Effective Hamiltonian Approach to the Master Equation

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Abstract

A method of exactly solving the master equation is presented in this letter. The explicit form of the solution is determined by the time evolution of a composite system including an auxiliary system and the open system in question. The effective Hamiltonian governing the time evolution of the composed system are derived from the master equation. Two examples, the dissipative two-level system and the damped harmonic oscillator, are presented to illustrate the solving procedure.

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The problem of open quantum systems has been around since the beginnings of quantum mechanics [1]. Important contributions to this general area have been made by researchers working in fields as diverse as cosmology [2], condensed matter [3], quantum optics [4,5], particle physics [6], quantum measurement [7], and quantum computation [8]. The problem can be described generally as interest in the effective dynamics of the open system surrounded by its environment. A formal framework to describe the effective dynamics of such an open system was set up in Ref.[9].

Generally speaking, interactions between a quantum system and its environment result in two kinds of irreversible effects: dissipation and decoherence. The first effect is due to the energy exchange between the system and its environment, whereas the second one comes from the system-environment interaction that does not change the system energy. A powerful tool to study the quantum dissipative system is the master equation, which can be obtained in Markovian limit [1,2,4]. This approximation is often very useful became it is valid for many physically relevant situations and became its numerical solutions can be found. As given by Gardiner, Walls and Millburn, Louisell in their textbook [4], the reduced density matrix ρ of the open system which is linearly coupled to its environment obeys the following master equation in Lindblad form [10]

$$
\begin{aligned}
\dot{\rho}(t) = {} & -i[H_0, \rho] \\
& + \frac{1}{2} \sum_m K_m (2 X_m^- \rho X_m^+ - X_m^+ X_m^- \rho - \rho X_m^+ X_m^-) \\
& + \frac{1}{2} \sum_m G_m (2 X_m^+ \rho X_m^- - X_m^- X_m^+ \rho - \rho X_m^- X_m^+)
\end{aligned}
\tag{1}
$$

with

$$
K_m = 2\mathrm{Re} \left[\int_0^\infty d\tau e^{i\omega_m \tau} \mathrm{Tr}_{env} \{ A_m(\tau) A_m^\dagger(0) \rho_{env} \} \right],
$$

$$
G_m = 2\mathrm{Re} \left[\int_0^\infty d\tau e^{i\omega_m \tau} \mathrm{Tr}_{env} \{ A_m^\dagger(\tau) A_m(0) \rho_{env} \} \right].
$$

Here, $\rho(t) = \rho(t, K_m, G_m)$ stands for the density operator of the system and ρ_{env} denotes the density operator of the environment, $X_m^\pm$ are eigenoperators of the system satisfying $[H_0, X_m^\pm] = \pm\hbar\omega_m X_m^\pm$, H_0 stands for the free Hamiltonian of the system, and $A_m(A_m^\dagger)$

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are operators of the environment through which the system and its environment coupled together. Notice from eq.(1) that G_m should vanish at zero temperature $T = 0$, while K_m should not if A_m are indeed destruction operators of some kind. Some efforts such as the short-time expansion[11], the exact solution for some special kinds of the master equation[12], the small lose rate expansion[13] and the method of stochastic unravelings[14] have been made to solve (or solve it alternatively) the master equation. Unfortunately, this kind of master equation has not a general exact analytical solution yet.

Here we shall construct an exact solution for the master equation to describe quantum dynamics of an open system with linear dissipation. The method is outlined as follows. After introducing an auxillary system and mapping the density matrix of the original system to a pure state of the composite system, we obtain an effective Hamiltonian describing the evolution of the composite system from the master equation satisfied by the density matrix. Then the solution of the master equation can be obtained in terms of the evolution of the composite system by mapping the pure state back to the density matrix. As its applications, we present two examples to illustrate the solving procedure. The first example is a two-level atom coupling to a bosonic environment, whereas the second example consists of a single mode field in a cavity with linewidth κ due to partial transmission through one mirror.

