $X(t)$ determined by the macroscopic experimental setup of the apparatus.

(iii) Due to the ergodicity of the flow $\sigma_t$, the long-time average agrees with the "ensemble average" for any $L^1$ function $G(\xi)$ on $M_X$:

$$\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, G(\xi_{-t}) = \int_{M_X} d\mu(\xi)\, G(\xi) \tag{2.13}$$

By exploiting some of these facts, it has been shown in ref. 4 that the initial time average

$$\lim_{T_0\to\infty} \frac{1}{T_0}\int_{-T_0}^{0} dt_0$$

in (2.8) always exists, being equal to the $\mu$-average over the hull $M_X$ of $\mathbb{X}$ if the external force $\mathbb{X}(t)$ is taken to be almost periodic:

$$\begin{aligned}\bar{P} &\equiv \lim_{T\to\infty} \frac{1}{T}\int_0^T dt \lim_{T_0\to\infty} \frac{1}{T_0}\int_{-T_0}^{0} dt_0\, P(t+t_0, t_0; \mathbb{X}) \\ &= \lim_{T\to\infty} \frac{1}{T}\int_0^T dt \int_{M_X} d\mu(\xi)\, P(t, 0; \xi)\end{aligned} \tag{2.14}$$

[To be precise, what has been shown in ref. 4 is the almost-periodicity of $P(t, 0; \mathbb{X})$ in $t$ which allows one to extend this function onto the hull as $P(t, 0; \xi)$ with $\xi \in M_X$, but the expression involving the Haar measure $\mu$ does not appear there.] Thus, it allows us to take the limit of "infinite past $t_0 \to -\infty$" even if the limit state $\lim_{t_0\to-\infty} \omega_\beta \circ \alpha_{t_0,t}$ itself does not exist [as in the case of oscillating perturbation $\mathbb{X}(t)$ without the damping factor for adiabatic switching control]. As for the final time averaging limit, $\lim_{T\to\infty}(1/T)\int_0^T dt$, however, it is *not uniquely* determined in general, and we need to choose some suitable subsequence $(T_n)_{n\in\mathbb{N}}$ tending to $+\infty$, the existence of which is ensured by Markov–Kakutani fixed-point theorem.[16]

At the end of this résumé of ref. 4, we note that the (Abelian) group structure did not play an essential role in the above except for ensuring the uniqueness of the initial-time averaging limit identified with the Haar measure $\mu$ on the hull $M_X$. Since the compact hull can be associated with any bounded, uniformly continuous function being defined as the Gel'fand spectrum of the commutative $C^*$-algebra generated by its translates,[17] the present setting can be extended to any external force $\mathbb{X}$ such that the dynamical system $(C(M_X), \sigma_t)$ associated with it has a *unique* ergodic measure $\mu$ on its hull $M_X$.

# 3. REFORMULATION OF ENTROPY PRODUCTION IN ENLARGED DYNAMICAL SYSTEM

## 3.1. Embedding of Time-Dependent Dynamics into Time-Independent Composite System

With the aid of the hull $M_X$ of external force $\mathbb{X}(t)$, we now reformulate the problem of external-force perturbation as the coupling between *two physical systems*, the microscopic object system $(\mathfrak{A}, \alpha_t)$ and the classical dynamical system $(C(M_X), \sigma_t)$ on the hull $M_X$. They are glued together through this coupling into a composite total system with time-independent dynamics as follows.(18),4

First, the algebra $\mathfrak{B}$ of this composite system is defined by

$$\mathfrak{B} \equiv C(M_X, \mathfrak{A}) = \mathfrak{A} \otimes C(M_X) \tag{3.1}$$

$\mathfrak{B}$ can be identified interchangeably as the $C^*$-algebra of $\mathfrak{A}$-valued continuous functions $\xi \mapsto \hat{B}(\xi)$ on $M_X$ or the tensor-product algebra of $\mathfrak{A}$ with the commutative $C^*$-algebra $C(M_X)$ through the correspondence between $\xi \mapsto f(\xi)A$ and $A \otimes f$ for $A \in \mathfrak{A}$ and $f \in C(M_X)$. The algebra $\mathfrak{A}$ of the original object system is embedded in $\mathfrak{B}$ through the map $\iota$ given by

$$\iota\colon \mathfrak{A} \ni B \mapsto B \otimes \mathbb{1} \equiv \iota(B) \in \mathfrak{B} \tag{3.2}$$

To define a *composite dynamics* on this composite algebra $\mathfrak{B}$, we extend the perturbed dynamics $\alpha_{s,t;\mathbb{X}}$ given in (2.4) with parameter dependence on $\mathbb{X}$ into $\alpha_{s,t;\xi}$ with the variable $\xi$ on the hull $M_X$. This is justified by the continuity of $\alpha_{s,t;\mathbb{X}}$ (ref. 4) with respect to $\mathbb{X}$. It is easily seen that $\alpha_{s,t;\xi}$ satisfies the following two properties:

$$\alpha_{s,t;\xi} \circ \alpha_{t,u;\xi} = \alpha_{s,u;\xi} \qquad \text{(chain rule)} \tag{3.3}$$

$$\alpha_{s+\lambda,t+\lambda;\xi} = \alpha_{s,t;\xi_{-\lambda}} \qquad \text{(covariance condition)} \tag{3.4}$$

Then we can define a dynamics $\beta_t$ on the algebra $\mathfrak{B}$ of composite system by(18)

$$[\beta_t(\hat{B})](\xi) \equiv \alpha_{0,t;\xi}(\hat{B}(\xi_{-t})) \qquad \text{for} \quad \hat{B} \in \mathfrak{B} \tag{3.5}$$

4 The author is deeply indebted to Prof. J. Bellissard for his detailed and enlightening instructions in this direction.

By virtue of (3.3) and (3.4), $\beta_t$ is seen to be a time-independent dynamics satisfying the group property

$$\beta_s \circ \beta_t = \beta_{s+t} \tag{3.6}$$

Due to the ergodicity (2.13) of $\mu$, we obtain for an arbitrary state $\omega$ of $\mathfrak{A}$ and $\hat{B} \in \mathfrak{B}$

$$\begin{aligned}(\omega \otimes \mu)[\beta_t(\hat{B})] &= \int_{M_X} d\mu(\xi)\, \omega(\beta_t(\hat{B})(\xi)) \\ &= \lim_{T_0 \to \infty} \frac{1}{T_0} \int_{-T_0}^{0} dt_0\, \omega(\alpha_{t_0, t+t_0; \xi}(\hat{B}(\xi_{-t-t_0})))\end{aligned} \tag{3.7}$$

which shows the equivalence of the Haar measure $\mu$ with the initial time averaging procedure appearing in (2.8). Namely, the fictitious procedure of adiabatic switching with initial-time limit has been here replaced by an ergodic *state* $\mu$ of the external force system.

