Non-Markovian dynamics of a qubit in a reservoir: different solutions of non-Markovian master equation*

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We present a non-Markovian master equation for a qubit interacting with a general reservoir, which is derived according to the Nakajima–Zwanzig and the time convolutionless projection operator technique. The non-Markovian solutions and Markovian solution of dynamical decay of a qubit are compared. The results indicate the validity of non-Markovian approach in different coupling regimes and also show that the Markovian master equation may not precisely describe the dynamics of an open quantum system in some situation. The non-Markovian solutions may be effective for many qubits independently interacting with the heated reservoirs.

Keywords: Nakajima–Zwanzig and time convolutionless projection operator technique, non-Markovian solutions, Markovian solutions, correlation function, qubit

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1. Introduction

All quantum systems are open,[1−3] because they often interact with their environments, such as the electromagnetic field. Due to its relevance to the applications of quantum mechanics and a deeper understanding in the theory of quantum dynamics itself, an open quantum system is a very interesting topic. Research of the interaction between a quantum system and its environment is a common subject in many fields, such as quantum measurement,[4] quantum communication,[5] quantum optics,[6] condensed matter theory, and quantum chemistry, etc. Markovian approach is often employed in the above fields and the Lindblad expression for the generator of a quantum dynamical semigroup[7,8] provides a benchmark result for both microscopic[9] and phenomenological approaches.[10] However, this situation is not satisfied when we go beyond the Born–Markovian approximation and without the assumption of a separation of time scales between the system and environment in a realistic description. The memory effect of reservoir then becomes important and a non-Markovian description is necessary. Although some results have been reported,[11−25] a general valid theory of this case has not been found yet. The important step is to develop a suitable measure that can identify the degree of non-Markovianity dynamics.[26]

In general, dynamics of an open system is not solved exactly, but it can be solved precisely in certain special case, for example the Jaynes–Cummings (JC) model.[1] Here two main perturbation expansions are exploited in the solution of dynamics of an open system. The projection operator technique of the Nakajima–Zwanzig (NZ)[27] contains a convolution kernel and the time convolutionless (TCL)[28] involves a time-local generator. They can be expanded to arbitrary orders, so it is not easy to decide which method is the best. In fact the two perturbation expansions are strongly dependent on the condition of systems studied. Though the non-Markovian dynamics of this model has been studied many times,[1,27−30] these methods seem too complicated. We consider a computation approach to this model, which makes this problem become easier to solve.

In this paper, a microscopic deduction of the non-Markovian master equation for a qubit interacting with a general reservoir is given. The master equation is expanded to the second order and the dynamics of a qubit inside a reservoir is solved by means of the NZ and TCL projection operator technique. Markovian and non-Markovian dynamics of the reduced system are compared and discussed. The results show the validity of non-Markovian master equations in different

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coupling regimes of the systems and meanwhile it is pointed out that the Markovian approach might not be applied to this area in a short time. The method may become an effective way for more qubits interacting with the heated reservoir, respectively.

2. Model and exact solution

2.1. Model

The physical system we studied is composed of a two-level atom (qubit) coupling to an external field which can be treated as a bosonic bath.[1] Assuming $\hbar = 1$, the Hamiltonian of the total system can be given as

$$H = H_0 + H_{\rm I}, \tag{1}$$

where

$$H_0 = \omega_0 \sigma_z + \sum_k \omega_k b_k^\dagger b_k. \tag{2}$$

H_0 is the unperturbed part containing the free Hamiltonian of a qubit as well as an environment; ω_0 is the transition frequency of a two-level system and σ_z denotes the Pauli operator describing a qubit. The bosonic reservoir is characterized by proper frequency ω_k; $b_k^\dagger$ and b_k are the creation and destruction operators, which accord with bosonic commutation relation, namely $\left[b_k, b_{k'}^\dagger\right] = \delta_{kk'}$.