We suppose that the Hilbert space of the system S is an N-dimension Hilbert space spanned by, for instance, all the eigenstates of H_0. To begin with, we rewrite the master equation given in eq.(1) as the following general form

$$i\frac{\partial \rho}{\partial t} = H\rho - \rho H^\dagger + i\sum_\alpha \gamma_\alpha L_\alpha \rho L_\alpha^\dagger, \tag{2}$$

where H and L_α are well defined time-independent operators of the system, which may not be Hermitian generally and γ_α are real parameters determined by the environment.

As the first step to solve this general master equation, we introduce an auxiliary system A which is the same with the original system we concern. That is to say, the original Hilbert space is extended to an N^2-dimensional Hilbert space, which is the Hilbert space of the original system S and the ancilla A. Let $\{|m_S\rangle|n_A\rangle\}$ be an orthonormal and complete basis

for this composite system.

A density matrix ρ of the system S, whose matrix elements under the basis $\{|m_S\rangle\}$ of the system are denoted as $\rho_{mn} = \langle m|\rho|n\rangle_S$, determines a pure bipartite state in the N^2-dimensional Hilbert space according to

$$|\psi_\rho\rangle = \sum_{m,n=1}^{N} \rho_{mn}|m_S\rangle|n_A\rangle. \tag{3}$$

We note that this corresponding pure bipartite state is generally not normalized unless the initial state ρ of the system is a pure state. In fact every operator of the original system determines a pure state of the bipartite system in the same manner [15].

With the density matrix ρ evolving with time, the corresponding pure state $|\psi_\rho\rangle$ changes accordingly into another pure state

$$|\psi_\rho(t)\rangle = \sum_{m,n=1}^{N} \rho_{mn}(t)|m_S\rangle|n_A\rangle. \tag{4}$$

Because the evolution of the density matrix is governed by the general master equation (2), the evolution of the pure state $|\psi_\rho(t)\rangle$ is governed by the following Schödinger-like equation

$$i\partial_t|\psi_\rho(t)\rangle = \tilde{H}|\psi_\rho(t)\rangle. \tag{5}$$

Here the effective Hamiltonian, which is generally not Hermitian, reads

$$\tilde{H} = H - H_A + i\sum_\alpha \gamma_\alpha L_\alpha L_{A\alpha}, \tag{6}$$

where operators H and L_α of the original system are the same as given in Eq.(2) and operators H_A and $L_{A\alpha}^*$ are operators of the auxiliary system whose matrix elements are specified by

$$\langle m|H_A|n\rangle_A = \langle n|H^\dagger|m\rangle_S, \tag{7}$$

$$\langle m|L_{A\alpha}|n\rangle_A = \langle n|L_\alpha^\dagger|m\rangle_S. \tag{8}$$

We note that the first two terms of the effective Hamiltonian $\tilde{H}$ describe free evolutions of the system and the auxiliary system governed by H and $-H_A$ and the third term describes an interaction between the system and the ancilla.

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Because the effective Hamiltonian $\tilde{H}$ of the composite system is time-independent, we can obtain formally the evolution of the pure state $|\psi_\rho(t)\rangle$ as

$$|\psi_\rho(t)\rangle = e^{-i\tilde{H}t}|\psi_\rho\rangle. \tag{9}$$

¿From the definition Eq.(4) of the pure state $|\psi_\rho(t)\rangle$, we obtain finally the time-dependence of the original density matrix as

$$\rho_{mn}(t) = \langle m_S|\langle n_A|\psi_\rho(t)\rangle = \langle m_S|\langle n_A|e^{-i\tilde{H}t}|\psi_\rho\rangle. \tag{10}$$

Since the effective Hamiltonian $\tilde{H}$ changes its sign under the complex conjugate together with an interchange of the system and the ancilla, the Hermicity of the density matrix is preserved during the evolution. Moreover if the master equation (2) preserves the trace of the density matrix, solution given in Eq.(10) has also trace 1 when the initial state is normalized.