On the other hand, the problem concerning the final time limit is more complicated: Although both the initial states $\omega_\beta$ and $\mu$ are ergodic, respectively, for component dynamical systems $(\mathfrak{A}, \alpha_t)$ and $(C(M_X), \sigma_t)$, the product state $\omega_\beta \otimes \mu$ is in general *neither* stationary *nor* ergodic with respect to the composite dynamical system $(\mathfrak{B}, \beta_t)$. Therefore, the discussion about the final time limit requires us to investigate the dynamical behavior of the state $\omega_\beta \otimes \mu$ under the dynamics $\beta_t$ of the *total* system.

## 3.2. Entropy Production and Stationarity in Composite System

For this purpose, it is convenient to introduce the GNS representations $(\pi, \mathfrak{H}, \Omega, U_t = \exp iH_\beta t)$ and $(\pi_\mu, L^2(M_X, \mu), \mu^{1/2}, V_t = \exp it\Delta)$ associated, respectively, with the states $\omega_\beta$ and $\mu$ of the dynamical systems $(\mathfrak{A}, \alpha_t)$ and $(C(M_X), \sigma_t)$:

$$\omega_\beta(B) = \langle \Omega, \pi(B)\Omega \rangle \qquad \text{for} \quad B \in \mathfrak{A} \tag{3.8}$$

$$\mathfrak{H} = \overline{\pi(\mathfrak{A})\Omega} \qquad \text{(cyclicity)} \tag{3.9}$$

$$\pi(\alpha_t(B)) = U_t \pi(B) U_t^*; \qquad U_t = \exp iH_\beta t; \qquad H_\beta \Omega = 0 \tag{3.10}$$

$$\mu(f) = \int_{M_X} d\mu(\xi)\, f(\xi) \equiv \langle \mu^{1/2}, \pi_\mu(f)\, \mu^{1/2} \rangle \tag{3.11}$$

$$[\pi_\mu(f)\psi](\xi) \equiv f(\xi)\, \psi(\xi) \qquad \text{for} \quad f \in C(M_X), \quad \psi \in L^2(M_X, \mu) \tag{3.12}$$

$$(V_t\psi)(\xi) \equiv \psi(\xi_{-t}); \qquad \pi_\mu(\sigma_t f) = V_t \pi_\mu(f)\, V_t^*; \qquad V_t = \exp it\Delta \tag{3.13}$$

Then, the dynamical system $(\mathfrak{B}, \beta_t)$ can be represented in the Hilbert space $\mathfrak{H} \otimes L^2(M_X, \mu) = L^2(M_X, \mathfrak{H}; \mu)$ of $\mathfrak{H}$-valued $L^2$-functions on $(M_X, \mu)$ as

$$[\{(\pi \otimes \pi_\mu)(\hat{B})\} \psi](\xi) = \pi(\hat{B}(\xi))\, \psi(\xi), \qquad \hat{B} \in \mathfrak{B}, \quad \psi \in L^2(M_X, \mathfrak{H}; \mu) \tag{3.14}$$

$$(\pi \otimes \pi_\mu)(\beta_t(\hat{B})) = e^{itH}(\pi \otimes \pi_\mu)(\hat{B})\, e^{-itH} \tag{3.15}$$

where the generator $H$ is given by

$$H \equiv H_\beta \otimes \mathbb{1} + \mathbb{1} \otimes \Delta - \sum_i \pi(A_i) \otimes \pi_\mu(\hat{X}_i) \equiv H_\beta \otimes \mathbb{1} + \mathbb{1} \otimes \Delta - \pi \otimes \pi_\mu(\mathbb{A} \otimes \hat{\mathbb{X}}) \tag{3.16}$$

It is easy to see that the product state $\omega_\beta \otimes \mu$ on the composite system $\mathfrak{B}$ is a KMS state with respect to the *decoupled* dynamics $\alpha_t \otimes \mathrm{Id}_{C(M_X)} \equiv \hat{\alpha}_t$ of the object system with the generator $H_\beta \otimes \mathbb{1}$ and that the *coupled* dynamics $\beta_t$ derives from it through the perturbation by the term $H - H_\beta \otimes \mathbb{1} = \mathbb{1} \otimes \Delta - \pi \otimes \pi_\mu(\mathbb{A} \otimes \hat{\mathbb{X}})$ in the generator. Through the replacement $\alpha_{s,t;\mathbb{X}} \to \beta_t$, $\omega_\beta \to \omega_\beta \otimes \mu$, $\varphi_t \to \omega_\beta \otimes \mu \circ \beta_t$, therefore, we can apply the formula (2.6) for the relative entropy to the composite system $(\mathfrak{B}, \beta_t)$ and obtain

$$\begin{aligned}
&S(\omega_\beta \otimes \mu \circ \beta_t \,|\, \omega_\beta \otimes \mu) \\
&\quad = \beta \int_0^t ds\, \langle \Omega \otimes \mu^{1/2}, e^{iHt}[iH_\beta \otimes \mathbb{1}, -\mathbb{1} \otimes \Delta \\
&\qquad + \pi \otimes \pi_\mu(\mathbb{A} \otimes \hat{\mathbb{X}})]\, e^{-iHt} \Omega \otimes \mu^{1/2} \rangle \\
&\quad = \beta \int_0^t ds \lim_{T_0 \to \infty} \frac{1}{T_0} \int_{-T_0}^0 dt_0\, \omega_\beta(\alpha_{t_0, s+t_0; \mathbb{X}}(\delta(\mathbb{A}))) \cdot \mathbb{X}(s) \\
&\quad = \lim_{T_0 \to \infty} \frac{1}{T_0} \int_{-T_0}^0 dt_0\, S(\varphi_{t+t_0} \,|\, \varphi_{t_0} = \omega_\beta)
\end{aligned} \tag{3.17}$$

The last two equalities are due to the ergodicity (3.7). Thus, we obtain a very simple expression for the mean entropy production $\bar{P}$ defined previously by (2.8) as follows:

$$\begin{aligned}
\bar{P} &= \lim_{n \to \infty} \frac{1}{T_n} S(\omega_\beta \otimes \mu \circ \beta_{T_n} \,|\, \omega_\beta \otimes \mu) \\
&= \beta \hat{\varphi}(\mathbb{J} \otimes \hat{\mathbb{X}}) \geqslant 0
\end{aligned} \tag{3.18}$$

where $\hat{\varphi}$ is one of the limit stationary states to which the initial equilibrium state $\omega_\beta \otimes \mu$ of the decoupled system $(\mathfrak{B}, \hat{\alpha}_t)$ tends, being driven by the time-independent dynamics $\beta_t$ of the coupled system:

$$\hat{\varphi} \equiv \lim_{n \to \infty} \frac{1}{T_n} \int_0^{T_n} dt\, (\omega_\beta \otimes \mu) \circ \beta_t \tag{3.19}$$

