Dissipation and entropy production in open quantum systems

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Abstract. A microscopic description of an open system is generally expressed by the Hamiltonian of the form: \( H_{\text{tot}} = H_{\text{sys}} + H_{\text{environ}} + H_{\text{sys-environ}} \). We developed a microscopic theory of entropy and derived a general formula, so-called “entropy-Hamiltonian relation” (EHR), that connects the entropy of the system to the interaction Hamiltonian represented by \( H_{\text{sys-environ}} \) for a nonequilibrium open quantum system. To derive the EHR formula, we mapped the open quantum system to the representation space of the Liouville-space formulation or thermo field dynamics (TFD), and thus worked on the representation space \( \mathcal{L} := \mathcal{H} \otimes \tilde{\mathcal{H}} \), where \( \mathcal{H} \) denotes the ordinary Hilbert space while \( \tilde{\mathcal{H}} \) the tilde Hilbert space conjugates to \( \mathcal{H} \).

We show that the natural transformation (mapping) of nonequilibrium open quantum systems is accomplished within the theoretical structure of TFD. By using the obtained EHR formula, we also derived the equation of motion for the distribution function of the system. We demonstrated that by knowing the microscopic description of the interaction, namely, the specific form of \( H_{\text{sys-environ}} \) on the representation space \( \mathcal{L} \), the EHR formulas enable us to evaluate the entropy of the system and to gain some information about entropy for nonequilibrium open quantum systems.

1. Introduction
Dynamical processes in dissipative (open) systems involve irreversible transformations of nonequilibrium states of the systems. An important physical quantity of the theory of nonequilibrium processes is the entropy production that is the rate at which entropy is produced as a result of irreversible processes \([1, 2]\). In the quantum theory of open systems the entropy production is usually related to the negative derivative of the relative entropy with respect to an invariant state in order to show the second law of thermodynamics \([1]\). However, conventional theories have not made clear the connection between the entropy production and the interactions between the system and its environment in open quantum systems. Indeed providing a microscopic expression for the entropy production has been one of the grand aims of statistical mechanics, going back to the seminal work of Boltzmann.

In this paper, we derive a general formula which relates the entropy of the system to the system-environment interactions in an open quantum system (generally represented by the Hamiltonian \( H_{\text{tot}} = H_{\text{sys}} + H_{\text{environ}} + H_{\text{sys-environ}} \)). To derive the formula, we adopt the Liouville-space formulation or the method of thermo field dynamics (TFD) \([3, 4]\) as a means for treating open quantum systems. In the formulation of the problem, we shall use the idea introduced in the theory of TFD, namely, doubling the degree of freedom by introducing the tilde Hilbert
space $\widetilde{H}$, and the rules defined in the representation spaces $\widetilde{H}$ and $H$ introduced in TFD. In concreteness, we map the open quantum system to the representation space of TFD. On the basis of the zeroth law of thermodynamics [5, 6, 7], it can be shown that the interactions between a system and its environment can be transformed into the nontilde-tilde interactions [8, 9]. Once the entropy of the system is expressed on the Hilbert space $H$ and is connected to the system-environment interaction expressed on the representation space $L := H \otimes \widetilde{H}$, we can examine the behavior of the entropy from the microscopic description of the interaction Hamiltonian $H_{\text{sys-env}}$. In other words, we can study the behavior of the entropy of the system microscopically from the knowledge of those interactions between the system represented on the space $\widetilde{H}$ and its environment represented on the space $H$ within the framework of TFD. By studying the interactions between the system and its environment mapped on the representation space $L$, we can generally derive a formula which connects the interaction Hamiltonian to the entropy of the system in open quantum systems.

We also show that the equation of motion for the distribution function of the system can be derived from the formula and it is shown that the entropy of the system is expressed in terms of the distribution function. Finally, we consider two possible example models as applications of the formulas obtained for the open quantum systems.

2. Entropy-Hamiltonian relation

In this section, we discuss an open quantum system in connection with the framework of TFD and derive the formula which connects the entropy and the Hamiltonian (so called entropy-Hamiltonian relation, EHR for short) for open quantum systems by using an entropy operator and the generalized Schrödinger-like equation in the representation space $L$.