The generalizations of the above effective Hamiltonian method to the systems with infinite many energy levels or with continuous spectra are straightforward. Also, the master equations with time-dependent γ_α and those master equations not posessing Lindblad form can be treated in the same manner, i.e., effective Hamiltonian can be obtained similarly. Thus the problem of solving the master equation becomes a problem of finding the time evolution of an effective Hamiltonian. Although the biorthogonal basis can be used to deal with general non-Hermitian Hamiltonian, for some special cases we can evaluate the evolution operator directly for finite-level system as illustrated by the first example and factorize the evolution operator directly for quadratic systems as illustrated by the second example.

In order to gain further insight into the content of the solution presented above, we shall consider at first the following master equation describing a two-level atom coupled to a bose-mode environment [4]

$$\dot{\rho} = -\frac{i\Omega}{2}[\sigma_z, \rho] + \frac{\gamma}{2}\{2\sigma_-\rho\sigma_+ - \rho\sigma_+\sigma_- - \sigma_+\sigma_-\rho\} \tag{11}$$

with

$$\gamma = 2\pi \mathrm{Re}\left[\int_0^\infty d\tau e^{i\omega_m\tau}\mathrm{Tr}_{env}\{b_m(\tau)b_m^\dagger(0)\rho_{env}\}\right],$$

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where $b_m^\dagger (b_m)$ stands for the creation (annihilation) operator of the m-th mode of the environment, Ω is the Rabi frequency, and $\sigma_z(\sigma_\pm)$ denote the Pauli matrices. The basis of the two-level system is chosen so that $\sigma_+|g_S\rangle = |e_S\rangle$ where $|g_S\rangle$ and $|e_S\rangle$ stand for the ground and excited states. This master equation is obtained under the condition that the environment is in its vacuum state.

The auxiliary system we shall introduce is another two-level system whose Pauli matrices are denoted as $\tau_z(\tau_\pm)$ which satisfy $\tau_+|g_A\rangle = |e_A\rangle$, where $|e_A\rangle$ denotes the upper level of the ancilla A. By rewriting the master equation above into the general form of Eq.(2), we obtain immediately $H = (\Omega\sigma_z - i\gamma\sigma_+\sigma_-)/2$ and $L = \sigma_-$. According to the definitions (7-8) we obtain $H_A = (\Omega\tau_z + i\gamma\tau_+\tau_-)/2$ and $L_A = \tau_-$. The effective Hamiltonian governing the time evolution of the bipartite system is therefore

$$\tilde{H} = H - H_A + i\gamma\sigma_-\tau_-. \tag{12}$$

As mentioned above, eq.(12) is the effective Hamiltonian corresponding to the master eq.(11), which is derived by neglecting the temperature effect of the environment. If we take the temperature effects into account, the effective Hamiltonian should be

$$
\begin{aligned}
\tilde{H}_T &= H - H_A + i\gamma\left(\bar{N}\sigma_+\tau_+ + (\bar{N}+1)\sigma_-\tau_- - \bar{N}\right) \\
&= \left\{\frac{\Omega}{2}(\sigma_z - \tau_z) - i\gamma\left(\bar{N} + \frac{1}{2}\right)\right\} \\
&\quad + i\gamma\left\{\bar{N}\sigma_+\tau_+ + (\bar{N}+1)\sigma_-\tau_- - \frac{\sigma_z + \tau_z}{4}\right\} \\
&\equiv H_0 + i\gamma J \tag{13}
\end{aligned}
$$

where $\bar{N} = (\exp(\Omega/k_B T) - 1)^{-1}$ is the Bose distribution. Further we have $[H_0, J] = 0$ and $J|e_S\rangle|g_A\rangle = J|g_S\rangle|e_A\rangle = 0$ which are sufficient to make an explicit calculation of the evolution operator

$$
e^{-i\tilde{H}_T t} = \frac{1}{2\bar{N}+1}
\begin{pmatrix}
\bar{N} + (\bar{N}+1)e^{-(2\bar{N}+1)\gamma t} & 0 & 0 & \bar{N}(1 - e^{-(2\bar{N}+1)\gamma t}) \\
0 & e^{-i\Omega t - (\bar{N}+1/2)\gamma t} & 0 & 0 \\
0 & 0 & e^{i\Omega t - (\bar{N}+1/2)\gamma t} & 0 \\
(\bar{N}+1)(1 - e^{-(2\bar{N}+1)\gamma t}) & 0 & 0 & \bar{N} + 1 + \bar{N}e^{-(2\bar{N}+1)\gamma t}
\end{pmatrix}
\tag{14}
$$

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where the bases of the composite system has been arranged as $|e_S, e_A\rangle$, $|e_S, g_A\rangle$, $|g_S, e_A\rangle$, and $|g_S, g_A\rangle$. For simplicity, we consider zero temperature Hamiltonian $\tilde{H}$ to study the time evolution of the density matrix $\rho(t)$ with $\bar{N} = 0$.