The interaction Hamiltonian reads

$$H_{\rm I} = \sigma_+ \sum_k g_k b_k + \sigma_- \sum_k g_k^* b_k^\dagger, \tag{3}$$

where σ_+ and σ_- are the raising and lowering operators of a qubit. The model describes the interaction between a qubit and a reservoir of electromagnetic field modes, which is labeled by an index k with corresponding frequencies ω_k and coupling constants g_k.

Recently, the non-Markovian dynamics stemming from Hamiltonian (1) has been analysed theoretically.[1,3] The TCL approach has been employed in order to study the non-Markovian dynamics, the time-dependent Schrödinger equation is solved exactly in another way in this article. The reduced density operator of the systems is deduced by the NZ projection operator technique and non-Markovian master equations are also acquired, therefore a comparison of exact and approximate solutions can be done in order to test the validity of perturbation expansions. In the following we work in Dirac picture with respect to H_0 and the interaction Hamiltonian in this picture is given by

$$H_{\rm I}(t) = \sigma_+ \sum_k g_k b_k \, {\rm e}^{{\rm i}(\omega_0 - \omega_k)t} + \sigma_- \sum_k g_k^* b_k^\dagger \, {\rm e}^{-{\rm i}(\omega_0 - \omega_k)t}. \tag{4}$$

2.2. Exact solution

It is easy to testify that the number operator can be written as

$$N = \sigma_+ \sigma_- + \sum_k b_k^\dagger b_k, \tag{5}$$

for the number of excitations in the total system commutes with both the total and interaction Hamiltonian, as a result of rotating wave approximation (RWA) applied in Eq. (3). Therefore, the number operator is a constant of motion. The state of the composite system along with time is

$$|\psi(t)\rangle = a(t)\,|1\rangle\,|0_k\rangle + \sum_k c_k(t)\,|0\rangle\,|1_k\rangle, \tag{6}$$

where $|1_k\rangle$ denotes a state with one photon in the k-th mode and satisfies formula $|1_k\rangle = b_k^\dagger\,|0_k\rangle$; $a(t)$ and $c_k(t)$ are probability amplitudes corresponding to states $|1\rangle\,|0_k\rangle$ and $|0\rangle\,|1_k\rangle$. Substituting Eq. (4) to the Schrödinger equation in the Dirac picture, we can obtain the equations of $a(t)$ and $c_k(t)$. Assuming $c_k(0) = 0$, which means the vacuum state of the reservoir, we can have the following equation[1]

$$\frac{{\rm d}a(t)}{{\rm d}t} = -\int_0^t a(t')\, f(t-t')\, {\rm d}t'. \tag{7}$$

The kernel $f(t-t')$ is given by the correlation function.[31] As usual, this kernel may be expressed in terms of the spectral density $J(\omega)$ of reservoir as follows:

$$f(t-t') = \int {\rm d}\omega J(\omega)\, {\rm e}^{{\rm i}(\omega_0 - \omega_k)(t-t')}. \tag{8}$$

Making use of Laplace transform, we obtain the solution of $a(t)$ is

$$\wp[a(t)] = \frac{a(0)}{p + \wp[f(t)]}, \tag{9}$$

where $\wp[a(t)]$ and $\wp[f(t)]$ denote the Laplace transform of $a(t)$ and $f(t)$ respectively, and $a(0)$ is the initial value. Once the spectral density $J(\omega)$ is fixed, it is quite easy to obtain the time evolution behaviour of $a(t)$, simply anti-transforming the amplitude $\wp[a(t)]$ supported by Eq. (9). The results will be discussed in Section 4.