The *stationarity* of the state $\hat{\varphi}$ under $\beta_t$ is easily seen as follows:

$$\begin{aligned}
&|(\hat{\varphi} \circ \beta_s - \hat{\varphi})(\hat{B})| \\
&\quad = \lim_{n \to \infty} \frac{1}{T_n} \left| \int_0^{T_n} dt\, [(\omega_\beta \otimes \mu) \circ \beta_{t+s} - (\omega_\beta \otimes \mu) \circ \beta_t](\hat{B}) \right| \\
&\quad \leqslant \lim_{n \to \infty} \frac{1}{T_n} \left| \left\{ \int_s^{T_n + s} - \int_0^{T_n} \right\} dt\, (\omega_\beta \otimes \mu) \circ \beta_t(\hat{B}) \right| \\
&\quad \leqslant \lim_{n \to \infty} \frac{2\,|s|}{T_n} \|\hat{B}\| = 0
\end{aligned} \tag{3.20}$$

As already noted, the final-time limit in (3.19) involves some subtle points: Although the state $\omega_\beta$ on the object system $(\mathfrak{A}, \alpha_t)$ and the external-force system $(C(M_X), \sigma_t)$ are ergodic, the composite system $(\mathfrak{B}, \beta_t)$ or the state $\hat{\varphi}$ on it may not be so in general, and the final-time average of the orbit $\omega_\beta \otimes \mu \circ \beta_t$ of the state $\omega_\beta \otimes \mu$ along the dynamics $\beta_t$ may not be uniquely determined. Since the state space on $\mathfrak{B}$ is convex and weak*-compact, the Markov–Kakutani theorem[16] guarantees the existence of a fixed point, which can be attained as a limit point of some *subsequence* with $t = T_n$ tending to $+\infty$. However, the resulting limit state $\hat{\varphi}$ will be changing depending upon the choice of such a subsequence. Therefore, there may exist many stationary states on $(\mathfrak{B}, \beta_t)$ and the state $\hat{\varphi}$ may be decomposed into the direct sum or integral of such stationary ergodic states. For further analysis of this problem, detailed information is required of the explicit structure of the dynamical system $(\mathfrak{A}, \alpha_t)$, but the general setting for the bifurcation problem in nonequilibrium stationarity should be formulated in the present framework as such a kind of ergodic decomposition.

Now the formula (3.18) is naturally interpreted as the quantized nonlinear version of Onsager's dissipation function, since it reduces to the product of the fluxes and the forces if the leading approximation is taken with respect to the correlations in the state $\hat{\varphi}$ as well as the coupling terms in the dynamics $\beta_t$ between the system $\mathfrak{A}$ and the external force system $C(M_X)$. The relations of (3.18) with the Kubo formula will be discussed in the next section from the viewpoint of the van Hove limit.

## 4. STATIONARITY AND DISSIPATIVITY

### 4.1. Object System As an Open Subsystem of Enlarged Total System

With the aid of the notions of the hull $M_X$, the Haar measure $\mu$ on it, and the "time-independent shape" $\hat{\mathbb{X}}$ of the time-dependent external force $\mathbb{X}(t)$, the problems concerning the initial- and final-time limits have been clearly separated in the expressions (3.18) and (3.19), not only at the technical level of limit procedures, but also at that of states and observables: In the original response-theoretic formulation, the physical meaning of the "adiabatic switching-on" process with the limit $t_0 \to -\infty$ has been obscured in the complicated formulas, being kept only at the level of the heuristic arguments. On the contrary, it is explicitly formulated here as the *initial state* $\mu$ of the dynamical system $(C(M_X), \sigma_t)$ of external force. The important role of this state $\mu$ in generating the dissipativity will be made clear in the following.

On the other hand, the problem concerning the final state is condensed in Eq. (3.19). While its stationarity is formulated there in the *enlarged system* $(\mathfrak{B}, \beta_t)$, we also need to know how the *original object system* $\mathfrak{A}$ behaves in this total system, in order to clarify what kind of physical system appears in the final long-time limit. For this purpose, it is necessary for us to control freely the shift of description levels between the microscopic total system with the uncontrollable "redundant" variables $\xi$ and the macroscopic observable subsystem of "relevant" variables. This can be achieved by the help of the embedding map $\imath$ given in (3.2) in combination with the following map $\hat{\mu}$ projecting out the variables in the total system $\mathfrak{B}$ onto its subsystem $\mathfrak{A}$:

$$\hat{\mu}: \quad \mathfrak{B} \ni \hat{B} \mapsto \hat{\mu}(\hat{B}) \equiv \int_{M_X} d\mu(\xi)\, \hat{B}(\xi) \in \mathfrak{A} \tag{4.1}$$

It is easily seen that they satisfy the following relations:

$$\omega \otimes \mu = \omega \circ \hat{\mu} \tag{4.2}$$

$$\hat{\mu} \circ \imath = \mathrm{Id}_{\mathfrak{A}} \tag{4.3}$$

In terms of these maps, the state $\hat{\varphi}$ and the dynamics $\beta_t$ on the total system $\mathfrak{B}$ can be pulled back onto the object system $\mathfrak{A}$ as follows:

$$\varphi \equiv \imath^*(\hat{\varphi}) \equiv \hat{\varphi} \circ \imath \tag{4.4}$$

$$\gamma_t \equiv \hat{\mu} \circ \beta_t \circ \imath \tag{4.5}$$

As a *conditional expectation* characterized by the properties

$$\hat{\mu}(\imath(B_1)\,\hat{B}_2\,\imath(B_3)) = B_1\,\hat{\mu}(\hat{B}_2)\,B_3 \tag{4.6}$$

$$\hat{\mu}(\hat{B}^*\hat{B}) \geqslant \hat{\mu}(\hat{B})^*\,\mu(\hat{B}) \tag{4.7}$$