Let us briefly explain TFD. TFD is constructed by doubling a representation space for a set of those tilde conjugate operators $\{\alpha\}$ defined on the Hilbert space $H$ by introducing the tilde conjugation Hilbert space $\widetilde{H}$ for a set of those tilde conjugate operators $\{\widetilde{\alpha}\}$. Utilizing this structure in the theory of TFD, we can conveniently express the interaction Hamiltonian of an open quantum system in terms of those operators on $H$ and on $\widetilde{H}$ in the representation space $L$ as will be shown shortly. Bosonic and fermionic tilde operators are, respectively, assumed to commute and anticommute with respective nontilde operators.

Each operator in $\{\alpha\}$ satisfies the tilde conjugation rules [4]. Thermal state $|\Psi(t)\rangle$ defined in TFD is expressed by

$$|\Psi_\alpha(t)\rangle = \rho^\alpha(t)|1\rangle \quad (0 \leq \alpha \leq 1),$$

where $\rho(t)$ is a density operator describing a system, and a state $|1\rangle$ is defined by $|1\rangle := e^{a|a^\dagger|}[0,0]$ for bosons and $|1\rangle := [0,0] + ia^\dagger|a|0,0\rangle$ for fermions. By using the thermal state $|\Psi_\alpha(t)\rangle$, we can obtain the mean value (i.e., finite temperature expectation value) of the microscopic description of physical quantity (denoted by $A$) at time $t$:

$$\langle A \rangle_t = \text{Tr}\{\rho(t)A\} = \langle \Psi_\alpha(t)|A|\Psi_\alpha(t)\rangle,$$

where $\langle \Psi_\alpha(t)|$ is defined by $\langle \Psi_\alpha(t)| := \langle 1|\rho^{1-\alpha}$. Here and in the following, time dependence of the expectation values $\langle \cdots \rangle_t$ is indicated by a subscript $t$. Entropy $S(t)$ may be expressed by the density operator $\rho(t)$:

$$S(t) = -k \text{Tr}\{\rho(t) \ln \rho(t)\} = \text{Tr}\{\rho(t)|-k \ln \rho(t)|\} = \langle -k \ln \rho(t) \rangle_t,$$

where $k$ is the Boltzmann constant. This equation defines entropy for nonequilibrium processes.

In what follows, it will be convenient to consider a dynamical variable

$$\eta(t) = -k \ln \rho(t)$$

(4)
as an **entropy operator** since its mean value \( \langle \eta(t) \rangle_t \) coincides with the nonequilibrium thermodynamic (von Neumann) entropy \( S(t) \) given by Eq. (3). Noticing that the density operator \( \rho(t) \) can be written in terms of the entropy operator \( \eta(t) \) as

\[
\rho(t) = e^{-\eta(t)/k},
\]

the thermal state \( |\Psi(t)\rangle \) in Eq. (1) can be expressed in terms of the entropy operator as

\[
|\Psi_\alpha(t)\rangle = e^{-\alpha \eta(t)/k} |1\rangle.
\]

The time derivative of Eq. (6) is given by

\[
\frac{\partial}{\partial t} |\Psi_\alpha(t)\rangle = -\frac{\alpha}{k} \int_0^1 K(\lambda) d\lambda |\Psi_\alpha(t)\rangle,
\]

where

\[
K(\lambda) = e^{-\lambda \eta} \frac{\partial \eta}{\partial t} e^{\lambda \eta} = \frac{\partial \eta}{\partial t} + \lambda \left[ \frac{\eta}{k} \frac{\partial \eta}{\partial t} \right] + \frac{\lambda^2}{2!} \left[ \frac{\eta}{k} \frac{\partial \eta}{\partial t} \right] + O(\lambda^3).
\]

Meanwhile, in TFD the thermal state evolves with time according to the Schrödinger-like equation [10, 11]:

\[
\frac{\partial}{\partial t} |\Psi_\alpha(t)\rangle = -\frac{i}{\hbar} \tilde{H}(t) |\Psi_\alpha(t)\rangle,
\]

where \( \tilde{H}(t) := \hat{H} + i \hat{\Gamma}(t) \) (\( \hat{H} := H - \hat{H} \)) denotes a total-Hamiltonian and \( \hbar \) is Planck’s constant. The operator \( \hat{H} \) defined on \( \mathcal{H} \) is a hermitian operator denoting the Hamiltonian of a system, and \( \hat{\Gamma} \) defined on \( \mathcal{L} \) is an arbitrary operator satisfying \( (\hat{\Gamma})^\sim = \hat{\Gamma} \).