3. The NZ and TCL master equation

In this section we apply the projection operator technique to obtain the non-Markovian master equation about the reduced density matrix $\rho_s(t)$ of systems.[1] It is convenient to define a super-operator P according to

$$\rho \mapsto P\rho = \mathrm{tr}_B\{\rho\} \otimes \rho_B = \rho_s \otimes \rho_B, \tag{10}$$

where ρ_B is some fixed state of a reservoir. The super-operator projects on the relevant part of the density matrix ρ and gives the complete information that is required to reconstruct the reduced density matrix ρ_s of an open system. Following the NZ approach, the corresponding equation for the relevant part of density matrix ρ is

$$\frac{\partial}{\partial t} P\rho(t) = \int_{t_0}^{t} \mathrm{d}s K(t,s) P\rho(s). \tag{11}$$

The convolution $K(t,s)$ represents a super-operator in the relevant subspace in the above equation. In order to discuss the reduced dynamics we perform a perturbation expansion of $K(t,s)$ with respect to interaction Hamiltonian.[1] The first and second order terms are

$$K_1(t,s) = PL(t)P, \tag{12}$$

and

$$K_2(t,s) = PL(t)QL(s)P. \tag{13}$$

A complementary super-operator Q projects on the irrelevant part of the density matrix ρ. $L(t)$ is the Liouville super-operator which satisfies $L(t)\rho(t) = -\mathrm{i}[H_{\mathrm{I}}(t), \rho(t)]$. Substituting Eqs. (12) and (13) into Eq. (11), we can obtain the second order NZ master equation. Then applying Eq. (4), it is easy to gain the reduced density of this composite system

$$\frac{\mathrm{d}\rho_s(t)}{\mathrm{d}t} = -\int_0^t \mathrm{d}t' \left\{ \begin{array}{l} A(t-t')[\sigma_-\rho_s(t'), \sigma_+] \\ +B(t-t')[\sigma_+, \rho_s(t')\sigma_-] \\ +A^*(t-t')[\sigma_-, \rho_s(t')\sigma_+] \\ +B^*(t-t')[\sigma_+\rho_s(t'), \sigma_-] \end{array} \right\}, \tag{14}$$

where

$$A(t-t') = \sum_k |g_k|^2 \, \mathrm{e}^{\mathrm{i}(\omega_0-\omega_k)(t-t')} \mathrm{tr}_R\left\{b_k b_k^\dagger \rho_B\right\} = \sum_k |g_k|^2 \, \mathrm{e}^{\mathrm{i}(\omega_0-\omega_k)(t-t')} \left\langle b_k b_k^\dagger \right\rangle_R,$$

$$B(t-t') = \sum_k |g_k|^2 \, \mathrm{e}^{-\mathrm{i}(\omega_0-\omega_k)(t-t')} \mathrm{tr}_R\left\{b_k^\dagger b_k \rho_B\right\} = \sum_k |g_k|^2 \, \mathrm{e}^{-\mathrm{i}(\omega_0-\omega_k)(t-t')} \left\langle b_k^\dagger b_k \right\rangle_R.$$

In the above two equations, $A(t-t')$ and $B(t-t')$ are the correlation function which corresponds to a thermal bath with $T \neq 0$ K, namely finite temperature. From Subsection 2.1, the initial condition of reservoir is the vacuum state, which means average photon $\bar{n}$ is zero and its mathematical representation is

$$\bar{n} = \left\langle b_k^\dagger b_k \right\rangle_R = \mathrm{tr}_R\left\{b_k^\dagger b_k \rho_B\right\} = 0. \tag{15}$$

Equation (14) reduces as follows:

$$\frac{\mathrm{d}\rho_s(t)}{\mathrm{d}t} = \int_0^t \mathrm{d}t' \left\{ \begin{array}{l} g(t-t')[\sigma_-\rho_s(t'), \sigma_+] \\ +g^*(t-t')[\sigma_-, \rho_s(t')\sigma_+] \end{array} \right\}, \tag{16}$$

where $g(t-t')$ is the correlation function, which coincides with $f(t-t')$ defined in Eq. (8) with $T = 0$ K.