$\hat{\mu}$ defined by (4.1) is a *completely positive* (CP) map preserving the positivity of the observables in the stronger sense than (4.7),

$$\left[\sum_{k=1}^{N} \hat{\mu}(\hat{B}_{ik}^*\hat{B}_{kj})\right]_{i,j=1}^{N} \geqslant 0, \qquad \forall(\hat{B}_{ij})_{i,j=1}^{N} \in \mathfrak{B}\otimes M_N(\mathbb{C}) \text{ for } \forall N \in \mathbb{N} \tag{4.8}$$

where $M_N(\mathbb{C})$ is the algebra of complex $N\times N$ matrices and $\mathfrak{B}\otimes M_N(\mathbb{C}) \simeq M_N(\mathfrak{B})$ is the algebra of matrices with each component in $\mathfrak{B}$. However, $\hat{\mu}$ is *not* a homomorphism between $\mathfrak{B}$ and $\mathfrak{A}$ preserving the multiplication law:

$$\hat{\mu}(AB) \neq \hat{\mu}(A)\,\hat{\mu}(B) \tag{4.9}$$

Therefore, unless the coupling between the system $\mathfrak{A}$ and the external force vanishes, the mapping $\gamma_t$ defined by (4.5) is not an automorphism of $\mathfrak{A}$, but a CP map which can transfer a pure state into a mixed state. In this sense, the system $(\mathfrak{A}, \gamma_t)$ defines a *dissipative* dynamics, but, due to the "memory effect," it *cannot* satisfy in general the Markov property:

$$\gamma_s \circ \gamma_t \neq \gamma_{s+t} \tag{4.10}$$

Therefore, contrary to the stationarity of the state $\hat{\varphi}$ of the composite system $(\mathfrak{B}, \beta_t)$ shown in (3.20), the pullback state $\varphi$ on $(\mathfrak{A}, \gamma_t)$ *cannot* be ensured straightforwardly to be stationary.

### 4.2. Van Hove Limit As Adiabatic Elimination of High Frequencies and Its Relation to Stationarity and Markov Property

To attain the nonequilibrium stationarity with positive entropy production, we note here the role of van Hove limit[19,20] in reducing the generalized master equation dragging memory effects to the Markovian master equation without memory.[21,22] Although this problem has been discussed traditionally in the context of the "*downhill process*" of *return to equilibrium*, which is just opposite to our "*uphill process*" aiming at non-equilibrium stationarity, the formulation of van Hove limit in terms of master equations seems to be quite useful here, at least for the qualitative understanding of the general relationships among scale changes, Markov property, and stationarity.

For this purpose, we introduce a (dimensionless) coupling parameter $\lambda$ in the coupling Hamiltonian (2.1),

$$H_I(t) = -\mathbb{A}\cdot\mathbb{X}(t) \to -\lambda\mathbb{A}\cdot\mathbb{X}(t) \tag{4.11}$$

which causes also a change in the third term of $H$ in (3.16) as

$$H_I \equiv -\pi\otimes\pi_\mu(\mathbb{A}\otimes\hat{\mathbb{X}}) \to -\lambda\pi\otimes\pi_\mu(\mathbb{A}\otimes\hat{\mathbb{X}}) \tag{4.12}$$

Then, the van Hove limit means the limit procedure to let the time parameter $t$ tend to infinity with the quantity $\lambda^2 t \equiv \tau$ fixed finite:

$$t\to\infty \qquad \text{with} \quad \lambda^2 t = \tau \text{ fixed} \tag{4.13}$$

Using the embedding map $\iota$ and the conditional expectation $\hat{\mu}$, we define a "projection" operator $P_0$ picking up the subalgebra $\mathfrak{A}\otimes\mathbb{1}$ in $\mathfrak{B}$ and its complement $P_1$ by

$$\iota\circ\hat{\mu} \equiv P_0 = P_0^2 \tag{4.14}$$

$$P_1 \equiv \mathrm{Id}_{\mathfrak{B}} - P_0 = P_1^2 \tag{4.15}$$

Then we can formulate (at least formally) the generalized master equation governing the non-Markovian dissipative dynamics $\gamma_t$ on $\mathfrak{A}$ with $t=\tau/\lambda^2$, in the following two forms adapted to discussing the asymptotic behaviors of states $\varphi$ and observables $C$, respectively:

$$\begin{aligned}\varphi\circ\alpha^{-1}_{\tau/\lambda^2}\circ\gamma_{\tau/\lambda^2} &= \varphi - \int_0^\tau du\int_0^{(\tau-u)/\lambda^2} ds\,\varphi\circ\alpha^{-1}_{u/\lambda^2+s}\circ\hat{\mu}\circ ad(\mathbb{A}\otimes\hat{\mathbb{X}})\circ P_1\circ e^{sZ}\\ &\quad\circ ad(\mathbb{A}\otimes\hat{\mathbb{X}})\circ\iota\circ\gamma_{u/\lambda^2}\end{aligned} \tag{4.16}$$

$$\begin{aligned}\gamma_{\tau/\lambda^2}(\alpha^{-1}_{\tau/\lambda^2}(C)) &= C - \int_0^\tau du\int_0^{(\tau-u)/\lambda^2} ds\,(\gamma_{u/\lambda^2}\circ\hat{\mu}\circ ad(\mathbb{A}\otimes\hat{\mathbb{X}})\circ P_1\circ e^{sZ}\circ ad(\mathbb{A}\otimes\hat{\mathbb{X}})\circ\iota)\\ &\quad\times(\alpha^{-1}_{u/\lambda^2+s}(C))\end{aligned} \tag{4.17}$$

Here $Z$ denotes the generator of the "renormalized" unperturbed dynamics given by

$$Z = \frac{d}{dt}\alpha_t\otimes\sigma_t\Big|_{t=0} - i\lambda P_1\,ad(\mathbb{A}\otimes\hat{\mathbb{X}})\,P_1 \tag{4.18}$$

on the assumption that $\mu(\hat{\mathbb{X}})=0$.

Thus, we see that the validity of the Markov property in the van Hove limit (4.13) is ensured if the following two points are verified: (i) *whether* the upper end $(\tau-u)/\lambda^2$ of the second integrals in the right-hand sides of (4.16) and (4.17) can be replaced by $+\infty$,

$$\int_0^{(\tau-u)/\lambda^2} ds \xrightarrow[\lambda\to 0]{} \int_0^{+\infty} ds \tag{4.19}$$

and (ii) (*adiabatic elimination of microscopic rapid motion*) *whether* the factors $\alpha_{\tau/\lambda^2}^{-1}$ and $\alpha_{u/\lambda^2+s}^{-1}$ can be absorbed by some conditions of "quasi-invariance" on the states $\varphi$ and/or the observables $C$ such as

$$\lim_{\lambda\to 0} \varphi\circ\alpha_{\tau/\lambda^2}^{-1}=\varphi \qquad \text{for} \quad \forall\tau>0 \tag{4.20}$$

$$\lim_{\lambda\to 0} \alpha_{\tau/\lambda^2}^{-1}(C)=C \qquad \text{for} \quad \forall\tau>0 \tag{4.21}$$

