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Reduced dynamics and the master equation of open quantum systems

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ABSTRACT

An exact reduced density operator of a quantum system interacting with a bosonic thermal reservoir is derived by means of the simple algebraic method. The necessary and sufficient condition is found that the time-convolutionless master equation becomes exact up to the second order with respect to the system-reservoir interaction. The result is examined by means of the boson-detector model. The reduced dynamics of a quantum system interacting with a classical reservoir is also discussed.

1. Introduction

A quantum system placed under the influence of a surrounding environment, which is referred to as a thermal reservoir, undergoes an irreversible time-evolution from an initial state to a thermal equilibrium state. It is one of the most important problems in non-equilibrium quantum statistical mechanics to formulate such an irreversible time-evolution of a quantum system [1–3]. For this purpose, the various kinds of mathematical methods such as the stochastic method [1], the path-integral method [4–6] and the projection-operator method [3,7,8], have been developed. Except for the several models, however, it is very difficult to derive an exact result for a reduced dynamics of an open quantum system. When the interaction between the relevant system and thermal reservoir is linear with respect to bosonic annihilation and creation operators and the reservoir consists of independent harmonic oscillators in the thermal equilibrium state, the exact time-evolution generator of the relevant system have been obtained both in the adiabatic coupling case [9–11] and in the non-adiabatic coupling case [12–14]. Essentially the same result was obtained in the path integral form [5] and was used to discuss the quantum Brownian motion [6]. In the adiabatic coupling case, the condition has been found that the time-convolutionless (TCL) quantum master equation [7,8] of the second-order perturbation with respect to the system-reservoir interaction becomes exact [11]. In the non-adiabatic coupling case, it has explicitly been checked [13] up to the fourth-order with respect to the system-reservoir interaction that the reduced density operator satisfies the TCL master equation derived by means of the projection operator method [8]. In other words, the exact time-evolution generator in the non-adiabatic case yields the TCL quantum master equation with the higher order terms. This is not in accordance with the assertion [14] that the TCL master equation of the second-order perturbation is exact. In this Letter, therefore, we will investigate the condition that the second-order TCL master equation becomes exact in both the adiabatic and non-adiabatic cases. This is the generalization of the results obtained in Ref. [11].

This Letter is organized as follow. In Section 2, using the simple algebraic method, we derive the exact reduced density operator of an open quantum system, though the result is the same as that obtained by means of the field-theoretical method [12,13] and the path-integral method [14]. As noted above, an equivalent path integral form of the solution was found in Ref. [5]. In Section 3, we obtain the necessary and sufficient condition for the second-order TCL master equation to be exact. In Section 4, we investigate the reduced dynamics for a propagating particle of the boson-detector model. We provide the concluding remarks in Section 5. In Appendix A, we briefly discuss the reduced dynamics when the thermal reservoir is classical.

2. Reduced dynamics of an open quantum system

We consider a reduced dynamics of a quantum system in contact with a thermal reservoir which is a large environmental system in thermal equilibrium. We denote Hamiltonians of the relevant quantum system and thermal reservoir as $\hat{H}_S$ and $\hat{H}_R$. In our treatment, we do not need to specify the system Hamiltonian $\hat{H}_S$. The thermal reservoir is assumed to be a set of independent harmonic oscillators in the thermal equilibrium state and thus $\hat{H}_R$ is given by $\hat{H}_R = \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k$, where ω_k is the frequency and $\hat{a}_k$ and