The TCL master equation is a nonlocal evolution equation[1]

$$\frac{\partial}{\partial t} P\rho(t) = K(t) P\rho(t), \tag{17}$$

where $K(t)$ is called the TCL generator. $K(t)$ can also be expanded to arbitrary order with respect to the interaction Hamiltonian. Substituting Eq. (4) into Eq. (17), the second TCL master equation for this model leads to the following equation

$$\frac{\mathrm{d}\rho_s(t)}{\mathrm{d}t} = \int_0^t \mathrm{d}t' \left\{ \begin{array}{l} g(t-t')[\sigma_-\rho_s(t), \sigma_+] \\ +g^*(t-t')[\sigma_-, \rho_s(t)\sigma_+] \end{array} \right\}. \tag{18}$$

From the master equations (16) and (18), we can also obtain the solutions which will be reported in the next section and two solutions are compared with the exact solution.

4. Comparisons

Exploiting the above results, we can analyse the dynamical behaviour of a qubit and compare the non-Markovian and Markovian solutions. The main purpose is to point out their ranges of validity and the difference of their approaches. In fact, there is no general theory which is more appropriate among the above three approaches. Generally speaking, their effective ranges depend strongly on specific property of the reservoir, such as interaction Hamiltonian and spectral density of reservoir.

In the following, we assume that the density of reservoir is Lorentzian spectral density[1]

$$J(\omega) = \frac{1}{2\pi} \frac{\gamma\lambda^2}{(\omega_0 - \omega)^2 + \lambda^2}. \tag{19}$$

The parameter λ defines the spectral width of coupling, which is connected to the reservoir correlation time τ_B by the relation $\tau_B = \lambda^{-1}$ and τ_R denotes the rate of change for a state of the system by $\tau_R = \gamma^{-1}$. Therefore the correlation function defined by Eq. (8) takes the form

$$f(t - t') = \frac{1}{2}\gamma\lambda\, \mathrm{e}^{-\lambda|t-t'|}. \tag{20}$$

The dynamics of the system can be analysed and the population of a qubit excitation state $P_{\mathrm{e}}(t)$ can be observed. In order to examine the validity of the NZ, the TCL and the Markovian approaches, we inspect the three different coupling regimes by varying the coupled width of the Lorentzian spectral density λ.

Figure 1 shows the comparison of the exact, the TCL, the NZ and the Markovian solutions when a large reservoir bandwidth is $\lambda = 20\gamma$. The horizontal axis of the figure is the dimensionless variable γt and the vertical axis is the population of a qubit excitation state $P_{\mathrm{e}}(t)$. For the Markovian solution, the decay rate is γ. We can see clearly that they are consistent perfectly among the exact, the NZ, the TCL and the Markovian solutions in large time scale and show the validity of our method. In a short time, they begin to display the differences among the above three solutions from the insets. The NZ and TCL solutions are better than the Markovian solution, which means that they are a better approximation in this case and the Markovian approach may not be suitable in short time. From the previous section, we have known that the TCL master equation might be preferred, since it involves a time-local first order differential equation that can be easily solved. It may be a better approach as compared to other methods.

Figure 2 shows the same quantity in a weak non-Markovian regime. From the inset in Fig. 2, the Markovian solution deviates completely from the exact solution in a short time. From Fig. 2, the solution of the TCL master equation is better than the result of the NZ master equation about long time behaviour, so under this condition the NZ master equation method is not a good approximation, and the population even appears negative values which do not match the real process. We may conclude that under this condition our exact solution and the TCL solution can show the virtual process, but the Markovian approach and the NZ projection operator technique are not introduced.

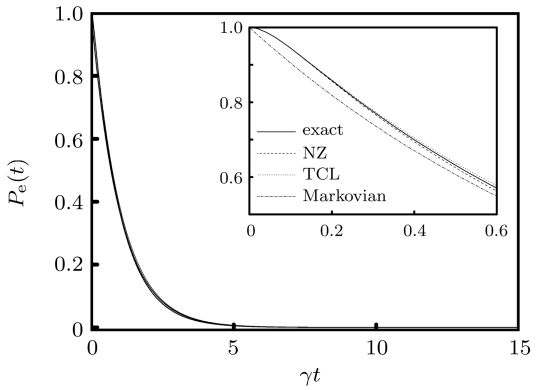


Fig. 1. The population of excitation state $|1\rangle$ along with time for a qubit initially prepared in excitation state and a reservoir in vacuum state. The width of Lorentzian spectral density is $\lambda = 20\gamma$. The short time evolution behaviour is also shown.