If these approximations are valid, then the generalized master equation (4.16)–(4.17) will be reduced to the Markovian master equation for $\tilde{\gamma}_\tau\equiv\gamma_{\tau/\lambda^2}$ with $\tau\geqslant 0$ satisfying

$$\tilde{\gamma}_{\tau+\sigma}=\tilde{\gamma}_\tau\circ\tilde{\gamma}_\sigma \tag{4.22}$$

and hence the stationarity of the state will be attained for any asymptotic limit state of the form

$$\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau d\tau\, \varphi\circ\tilde{\gamma}_\tau$$

In the usual formulation of the master equation in the processes of return to equilibrium, the state $\varphi\circ\alpha_{\tau/\lambda^2}^{-1}$ in (4.16) is replaced by the density matrix of the Gibbs state $e^{\beta(F-H)}$, which obscures the relevance of the second problem (ii) of the adiabatic elimination of microscopic rapid motion in the infinite future time ($\tau/\lambda^2$ with $\lambda\sim 0$, $\tau\geqslant 0$). Consequently, the natural meaning of van Hove limit has been lost, being taken only as a formal recipe to derive a Markovian stochastic dynamics. Taking account properly of the adiabatic elimination, however, we can interpret the van Hove limit in a more realistic way as a scale transformation controlling the *change of units between the two different times* $t=t_{\mathrm{micro}}$ and $\tau=t_{\mathrm{macro}}$ of the microscopic and macroscopic levels:

$$\lambda^2 t_{\mathrm{micro}}=t_{\mathrm{macro}} \tag{4.23}$$

If we take the microscopic time $t_{\mathrm{micro}}$ finite in (4.23), the limit $\lambda\to 0$ takes us literally to the situation of *weak coupling* or approximate decoupling between the macroscopic external force $\mathbb{X}$ and the microscopic object system $\mathfrak{A}$, where we "observe" the purely dynamical motion of the latter with time $t_{\text{micro}}$. On the contrary, the situation of the van Hove limit (4.13) in combination with the adiabatic elimination (4.20)–(4.21) brings into focus the macroscopic level of *state-changing process* with finite time $t_{\text{macro}}$. In spite of the small coupling parameter $\lambda \to 0$, the effects of the coupling term (4.11) accumulate into macroscopically visible state changes through the infinite repetitions of "invisible" microscopic dynamical motions of high frequencies during the *infinite* time interval $t_{\text{micro}} = t_{\text{macro}}/\lambda^2 \to \infty$, as is seen in (4.16)–(4.17).

The physical basis of such an interpretation is that the notion of *time* emerges from the correlations among physical motions which are "fibered" into different levels with certain typical motions in each regime (i.e., *different* "standard clocks" at each size level), and hence that the standard scales of time differ from level to level according to the changes of the "standard physical motions." Such a scale transformation as (4.23) is just a "calibration" between different "clocks" belonging to different size regimes. In the *idealization limit* of $\lambda \to 0$, simple approximate descriptions emerge as above for either the microscopic dynamical motions *or* macroscopic state-changing processes, according to the choice between $\{t_{\text{micro}} = \text{finite with } t_{\text{macro}} \to 0\}$ and $\{t_{\text{macro}} = \text{finite with } t_{\text{micro}} \to \infty\}$. This interpretation leads to a natural reformulation of the Kubo formula in direct relation to entropy production in the next subsection.

## 4.3. Entropy Production and van Hove Limit As Scale Change

If we adopt the above physical viewpoint, the inverse temperature $\beta$ appearing in the mean entropy production $\bar{P}$, (3.18), should also be transformed in parallel with the time[5] corresponding to the time-scale change (4.23):

$$\text{microscopic } \beta \to \text{macroscopic } \lambda^2\beta \equiv \beta_{\text{eff}} \tag{4.24}$$

Therefore, we obtain the following expression for the mean entropy production $\bar{P}$ in van Hove limit (4.13):

$$\begin{aligned}
0 \leqslant \bar{P} &= \beta\hat{\varphi}_{\lambda\mathbb{X}}(\lambda\mathbb{J} \otimes \hat{\mathbb{X}}) = \beta_{\text{eff}}\lambda^{-1}\hat{\varphi}_{\lambda\mathbb{X}}(\mathbb{J} \otimes \hat{\mathbb{X}}) \\
&\xrightarrow[\lambda \to 0]{} \beta_{\text{eff}} \frac{d}{d\lambda} \hat{\varphi}_{\lambda\mathbb{X}}(\mathbb{J} \otimes \hat{\mathbb{X}})\Big|_{\lambda=0} \\
&= \frac{1}{2} \beta_{\text{eff}} \frac{d^2}{d\lambda^2} \hat{\varphi}_{\lambda\mathbb{X}}(\lambda\delta(\mathbb{A}) \otimes \hat{\mathbb{X}})\Big|_{\lambda=0} \\
&= \frac{1}{2} L_{ij}\hat{X}^i\hat{X}^j \geqslant 0
\end{aligned} \tag{4.25}$$

with $L_{ij}$ defined by

$$L_{ij} \equiv \beta_{\text{eff}} \frac{\partial^2}{\partial X^i \, \partial X^j} \hat{\varphi}_{\mathbb{X}}(\delta(\mathbb{A}) \otimes \hat{\mathbb{X}}) \bigg|_{\mathbb{X}=0} \tag{4.26}$$

Here the $\lambda\mathbb{X}$ dependence of the state $\hat{\varphi}$ is made explicit as $\hat{\varphi}_{\lambda\mathbb{X}}$ and we have used the simple facts that

$$\hat{\varphi}_{\lambda\mathbb{X}}(\mathbb{J} \otimes \hat{\mathbb{X}})|_{\lambda=0} = (\omega_\beta \otimes \mu)(\delta(\mathbb{A}) \otimes \hat{\mathbb{X}})) = 0$$

and that the external force $\mathbb{X}$ is proportional to the coupling constant $\lambda$.