For a general initial state $\rho(0) = \sum_{i,j=g,e} \rho_{ij}|i_S\rangle\langle j_S|$ where $\rho_{ij} = \langle i_S|\rho(0)|j_S\rangle$, the corresponding initial state of the bipartite system is $|\psi_\rho(0)\rangle = \sum_{i,j=g,e} \rho_{ij}|i_S, j_A\rangle$. With this initial condition the final state of the composed system at time t reads

$$|\psi_\rho(t)\rangle = \rho_{ee}e^{-\gamma t}|e_S, e_A\rangle + (\rho_{gg} + \rho_{ee}(1 - e^{-\gamma t}))|g_S, g_A\rangle$$

$$+\rho_{eg}e^{-\frac{\gamma}{2}-i\Omega t}|e_S, g_A\rangle + \rho_{ge}e^{-\frac{\gamma}{2}+i\Omega t}|g_S, e_A\rangle. \tag{15}$$

That is

$$\rho_{ee}(t) = \rho_{ee}e^{-\gamma t}, \quad \rho_{gg}(t) = \rho_{ee}(1 - e^{-\gamma t}) + \rho_{gg},$$

$$\rho_{eg}(t) = e^{-\frac{\gamma}{2}t-i\Omega t}\rho_{eg}, \quad \rho_{ge}(t) = e^{-\frac{\gamma}{2}t+i\Omega t}\rho_{ge}. \tag{16}$$

The results show that the off-diagonal elements of the density matrix are damped-oscillation function of time, while the diagonal element ρ_{ee} decay exponentially. If $\Omega > \gamma$, there are several Rabi oscillations in ρ_{eg} (or ρ_{ge}) with the time evolution, otherwise ρ_{eg} (or ρ_{ge}) decay directly. Especially we consider a state $\rho = |e_S\rangle\langle e_S|$ as the initial condition of the density operator ρ, At time t we have

$$\langle e_S|\rho(t)|e_S\rangle = e^{-\gamma t}, \langle g_S|\rho(t)|g_S\rangle = 1 - e^{-\gamma t},$$

$$\langle e_S|\rho(t)|g_S\rangle = \langle g_S|\rho(t)|e_S\rangle = 0. \tag{17}$$

It is well known that the element $\langle e_S|\rho(t)|e_S\rangle$ of the density operator $\rho(t)$ represents the population of the system in its upper level $|e_S\rangle$. The results (17) show that the population of the upper level $|e_S\rangle$ decay exponentially with the time evolution, this coincides with the results given in most textbooks [4].

The second example presented here is a single-mode field in a lossy cavity. The density operator for that mode obeys the following master equation in the Schrödinger picture[4],

$$\dot{\rho} = -i[\omega_f a^\dagger a, \rho] + \frac{\kappa}{2}(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a), \tag{18}$$

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where κ is the linewidth of the cavity mode with frequency ω_f. In most textbooks, the solution of the master equation is given in terms of diagonal matrix elements $\langle n|\rho|n\rangle$ in a stationary state. Given an initial condition for the density operator, the evolution of ρ, however, is more useful than the stationary solution. In contrast with the solution in P-representation[4], in what follows, we present a solution of the master equation in a number state (Fock state) basis.