A general relation that connects the entropy operator \( \eta(t) \) (defined by Eq. (4)) and the time dependent total Hamiltonian \( \tilde{H}(t) \) can be obtained from Eqs. (7) and (9) as

\[
\int_0^1 K(\lambda) d\lambda = \frac{ik}{\alpha \hbar} \tilde{H}(t).
\]

This is the most general EHR. It should be noted however that the time-dependent total Hamiltonian \( \tilde{H}(t) \) depends on the particular physical situation under study. Taking the expectation value of Eq. (10) and noticing \( \langle H - \hat{H} \rangle_t = 0 \), the EHR in Eq. (10) can be expressed as

\[
\int_0^1 \langle K(\lambda) \rangle_t d\lambda = -\frac{k}{\alpha \hbar} \langle \tilde{H}(t) \rangle_t.
\]

Accordingly, if we assume \( [\eta(t), \partial \eta(t)/\partial t] = 0 \), the EHR in Eq. (11) can be expressed in a simple form:

\[
\langle \frac{\partial \eta(t)}{\partial t} \rangle_t = -\frac{k}{\alpha \hbar} \langle \tilde{H}(t) \rangle_t.
\]

It should be noted here that owing to the \( \langle H - \hat{H} \rangle = 0 \) setting in TFD, the EHR is expressed in terms of the entropy operator \( \eta(t) \) and an arbitrary operator \( \hat{\Gamma}(t) \) only. In other words, we can say that the entropy production can be evaluated from the microscopic description of the operator \( \hat{\Gamma}(t) \). These general formulas expressing the EHR can be applied for open quantum systems.
Let us consider an open quantum system within the framework of TFD in order to utilize the formulas obtained above. It is then worth reconsidering the physical foundation of TFD. We consider an open quantum system described by the Hamiltonian:

\[ H_{\text{tot}}(t) = H_{\text{sys}}(t) + H_{\text{environ}}(t) + H_{\text{sys-environ}}(t), \]  

(13)

where we assume \([H_{\text{sys}}, H_{\text{environ}}] = 0\) (i.e. the system and its environment are uncorrelated in the absence of the interactions between them). When this open system is in a thermal equilibrium state, the system is thermally equilibrium with its environment at the same temperature. In such a case, it is by no means to discriminate the state of the system thermodynamically from that of its environment, meaning that the environment in equilibrium is of de-individuation from the system in equilibrium [8]. Therefore, we do not care about the specific form of the environment Hamiltonian as far as those systems (the system of interest and its environment) are in the same thermal equilibrium state. Accordingly, the environment having the same thermodynamic property of the system can be regarded as the copy of the system of interest. Indeed, this allows us to assign the system of interest to the non-tilde space \(H\) and its environment to the tilde space \(\tilde{H}\) in the representation space \(L := \mathcal{H} \otimes \tilde{\mathcal{H}}\) introduced in TFD. Regarding the environment as the copy of the system, we can make the transformation of the system under consideration onto the non-tilde Hilbert space \(\mathcal{H}\) (i.e. \(H_{\text{sys}} \rightarrow H\)) and the environment onto the tilde Hilbert space \(\tilde{\mathcal{H}}\) (i.e. \(H_{\text{environ}} \rightarrow \tilde{H}\)). With this prescription, a natural transformation of an open quantum system within the theoretical structure of TFD can be accomplished by the following way: the interaction Hamiltonian \(H_{\text{sys-environ}}\) is mapped to the representation space \(L\) by the mapping \(H_{\text{sys-environ}} \rightarrow H_{\text{nontilde-tilde}}(\equiv i\tilde{\Gamma})\). The mapping of an open system to TFD is summarized in Table 1.