In order to rewrite the formula (4.25) in a more convenient form, we utilize an integral equation for the state $\omega_\beta \otimes \mu \circ \beta_t$,

$$\omega_\beta \otimes \mu \circ \beta_t(\hat{B}) = \omega_\beta \otimes \mu(\hat{B}) - \int_0^t ds \, \omega_\beta \otimes \mu([i\lambda\mathbb{A} \otimes \hat{\mathbb{X}}, \beta(\hat{B})]) \tag{4.27}$$

which follows from the expression (3.16) (with $\lambda$ inserted) of the infinitesimal generator of dynamics $\beta_t$ together with the stationarity of the product state $\omega_\beta \otimes \mu$ under the decoupled dynamics $\alpha_t \otimes \sigma_t$. From this we obtain another expression for the mean entropy production $\bar{P}$,

$$\begin{aligned}
\bar{P} &= \beta\lambda^2 \lim_{n \to \infty} \frac{1}{T_n} \int_0^{T_n} dt \, (T_n - t)(\omega_\beta \otimes \mu)([\beta_t(\delta(\mathbb{A}) \otimes \hat{\mathbb{X}}), i\mathbb{A} \otimes \hat{\mathbb{X}}]) \\
&= \beta_{\text{eff}} \lim_{n \to \infty} \int_0^{T_n} dt \left(1 - \frac{t}{T_n}\right) \\
&\quad \times \int d\mu(\xi) \, \omega_\beta(i[\alpha_{0,t;\xi}(\delta(\mathbb{A})) \cdot \hat{\mathbb{X}}(\xi_{-t}), \mathbb{A} \cdot \hat{\mathbb{X}}(\xi)]) \\
&= \beta_{\text{eff}} \lim_{n \to \infty} \int_0^{T_n} dt \left(1 - \frac{t}{T_n}\right) \\
&\quad \times \int d\mu(\xi) \int_0^\beta d\tau \, \hat{\mathbb{X}}(\xi_{-t}) \cdot \omega_\beta(\alpha_{-i\tau}\alpha_{0,t;\xi}(\mathbb{J})\mathbb{J}) \cdot \hat{\mathbb{X}}(\xi)
\end{aligned} \tag{4.28}$$

If the initial equilibrium state $\omega_\beta$ satisfies the *mixing property* suppressing the long-time correlation in the form

$$\omega_\beta(\alpha_t(\mathbb{J})\mathbb{J}) = O(t^{-1-\varepsilon}), \qquad \varepsilon > 0 \tag{4.29}$$

it is easy to see that this formula can be approximated in the van Hove limit by the formula valid in the *linear response* regime

$$\begin{aligned}
\bar{P} \underset{\lambda \to 0}{\overset{(<)}{\sim}} \; & \beta_{\text{eff}} \int_0^\infty dt \int d\mu(\xi) \\
& \times \int_0^\beta d\tau \, \hat{\mathbb{X}}(\xi_{-t}) \cdot \omega_\beta(\alpha_{t-i\tau}(\mathbb{J})\mathbb{J}) \cdot \hat{\mathbb{X}}(\xi) \bigg|_{\beta = \beta_{\text{eff}}/\lambda^2}
\end{aligned} \tag{4.30}$$

This can be checked by dividing the integral $\int_0^{T_n}$ into two parts,

$$\int_0^{T_n} = \int_0^M + \int_M^{T_n}$$

with sufficiently large $M > 0$, and by estimating the contribution of the term $-t/T_n$ in view of (4.29). Further, when applied to the almost-periodic external force $\mathbb{X}$ given by

$$\mathbb{X}(t) = \sum_k \mathbb{X}(\omega_k)\, e^{i\omega_k t} = \mathbb{X}(t)^* \tag{4.31}$$

it reproduces the following result obtained in ref. 4, Eq. (5.15):

$$\begin{aligned} \bar{P} \sim \beta_{\text{eff}} \sum_{\omega_k \geqslant 0} (\hbar\omega_k)^{-1} \tanh(\beta_{\text{eff}} \hbar\omega_k/2) \\ \times \sum_{i,j} X^i(\omega_k)^*\, L_{ij}(\omega_k)\, X^j(\omega_k) \end{aligned} \tag{4.32}$$

where the reality condition of $\mathbb{X}(t)$, $\mathbb{X}(\omega_k)^* = \mathbb{X}(-\omega_k)$, is used and the coefficient matrix $\{L_{ij}(\omega_k)\}$ is defined by

$$\begin{aligned} L_{ij}(\omega_k) &\equiv \int_{-\infty}^{\infty} d\tau\, e^{i\omega_k \tau} \omega_\beta(\{\alpha_\tau(J^i), J^j\}) \\ &= L_{ji}(\omega_k)^* = L_{ij}(-\omega_k)^* \end{aligned} \tag{4.33}$$

In view of the remark in ref. 3 on the relation between kinetic-theoretic approaches and linear-response theoretic ones toward the understanding of dissipativity, it would be interesting to consider here the problem of ordering consistency between *stochastization* and *linearization*: It is usually said[2,3] that in the former case the stochastization procedure comes first, followed by linearization, and that it is just in the opposite order in the latter. Here in the above discussion of the master equation as one of the kinetic-theoretic approaches, the *stochastization* is due to the conditional expectation map $\hat{\mu}$, which induces a non-Markovian dissipative dynamics $\gamma_t = \hat{\mu} \circ \beta_t \circ \iota$ governed by the generalized master equation (4.16), (4.17). To attain a genuine kinetic equation in the form of a Markovian master equation, the adiabatic elimination mechanism of the van Hove limit to focus upon the state-changing processes is indispensable as a kind of "*linearization*" procedure. However, we can see, from such an expression as

$$\begin{aligned} \varphi \circ \tilde{\gamma}_\tau &= \varphi \circ \Big( \underbrace{\lim_{\lambda \to 0}}_{\substack{\text{final-time} \\ \text{linearization}}} \underbrace{\hat{\mu}}_{\substack{\text{initial-time} \\ \text{stochastization}}} \circ \beta_{\tau/\lambda^2} \circ \iota \Big) \\ &= \lim_{\lambda \to 0} \underbrace{(\varphi \otimes \mu)}_{\substack{\text{initial} \\ \text{average}}} \circ \underbrace{([\alpha_{\tau/\lambda^2} \otimes \sigma_{\tau/\lambda^2}]^{-1} \circ \beta_{\tau/\lambda^2})}_{\text{linearization}} \circ \iota \end{aligned}$$

that the "difference in the ordering" of the "stochastization" $\hat{\mu}$ and the "linearization" $\lambda \to 0$ is at most in their *appearances* of the same procedures viewed from the "Heisenberg picture" for *observable* dynamics and from the "Schrödinger one" for *state-changing* dynamics, which are *contragrediently* related through the duality between algebras and states.