Comparing the above master equation with the general form eq.(2), we see that $H = (\omega_f - i\kappa/2)a^\dagger a$ and $L = a$. The auxiliary system is another single-mode field whose annihilation and creation operators are denoted as b and $b^\dagger$ respectively. By definitions eqs.(7-8) we have $H_A = (\omega_f + i\kappa/2)b^\dagger b$ and $L_A = b$. Hence the effective Hamiltonian governing the time evolution of the bipartite system is

$$\tilde{H} = (\omega_f - \frac{i\kappa}{2})a^\dagger a - (\omega_f + \frac{i\kappa}{2})b^\dagger b + i\kappa ab, \tag{19}$$

The time evolution operator $U(t)$ corresponding the effective Hamiltonian (19) reads

$$U(t) = e^{-i(\omega_f - \frac{i\kappa}{2})a^\dagger at} e^{i(\omega_f + \frac{i\kappa}{2})b^\dagger bt} e^{g_t ab}, \tag{20}$$

where $g_t = 1 - e^{-\kappa t}$. We consider a general initial state $\rho(0) = \sum_{mn} \rho_{mn}|m\rangle\langle n|$, where $\rho_{mn} = \langle m|\rho(0)|n\rangle$ is the element of the density operator at $t = 0$. Under the Fock state basis of the bipartite system, since $|\psi_\rho(0)\rangle = \sum_{m,n} \rho_{mn}|m\rangle|n\rangle_b$, with $|n\rangle_b$ satisfying $b^\dagger b|n\rangle_b = n|n\rangle_b$ we arrive at

$$\langle p|\rho(t)|q\rangle = e^{-i\omega_f(p-q)t - \kappa(p+q)t} \times$$
$$\times \sum_{m=0}^{\infty} \frac{\sqrt{(p+m)!(q+m)!}}{(m!)^2} g_t^m \rho_{p+m,q+m}. \tag{21}$$

It is obvious that all elements of the density operator are damped-oscillation function of time, the decay rate $\kappa(p+q)$ depends on the sum of p and q, which are initial condition-independent. Furthermore, we notice that the diagonal elements of the density operator, which represent the population in the corresponding state decay with different damped rate, the higher the state, the faster the decay. When the single-mode is initially at a thermal

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state $\rho(0) = e^{-\beta a^\dagger a}$ with the partition function as its normalization, we find that after time t the system is still at a thermal state $\rho(t) = e^{-\beta(t)a^\dagger a}$ with

$$\beta(t) = \beta + \kappa t + \ln(1 - e^{-\beta}(1 - e^{-\kappa t})). \tag{22}$$

Based on equation (21), for the bipartite system in the initial state corresponding to $\rho(0)$ we have

$$\rho(t) = \sum_{m=0}^{\infty} A_m(t)\rho(0)A_m^\dagger(t)$$
$$A_m(t) = \sqrt{\frac{g_t^m}{m!}}e^{-(i\omega_f + \kappa/2)a^\dagger a t}a^m, \tag{23}$$

which shows explicitly that the evolution is completely positive and trace preserving. Therefore there exist an environment and an evolution $U(t)$ of the system and the environment such that

$$\rho(t) = \mathrm{Tr}_E(U(t)(\rho(0) \otimes |0\rangle\langle 0|_E)U^\dagger(t)) \tag{24}$$

satisfies the master equation. It should be emphasized that the environment is exact. For the simple case of a single-mode field in lossy cavity, the environment is another single-mode field and the evolution is

$$U(t) = e^{-i\omega_f t a^\dagger a}e^{\theta_t(a^\dagger b - b^\dagger a)} \tag{25}$$

with $\cos\theta_t = e^{-\kappa t/2}$. In fact $A_m(t) = \langle m_b|U(t)|0_b\rangle$. This provides another Hamiltonian approach to this kind of problem: two-mode field interacting with one another with a time-dependent interaction.

In summary, we propose a method to approach solving the master equation exactly. For this end, we first of all introduce an auxiliary system, which has the same dimension as the system that we are interested in. The original system and the ancilla interact on each other, and the Hamiltonian which governs the time evolution of the composite system are determined by the master equation. In this sense, the solution of the master equation might be computed through the Schrödinger equation of the composed system. We would like to

note that whether we can obtain the solution of the master equation in an explicit form or not depends on the form of the effective Hamiltonian, but the method presented here provides a new approach to the exact solution of the master equation.

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