In the following, we assume the case where the system is very close to the equilibrium state of its environment (in other words, the interaction between the system and its environment is very weak). In such a case we can safely employ the mapping described above for the system and its environment and we generalize Eqs. (11) and (12) for the case where there exists some interactions between the system and its environments. For an open quantum system, the interaction between the system and its environment possibly plays a special role in the dynamics (e.g. the spontaneous, irreversible thermodynamic processes) of the system. Obviously if there is some interaction between them, the system may be in non-equilibrium states. Whether the system is equilibrium or non-equilibrium due to the interaction can be judged from the study of entropy \(S(t)\). Hereafter we assume the entropy for an open quantum system is evaluated from

\[ \left\langle \frac{\partial \eta(t)}{\partial t} \right\rangle \equiv \frac{\partial \langle \eta(t) \rangle_t}{\partial t} = \frac{\partial S(t)}{\partial t}, \]

(14)

where \(\langle \partial \eta(t)/\partial t \rangle\) is given by Eq. (12).
By applying the prescription for the transformation given above, Eqs. (11) and (12) are able to express an entropy production rate induced by e.g. the spontaneous or irreversible process, and therefore relate the entropy of the system to a possible interaction described by the microscopic interaction Hamiltonian \( \tilde{\Gamma} \). The general formulas (11) and (12) will be used to investigate the effect of interaction directly on the system by the spontaneous or irreversible process for open quantum systems by giving the explicit form of interactions expressed by non-tilde and tilde operators. It should be noted that this interaction Hamiltonian \( H_{\text{sys-env}}(t) \) can be represented by the transformation \( H_{\text{sys-env}} \rightarrow H_{\text{nontilde-tilde}} \) in the representation space \( \mathcal{L} \) of TFD as expressed by the operators comprised of non-tilde and tilde operators.

3. Distribution function

Entropy is often expressed in terms of a distribution function \( f(t) \):

\[
S(t) = -k \{ f(t) \ln f(t) \pm [1 \pm f(t)] \ln [1 \pm f(t)] \},
\]

where the upper sign is for bosons while the lower sign is for fermions.

In this section, we will derive the expression for the entropy production in terms of a distribution function and also derive an equation of motion for a distribution function for open quantum systems.

Let us consider the entropy given by Eq. (15). Differentiating the entropy with respect to time \( t \), we immediately obtain the expression for the entropy production of the system in terms of the distribution function \( f(t) \):

\[
\frac{\partial S(t)}{\partial t} = \begin{cases}
-k \frac{\partial f(t)}{\partial t} \ln \frac{f(t)}{1 + f(t)} & \text{(bosons)}, \\
-k \frac{\partial f(t)}{\partial t} \ln \{ f(t) [1 - f(t)] \} & \text{(fermions)}.
\end{cases}
\]

This indicates that the entropy for an open system can be determined by the knowledge of the distribution function only. Equating Eq. (12) to Eq. (16) and noting Eq. (14), we also obtain the equation of motion for the distribution function \( f(t) \):

\[
\hbar \frac{\partial f(t)}{\partial t} = \begin{cases}
\frac{\langle \hat{\Gamma}(t) \rangle_t}{\alpha \ln \{ f(t) [1 - f(t)] \}} & \text{(bosons)}, \\
\frac{\langle \hat{\Gamma}(t) \rangle_t}{\alpha \ln \{ f(t) [1 - f(t)] \}} & \text{(fermions)}.
\end{cases}
\]

It should be noted that the distribution function \( f(t) \) for open systems could be determined with a given value of \( \langle \hat{\Gamma}(t) \rangle \) by solving the self-consistent Eq. (17) for \( f(t) \).