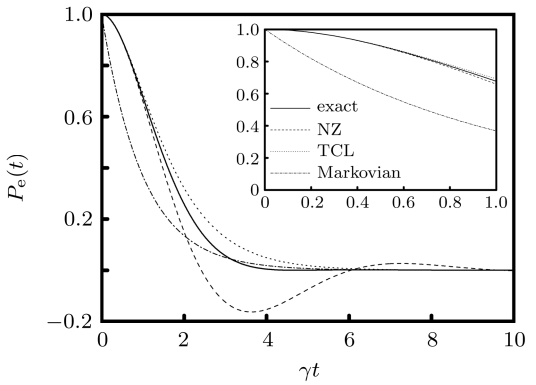


Fig. 2. Time evolution of the population of excitation state $|1\rangle$ for a composite system initially prepared in the product of excitation state $|1\rangle$ and vacuum state $|0\rangle$. The width of Lorentzian spectral density is $\lambda = \gamma$. The dynamics of a qubit in short time is presented in the inset.

In the end, the same quantity is presented in Fig. 3 when we choose $\lambda = 0.01\gamma$, which corresponds to strong reservoir correlation and long memory time. We can clearly observe a good agreement between the two non-Markovian approaches in short time and the Markovian approach still cannot coincide with the exact solution. From Fig. 3, the result of the NZ master equation can show the oscillation behaviour which is called Rabi oscillation, as shown by the exact solution. Because of the interaction between a qubit and its reservoir, the oscillation eventually decays to zero in the end due to the cavity loss. The solution of the TCL master equation decays exponentially and finally arrives at zero.

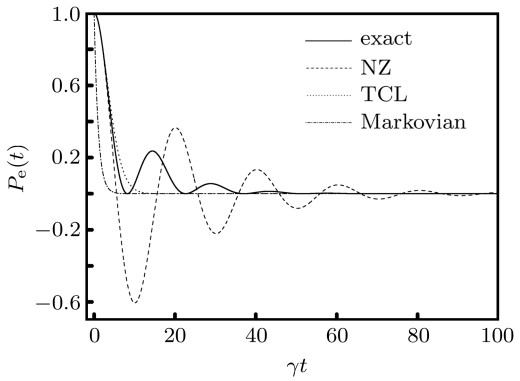


Fig. 3. Time evolution of the population of excitation state $|1\rangle$ for a composite system initially prepared in the product of excitation state and vacuum state $|0\rangle$. The width of Lorentzian spectral density is $\lambda = 0.01\gamma$.

5. Discussion and conclusion

We pay attention to two prevalent methods for the non-Markovian dynamics of an open quantum system. Exploiting an exact solution of the dynamics of a qubit coupling to a reservoir, we have shown that the TCL approach can produce most properties of non-Markovian dynamics for a range of parameters much wider than that which the NZ master equation gives. In the strong reservoir correlation regime, the solution of NZ can reflect the oscillator behaviour. Therefore, the NZ and the TCL approaches are better methods for treating the non-Markovian dynamics in short correlation time, while the NZ and the TCL approaches are often applied in large correlation time. We also investigate the Markovian dynamics, which violates the fact completely in large correction time. Therefore, the non-Markovian dynamics can show the virtual process. From the above discussions, we can find that our exact solution may be better than the methods mentioned in the former reference papers either in large time scale or in small time scale.

Finally we note that the model is very simple, but it can indeed point out the non-Markovian solutions which agree with the exact solution. They can solve two coupled or uncoupled qubits independently coupling to a reservoir. The projection operator techniques may also study entanglement and quantum discord dynamics of two qubits independently interacting with two coupling reservoir, this will be the subject of our future research.

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