Finally, we stress the intrinsic dynamical natures of the above two "procedures." First, the *probability* measure $\mu$ on $C(M_X)$ occupying the pivotal position responsible for the *stochastization* should not be taken as an *ad hoc* device, but its origin should be traced to the ergodicity of the *dynamics* of the external force system which couples to the object system. Second, the validity of the van Hove limit as a *level-transition* mechanism requires the consistency between macroscopic *stochasticity* and the long-time asymptotic behaviors of the microscopic *dynamics* in such a form as the *mixing property* (4.29), which is of renormalization-group-theoretic nature in essence. Namely, the total dynamical system $(\mathfrak{B}, \beta_t)$ should choose $\lambda = 0$ as its *infrared-stable* fixed point for the consistency of our discussion. If $\lambda = \infty$ is infrared-stable, on the contrary, the roles of $t_{\text{micro}}$ and $t_{\text{macro}}$ should be just interchanged, and hence we would encounter the situation where the singular coupling limit[23],[5] is relevant.

## 5. NONEQUILIBRIUM AND INHOMOGENEOUS STRUCTURES. FAMILY OF STATES AND GROUPOID DYNAMICS

Up to now, we have been concerned mainly with the formulation of stationarity. We discuss here some aspects of nonequilibrium states from the viewpoint of entropy production and their inhomogeneous internal structures.

We first recall that in the *zeroth law of thermodynamics* the abstract physical characterization of temperature *equilibrium* is given as a stable contact relation between *two* physical systems constituting an *equivalence relation* and that the equivalence classes of this relation are just parametrized by the absolute temperatures $T$ by taking the ideal gases as the standard reference systems. It is the transitivity of this equivalence relation that allows one to talk about a temperature equilibrium state of *one* physical system with no mention of another one (="reservoirs") constituting this *binary* relation. This well-known fact suggests the relevance of *multiple-reservoir systems* proposed by Lebowitz[6] to the nonequilibrium structures which negate equilibrium situations as an equivalence relation. As its simplest realization can be found in the classical

[5] See also the references cited in ref. 22.

Carnot *cycle* involving two heat baths at high and low temperatures, the notion of nonequilibrium *states* should encompass stationary *cyclic processes*, extending the classical thermodynamic notion of a state restricted by definition to the equilibrium.

From this viewpoint of multiple-reservoir systems, the structure of the entropy production formula (4.32) for the almost-periodic external force seems to be quite interesting in the following reinterpretation. In view of the ergodicity of the dynamical system $(C(M_X), \sigma_t, \mu)$, we can interpret the probability measure $\mu$ as a *microcanonical ensemble* state on this classical system. Then, the asymptotic decouplings among different modes $\{\omega_k\}$ in the van Hove limit (4.13) allow us to attach to each frequency $\omega_k$ a harmonic oscillator in a "local" canonical ensemble state embedded in the microcanonical ensemble $\mu$. On the assumption of the "local" detailed balance, the corresponding "local" effective temperature $T_k$ will be given by

$$\hbar\omega_k = \frac{1}{2} k_B T_k = \frac{1}{2} \beta_k^{-1} \tag{5.1}$$

Then the mean entropy production can be rewritten as

$$\begin{aligned} k_B \bar{P} &= \sum_k \frac{1}{T_k} 2\beta_{\text{eff}} \tanh\left(\frac{\beta_{\text{eff}}}{4\beta_k}\right) \sum_{i,j} X^i(\omega_k)^* L_{ij}(\omega_k) X^j(\omega_k) \\ &= \sum_k \frac{-(\Delta Q/\Delta t_{\text{macro}})_k}{T_k} \geqslant 0 \end{aligned} \tag{5.2}$$

where

$$(\Delta Q/\Delta t_{\text{macro}})_k \equiv -2\beta_{\text{eff}} \tanh(\beta_{\text{eff}}/4\beta_k) \sum_{i,j} X^i(\omega_k)^* L_{ij}(\omega_k) X^j(\omega_k) \tag{5.3}$$

Thus, with the interpretation of $-(\Delta Q/\Delta t_{\text{macro}})_k$ as the rate of heat exchange at the $k$th "reservoir" with "local" temperature $T_k$, (5.2) gives the connection between the Clausius formula for entropy changes in thermodynamics and the mean entropy production $\bar{P}$ given response-theoretically in a quantum dynamical system prepared with temperature $1/k_B\beta_{\text{eff}}$ at infinite past.

The inhomogeneous temperature distribution of the reservoir systems in (5.2) can be supplied not only by the *spatial* local configuration of heat baths, but also by such *internal* degrees of freedom as the *mode* differences in energy spectrum or the particle spectrum (as in the case of cosmological evolution processes). Although we have so far neglected these spatial and internal degrees of freedom, concentrating upon the *time* development of the system, it would be important to take them into account for the satisfactory treatment of the nonequilibrium processes of quantum dynamical systems. For this purpose, we add here a few comments on the relevance of Connes' noncommutative integration theory[8] and groupoid dynamical systems[7] to the present context. Since our external force $\mathbb{X}(t)$, *not* necessarily periodic, gives rise to an *ergodic* system $(C(M_X), \sigma_t)$ on its hull $M_X$, the groupoid approach is particularly relevant to us in its relation to Mackey's virtual group,[24] which arises in the situation that the group action is *ergodic* but *not* transitive. It may be interesting in this context to note that for $\mathbb{X}(t)$ having two frequencies $\omega_1$ and $\omega_2$ with an irrational ratio $\theta \equiv \omega_1/\omega_2$ $(<1)$ the crossed product $C(M_X) \rtimes_\sigma \mathbb{R}$ of the external force system becomes (stably isomorphic to) the irrational rotation algebra $A_\theta$,[25,26] and that the parameter $\theta$ can be related to the *efficiency* $\eta$ of the Carnot cycle through $\eta = 1 - \theta = 1 - \omega_1/\omega_2 = (T_2 - T_1)/T_2$.

Now we note that, in view of the covariance condition (3.4), the time-inhomogeneous dynamics $\alpha_{0,t;\xi}$ on $\mathfrak{A}$ can be interpreted as a *representation of a groupoid* $\Gamma \equiv \mathbb{R} \times_\lambda M_X$ associated with the action $\lambda$ of $\mathbb{R}$ on $M_X$. The multiplication law of this groupoid $\Gamma$ is defined for any pairs $\gamma_1 \equiv (t_1, \xi_1)$ and $\gamma_2 \equiv (t_2, \xi_2)$ satisfying $\lambda_{-t_1}(\xi_1) = \xi_2$ by

$$(t_1, \xi_1) \cdot (t_2, \xi_2) \equiv (t_1 + t_2, \xi_1) \tag{5.4}$$

and the hull $M_X$ can be identified with the space $\Gamma^{(0)} = \{0\} \times M_X$ of units of $\Gamma$ with respect to this multiplication. Each groupoid element $\gamma = (t, \xi)$ can be interpreted as a shift by $t$ from its *source* $s(\gamma) \equiv \lambda_{-t}(\xi)$ to its *target* $r(\gamma) \equiv \xi$ in $\Gamma^{(0)}$. Then, by denoting $\alpha_{0,t;\xi} \equiv \alpha_\gamma$ with $\gamma \equiv (t, \xi) \in \Gamma$, the covariance condition (3.4) together with the chain rule (3.3) yields the relation

$$\alpha_{\gamma_1} \circ \alpha_{\gamma_2} = \alpha_{\gamma_1 \cdot \gamma_2} \tag{5.5}$$

which defines a *groupoid dynamical system* $(\mathfrak{A}, \alpha_\gamma, \Gamma)$.[7]