4. Applications of EHR

In this section, we apply the EHR formula obtained in Sec. 2 to various types of boson model and consider how entropy is affected by the interactions between the system and its environment in open quantum systems. For the sake of convenience of calculations, we adopt the c-number parameter taken as \( \alpha = 1 \). It is noted that in the case \( \alpha = 1 \) the tilde operator and the non-tilde operator are related by the thermal state condition for the bra vacuum:

\[
\langle 1 | a^\dagger = \langle 1 | \hat{a},
\]

where \( \langle 1 | = \langle \Psi_{n=1} | \).
4.1. Dissipative interactions
Let us consider the interaction which causes energy dissipation and instability of the system [13, 14, 15]: In TFD, such an interaction may be expressed in the form of
\[ \hat{\Gamma} = g(t)(a^\dagger a - \bar{a}a). \] (19)

We note that the above interaction ensures the condition \( (\hat{\Gamma})^\dagger = \hat{\Gamma} \) for the interaction Hamiltonians in open quantum systems. By substituting Eq. (19) into Eq. (12) and Eq. (17) and noticing Eq. (14), we obtain the equation for the entropy production rate:
\[ \frac{\partial S(t)}{\partial t} = \frac{\partial \eta(t)}{\partial t} = -\frac{k}{\hbar} g(t), \] (20)

and the equation of motion for the distribution function:
\[ \hbar \frac{\partial f(t)}{\partial t} = \frac{g(t)}{\ln \frac{1 + f(t)}{1 - f(t)}}. \] (21)

respectively. From Eq. (20), the entropy at time \( t \) is expeditiously evaluated by
\[ S(t) = S(0) - \frac{k}{\hbar} \int_0^t g(t) dt. \] (22)

It should be noted again that the entropy and the distribution function can be evaluated when the coupling function \( g(t) \) of the system-environment interaction Hamiltonian [see Eq. (19)] is specifically given.

4.2. A relaxation process
A relaxation process is often described by the equation of motion for the distribution function [16]:
\[ \hbar \frac{\partial f(t)}{\partial t} = -2\kappa \{ f(t) - \bar{f} \}, \] (23)

where \( \kappa \) is an arbitrary positive c-number parameter and \( \bar{f} \) is an equilibrium distribution function specified by e.g. the Planck distribution function with temperature \( T \):
\[ \bar{f} = \frac{1}{e^{\hbar \omega / kT} - 1}. \] (24)

Solving Eq. (23) for \( f(t) \), we obtain
\[ f(t) = \bar{f} - (\bar{f} - f_0) e^{-2\kappa t / \hbar}, \] (25)

where \( f_0 \) is an initial distribution function.

Now we consider the Hamiltonian for an open quantum system, whose Hamiltonian in TFD can be expressed in a general form:
\[ \hat{H} = H - \hat{\Gamma} + i\hat{\Gamma}, \] (26)

where we consider the case \( H - \hat{\Gamma} \) and \( \hat{\Gamma} \) are specifically given by
\[ H - \hat{\Gamma} = \hbar \omega (a^\dagger a - \bar{a}^\dagger \bar{a}), \] (27)
\[ \hat{\Gamma} = -\kappa (a^\dagger a + \bar{a}^\dagger \bar{a} - 2\bar{f}) \left\{ \ln f(t) - \ln [1 + f(t)] \right\}. \] (28)
Here we note that the \( \tilde{\Gamma} \) in Eq. (28) ensures the condition \( \langle \tilde{\Gamma} \rangle^\sim = \tilde{\Gamma} \). We can easily confirm that this Hamiltonian leads to the equation of motion for the distribution function given by Eq. (23) with the use of Eq. (17). Solving the self-consistent equations, Eqs. (23) and (28) for \( f(t) \), we can obtain \( f(t) \) and \( \tilde{\Gamma}(t) \) at time \( t \). Taking the same path to obtain Eq. (20), we obtain the equation for the entropy production rate for an open system:

\[
\frac{\partial S(t)}{\partial t} = -\frac{k}{\hbar} \langle \tilde{\Gamma}(t) \rangle_t = \frac{2k\kappa}{\hbar} \{ f(t) - \bar{f} \},
\]

(29)

where we used Eq. (28) for the interaction Hamiltonian. Substituting Eq. (25) into the right-hand side of Eq. (29), Eq. (29) can be written in the form:

\[
\frac{\partial S(t)}{\partial t} = -\frac{2k\kappa}{\hbar} (\bar{f} - f_0) e^{-2\kappa t / \hbar}.
\]