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$\hat{a}_k^\dagger$ are bosonic annihilation and creation operators of the kth reservoir oscillator. We further assume that the interaction Hamiltonian $\hat{H}_{SR}$ between the relevant system and thermal reservoir is $\hat{H}_{SR} = \hbar\hat{S}\hat{X}$, where $\hat{S}$ stands for a Hermitian operator of the relevant system and the reservoir operator $\hat{X}$ is given by $\hat{X} = \sum_k (g_k\hat{a}_k + g_k^*\hat{a}_k^\dagger)$. In the interaction picture, we have $\hat{H}_{SR}(t) = \hbar\hat{S}(t)\hat{X}(t)$ with $\hat{S}(t) = e^{(it/\hbar)\hat{H}_S}\hat{S}e^{-(it/\hbar)\hat{H}_S}$ and $\hat{X}(t) = \sum_k (g_k e^{-i\omega_k t}\hat{a}_k + g_k^* e^{i\omega_k t}\hat{a}_k^\dagger)$. It is important to note that $\hat{S}(t)$ and $\hat{X}(t')$ are commutable for any t and t', namely, $[\hat{S}(t), \hat{X}(t')] = 0$.

A density operator $\hat{W}(t)$ of the total system in the interaction picture is subject to the Liouville–von Neumann equation,

$$\frac{\partial}{\partial t}\hat{W}(t) = -i\big[\hat{S}(t)\hat{X}(t), \hat{W}(t)\big]. \tag{1}$$

For our purpose, it is convenient to introduce superoperator $\check{M}$ corresponding to an operator $\hat{M}$ by the relation $\check{M}\bullet = \bullet\hat{M}$. It is easy to check that $[\hat{M}, \check{N}] = [\check{M}, \hat{N}] = 0$ for any $\hat{M}$ and $\hat{N}$. Furthermore the relations $\mathrm{Tr}\check{L}\check{M}\hat{N} = \mathrm{Tr}\hat{M}\hat{L}\hat{N}$ and $(MN)\check{} = \check{N}\check{M}$ are also fulfilled. Then we can express the Liouville–von Neumann equation in terms of the superoperators,

$$\frac{\partial}{\partial t}\hat{W}(t) = -i\big[\hat{S}(t)\hat{X}(t) - \check{S}(t)\check{X}(t)\big]\hat{W}(t), \tag{2}$$

the formal solution of which is given by

$$\hat{W}(t) = \mathrm{T}\exp\left(-i\int_0^t dt'\,\big[\hat{S}(t')\hat{X}(t') - \check{S}(t')\check{X}(t')\big]\right)\hat{W}(0), \tag{3}$$

where T stands for the time-ordering operation such that superoperators $\hat{S}(t)$, $\check{S}(t)$, $\hat{X}(t)$ and $\check{X}(t)$ are placed from the right to the left in the chronological order. The initial density operator of the total system is

$$\hat{W}(0) = \hat{\rho}_S(0)\otimes\hat{\rho}_R, \tag{4}$$

where $\hat{\rho}_S(0)$ is an arbitrary density operator of the relevant system and $\hat{\rho}_R$ is the thermal equilibrium state of the reservoir, that is, $\hat{\rho}_R = e^{-\hat{H}_R/k_\mathrm{B}T}/\mathrm{Tr}_R\, e^{-\hat{H}_R/k_\mathrm{B}T}$. Here Tr_R is the trace operation over the reservoir Hilbert space and T is an absolute temperature of the thermal reservoir.

To proceed further, we note that since $[\hat{S}(t), \hat{X}(t')] = 0$ and $[\check{S}(t), \check{X}(t')] = 0$ are always satisfied for any t and t', the time-ordering operation can be decomposed into $\mathrm{T}_S\mathrm{T}_R$ [12], where T_S (T_R) stands for the time-ordering operations for $\hat{S}(t)$'s and $\check{S}(t)$'s ($\hat{X}(t)$'s and $\check{X}(t)$'s). Then the density operator $\hat{W}(t)$ can be written in the following form:

$$\hat{W}(t) = \mathrm{T}_S\left[\mathrm{T}_R\exp\left(-i\int_0^t dt'\,\hat{S}(t')\hat{X}(t')\right)\right.$$
$$\left.\times\,\mathrm{T}_R\exp\left(i\int_0^t dt'\,\check{S}(t')\check{X}(t')\right)\right]\hat{W}(0). \tag{5}$$

To obtain the time-evolution of the total system, we first calculate the unitary superoperator,

$$\hat{U}(t) = \mathrm{T}_R\exp\left(-i\int_0^t dt'\,\hat{S}(t')\hat{X}(t')\right). \tag{6}$$

Since the operator $\hat{U}(t)$ always appears under the time-ordering operation T_S of the relevant system, we can teat the operator $\hat{S}(t)$ as a c-number when we calculate the unitary operator $\hat{U}(t)$.