Now, the construction (3.5) of the composite dynamics $\beta_t$ can be properly viewed from the more general context as follows. Let $(\mathfrak{A}, \alpha, \Gamma)$ denote a $C^*$-groupoid dynamical system with a groupoid $\Gamma = G \times_\lambda M$ associated with an action $\lambda$ of a locally compact group $G$ on a locally compact manifold $M$, in which the groupoid product is defined by $\gamma_1 \cdot \gamma_2 = (g_1 g_2, \xi_1)$ for any pair $\gamma_1 = (g_1, \xi_1)$, $\gamma_2 = (g_2, \xi_2) \in G \times M$ satisfying

$$s(\gamma_1) = \lambda_{g_1^{-1}}(\xi_1) = \xi_2 = r(\gamma_2)$$

Then this groupoid dynamical system is in a canonical correspondence with a $C^*$-dynamical system $(\mathfrak{B} \equiv \mathfrak{A} \otimes C_0(M), \beta, G)$ in the sense that their crossed products $\mathfrak{A} \rtimes_\alpha \Gamma$ and $\mathfrak{B} \rtimes_\beta G$ are isomorphic,[7] where the dynamics $\beta_g$ on $\mathfrak{B}$ is defined by

$$[\beta_g(\hat{B})](\xi) \equiv \alpha_{(g,\xi)}(\hat{B}(\lambda_{g^{-1}}(\xi))), \qquad \text{for} \quad \hat{B} \in \mathfrak{B} \tag{5.6}$$

Our definition (3.5) of the time-independent composite dynamics $\beta_t$ is just a special case of the dynamics $\beta$ on $G$ for $G = \mathbb{R}$. Thus, this formulation allows us to incorporate the spatial as well as internal degrees of freedom with suitable choices of the "gauge group" $G$ and the "internal and external spacetime" $M$.

We note further that the Haar measures $dv^{\xi} \equiv dt$ and $\Lambda_v \equiv \mu$ on the group $G = \mathbb{R}$ and the hull space $M = M_X$ constitute, respectively, a transverse function and a transverse measure in Connes' noncommutative integration theory[8] on the groupoid $\Gamma = \mathbb{R} \times_{\lambda} M_X$:

$$\Lambda(f) = (\Lambda_v \circ v)(f) = \int_{\Gamma^{(0)}} d\mu(\xi) \int_{\Gamma^{\xi}} dv^{\xi}(\gamma)\, f(\gamma)$$

$$= \int_{M_X} d\mu(\xi) \int_{-\infty}^{\infty} dt\, f(t, \xi) \tag{5.7}$$

It seems interesting to note that the formula (2.14) or (3.18) for the mean entropy production $\bar{P}$ can be rewritten as

$$\begin{aligned}
\bar{P} &= \beta \lim_{n \to \infty} \int_{M_X} d\mu(\xi) \\
&\quad \times \int_{-\infty}^{\infty} dt\, \omega_{\beta}(\alpha_{0,t;\xi}(\delta(\mathbb{A}))\, \hat{\mathbb{X}}(\xi_{-t}) \frac{\chi_{[0, T_n]}(t)}{T_n} \\
&= \beta \lim_{n \to \infty} \int_{M_X} d\mu(\xi) \\
&\quad \times \int_{\Gamma^{\xi}} dv^{\xi}(\gamma)\, \omega_{\beta}(\alpha_{\gamma}(\delta(\mathbb{A}))(\hat{\mathbb{X}} \circ s)(\gamma) \frac{\chi_{M_X \times [0, T_n]}(\gamma)}{\Lambda(\chi_{M_X \times [0, T_n]})} \\
&= \lim_{n \to \infty} \int d\mu(\xi) \int dv^{\xi}(\gamma)\, \omega_{\beta} \circ \alpha_{\gamma}(\beta\delta(\mathbb{A})) \cdot f_n(\gamma)\, s^*(\hat{\mathbb{X}})(\gamma)
\end{aligned} \tag{5.8}$$

where $\chi_S$ denotes the characteristic function of a set $S$: $\chi_S(x) = 1$ or $0$ according as $x \in S$ or not, and $s$ is a source mapping $\Gamma \ni \gamma = (t, \xi) \mapsto s(\gamma) \equiv \lambda_{-t}(\xi)$. The function $f_n$ defined by

$$f_n(\gamma) \equiv f_n(t, \xi) = \chi_{M_X \times [0, T_n]}(\gamma)/T_n \tag{5.9}$$

plays the role of a normalized test function.

We note here that the composite state $\hat{\varphi}$ on $\mathfrak{B}$ can be decomposed into its "component states" $\varphi_{\xi}$ on $\mathfrak{A}$ as

$$\hat{\varphi}(\hat{B}) = \int_{M_X} d\mu(\xi)\, \varphi_{\xi}(\hat{B}(\xi)) \tag{5.10}$$

with $\varphi_\xi$ defined by

$$\varphi_\xi = \lim_{n \to \infty} \frac{1}{T_n} \int_0^{T_n} dt\, \omega_\beta \circ \alpha_{0,t;\xi_t} \tag{5.11}$$

Then these $\varphi_\xi$ are easily seen to satisfy Bellissard's condition[18] for the stationarity of $\hat{\varphi}$ formulated in terms of *family of states* on the object system $\mathfrak{A}$,

$$\varphi_{\xi_{-t}} = \varphi_\xi \circ \alpha_{0,t;\xi} \tag{5.12}$$

which can be viewed as the equivariance condition in the groupoid notation:

$$\varphi_{r(\gamma)} = \varphi_{s(\gamma)} \circ \alpha_{\gamma^{-1}} = \alpha^*_{\gamma^{-1}} \varphi_{s(\gamma)} \tag{5.13}$$

Since the role of the transverse measure $\mu$ consists in the averaging over the fluctuating "random variables" $\xi$ which perturb the dynamics, this kind of reformulation will clarify the proper connections of our present setup with various "adiabatic theorems"[26,27] related to the "Berry phase" as well as the stochastic process approaches.[28] Investigation along these lines will be reported elsewhere.

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