(30)

Furthermore integrating Eq. (30) with respect to time \( t \), we obtain the entropy of the system at time \( t \) for the open quantum system described by the specific Hamiltonian \( \mathcal{H} \) given by Eqs. (27) and (28):

\[
S(t) = S(\infty) + k(\bar{f} - f_0) e^{-2\kappa t / \hbar}.
\]

(31)

This equation implies that the entropy of the system will relax exponentially to \( S(\infty) \) with the relaxation time \( \tau := \hbar / 2\kappa \) due to the presence of the interaction given by Eq. (28).

5. Summary and concluding remarks

We developed a microscopic theory of entropy and derived a general formula which connects entropy to a system Hamiltonian. This formula, so-called the “entropy-Hamiltonian relation” (EHR), is applied for an open quantum system with the help of the Liouville-space formulation or thermo field dynamics (TFD). When an open system is in a thermal equilibrium state, the system is thermally equilibrium with its environment at the same temperature. On the basis of the zeroth law of thermodynamics, it is by no means to discriminate the state of the system thermodynamically from that of its environment, meaning that the environment in equilibrium is of de-individuation from the system in equilibrium. As shown in Sec. 2, this allows us to relate the interactions to the entropy of the system and to investigate the effect of interactions in nonequilibrium open quantum systems by assuming that we can consider the environment to be a copy of the system. Therefore, we can assign the system of interest to the non-tilde Hilbert space \( \mathcal{H} \) and its environment to the tilde space \( \tilde{\mathcal{H}} \) in the representation space \( \mathcal{L} := \mathcal{H} \otimes \tilde{\mathcal{H}} \) introduced in TFD. Regarding the environment as the copy of the system, we can indeed make the transformation of the system under consideration onto the non-tilde Hilbert space \( \mathcal{H} \) (i.e. \( H_{\text{sys}} \mapsto H \)) and the environment onto the tilde Hilbert space \( \tilde{\mathcal{H}} \) (i.e. \( H_{\text{environ}} \mapsto \tilde{H} \)). With this prescription, we accomplished a natural transformation of an open quantum system within the theoretical structure of TFD in the following way: the interaction Hamiltonian \( H_{\text{sys-environ}} \) is mapped to the representation space \( \mathcal{L} \) by the mapping \( H_{\text{sys-environ}} \mapsto H_{\text{nontilde-tilde}}(\equiv i\tilde{\Gamma}) \).

We derived the EHR formulas (11) and (12) which connect the interaction Hamiltonian to the entropy of the system in nonequilibrium open quantum systems. The equation of motion for the distribution function (17) is also obtained from the entropy represented by the distribution function. We apply the EHR formula and the equation of motion for a distribution function obtained in Sec. 2 to two different kinds of boson model. In particular, we considered the case where the interaction causes dissipation and the case where the interaction causes a relaxation process to show the applicability of obtained formulas. We obtained the entropy production by using these interaction Hamiltonians to the EHR formula. If we find the microscopic description
of the interaction Hamiltonian $\hat{\Gamma}$, all we need to do is to utilize the EHR formulas (11) and (12), and we will have the entropy production from which we can obtain some information about the interaction through the entropy of the system for the open quantum system.

Finally, one important remark is relevant here. The quantum effects play a very essential role in the nanoscale tribology [17, 18, 19, 20, 21]. For instance, the Caldeira-Leggett model introduced to elucidate the role of (quantal) friction is successfully formulated by considering a macroscopic quantum tunneling in terms of path-integral method [17]. However, their formulation is difficult to treat and calculate analytically. While, our theory is based on canonical formulation and therefore it can be more intuitively understood the interacting phenomena, and easier to treat and evaluate than the path-integral method. Indeed, our new formulation presented in this article (i.e. the EHR) enables us to calculate the entropy production directly from system-environment interactions. This means that it allows us to conjecture what type of interactions play an essential role for frictional effects on the system just using a conjectured form of the interaction Hamiltonian $\hat{\Gamma}$.

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