Differentiating the unitary operator $\hat{U}(t)$ with respect to time t, we obtain

$$\frac{\partial}{\partial t}\hat{U}(t) = -i\hat{S}(t)\big[\hat{A}(t) + \hat{A}^\dagger(t)\big]\hat{U}(t), \tag{7}$$

where $\hat{A}(t)$ is the positive frequency part of $\hat{X}(t)$, that is, $\hat{A}(t) = \sum_k g_k e^{-i\omega_k t}\hat{a}_k$. We can easily obtain the commutation relations,

$$\big[\hat{S}(t)\hat{A}(t), \hat{S}(t')\hat{A}(t')\big] = 0,$$
$$\big[\hat{S}(t)\hat{A}(t), \hat{S}(t')\hat{A}^\dagger(t')\big] = \hat{S}(t,t'), \tag{8}$$
$$\big[\check{S}(t)\check{A}(t), \check{S}(t')\check{A}(t')\big] = 0,$$
$$\big[\check{S}(t)\check{A}(t), \check{S}(t')\check{A}^\dagger(t')\big] = -\check{S}(t,t'), \tag{9}$$

with

$$\hat{S}(t,t') = \hat{S}(t)\hat{S}(t')\sum_k |g_k|^2 e^{-i\omega_k(t-t')},$$
$$\check{S}(t,t') = \check{S}(t)\check{S}(t')\sum_k |g_k|^2 e^{-i\omega_k(t-t')}. \tag{10}$$

Introducing the operator $\hat{U}'(t)$ by

$$\hat{U}(t) = \exp\left[-i\int_0^t dt'\,\hat{S}(t')\hat{A}(t')\right]\hat{U}'(t), \tag{11}$$

and using the commutation relations given by Eq. (8), we can derive

$$\frac{\partial}{\partial t}\hat{U}'(t) = \left[-i\hat{S}(t)\hat{A}^\dagger(t) + \int_0^t dt'\,\hat{S}(t',t)\right]\hat{U}'(t). \tag{12}$$

Solving this equation, we obtain

$$\hat{U}(t) = \exp\left(\int_0^t dt'\int_0^{t'} dt''\,\hat{S}(t'',t')\right)\exp\left(-i\int_0^t dt'\,\hat{S}(t')\hat{A}(t')\right)$$
$$\times\exp\left(-i\int_0^t dt'\,\hat{S}(t')\hat{A}^\dagger(t')\right). \tag{13}$$

Combining the second and third exponentials, we find the expression of the unitary operator $\hat{U}(t)$ without the time-ordering operation T_R,

$$\hat{U}(t) = \exp\left(-\frac{1}{2}\int_0^t dt'\int_0^{t'} dt''\,\big[\hat{S}(t',t'') - \hat{S}(t'',t')\big]\right)$$
$$\times\exp\left(-i\int_0^t dt'\,\hat{S}(t')\hat{X}(t')\right). \tag{14}$$

For the unitary operator obtained by replacing $\hat{S}(t)$ and $\hat{X}(t)$ with $\check{S}(t)$ and $-\check{X}(t)$ in Eq. (6), using the commutation relations given by Eq. (9), we can derive the similar result. Thus the density operator $\hat{W}(t)$ of the total system becomes

$$\hat{W}(t) = \mathrm{T}_S\left[\hat{\mathcal{U}}_S(t)\exp\left(-i\int_0^t dt'\,\hat{S}(t')\hat{X}(t')\right)\right.$$
$$\left.\times\exp\left(i\int_0^t dt'\,\check{S}(t')\check{X}(t')\right)\right]\hat{W}(0), \tag{15}$$