Non-Markovian quantum jump with generalized Lindblad master equation

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The Monte Carlo wave function method or the quantum-trajectory–jump approach is a powerful tool to study dissipative dynamics governed by the Markovian master equation, in particular for high-dimensional systems and when it is difficult to simulate directly. We extend this method to the non-Markovian case described by the generalized Lindblad master equation. Two examples to illustrate the method are presented and discussed. The results show that the method can correctly reproduce the dissipative dynamics for the system. The difference between this method and the traditional Markovian jump approach and the computational efficiency of this method is also discussed.

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I. INTRODUCTION

Since the pioneering work of Albert Einstein, who explained the phenomenon of dissipation and Brownian motion in his *annus mirabilis* of 1905 by use of statistical methods, a rich variety of methods to tackle quantum fluctuations and quantum dissipation in open systems has been proposed [1,2]. Among them, the quantum master equation (QME) approach and the quantum Langevin description (QLE) [3] are two powerful functional integral techniques for the study of the time evolution of open quantum systems. The quantum master equation can be divided into two categories: Markovian and non-Markovian. The Markovian master equation [4] (especially in the Lindbald form) can be derived with the weak-coupling limit (or the Born approximation) and the Markovian approximation. It can be solved analytically [5] for some special cases, but for most cases we have to solve and simulate it numerically by the Monte Carlo wave function method or quantum-trajectory–jump approach [6–11]. This method is very effective for qubit systems even with a large number of qubits—say, $n=24$ [9].

However, the dynamics of an open system is not always Markovian. Strong system-environment couplings, correlation and entanglement in the initial state, and structured reservoirs may lead the dynamics far from Markovian. Many methods have been proposed to describe the non-Markovian process, including the Lindblad equation with time-dependent decay rates [12], generalized Lindblad equation [13] obtained from the correlated projection superoperator techniques [14,15], phenomenological memory kernel master equation [16,17], and the post-Markovian master equation [18–20]. The first two methods are local in time, while the last two involve an integral of time. For the first method, the only difference from the Markovian master equation is that the decay rates in the equation are time dependent. These decay rates may take not only positive values, but also negative ones. When decay rates are positive, the Markovian Monte Carlo wave function method can directly be used. However, the method is not available when the decay rates are negative. This problem was solved in Ref. [21] by introducing reversed jumps.

The generalized Lindblad master equation can well describe the dynamics of an open system beyond the Markovian limit; especially, it is very effective for an environment composed of spins [22–24] and structured reservoirs [25]. However, the extension of the Monte Carlo simulation to this equation remains untouched. In this paper, we will explore the unraveling and quantum trajectory approach for the generalized Lindblad equation. The structure of this paper is organized as follows. In Sec. II we briefly review the generalized Lindblad equation. In Sec. III we give the unraveling of this equation and generalize the Monte Carlo method to this equation. Two examples are presented in Sec. IV. Finally, we conclude our results in Sec. V.

II. GENERALIZED LINDBLAD MASTER EQUATION

The equation that governs the dynamics of an open quantum system can be derived by means of the projection superoperator technique [12,14]. The form (Markovian or non-Markovian) of the master equation crucially depends on the approximation used in the derivation, reflected in the projection superoperator chosen. When we project the total system state onto a tensor product, we can obtain the Markovian master equation, whereas a non-Markovian master equation can be obtained when we use a correlated projection. The following is the master equation derived by this method, and it is called the generalized Lindblad master equation [13]:

$$\frac{d}{dt}\rho_m = -i[H_m,\rho_m] + \sum_{n\lambda}\left(R^{\lambda}_{mn}\rho_n R^{\lambda\dagger}_{mn} - \frac{1}{2}\{R^{\lambda\dagger}_{nm}R^{\lambda}_{nm},\rho_m\}\right), \tag{1}$$

where H_m are Hermitian operators and R^{λ}_{mn} are arbitrary system operators depending on the form of system-environment interactions. If we have only a single component $\rho_S=\rho_1$, this equation obviously reduces to the ordinary Markovian master equation. In this paper we will focus on the case where we have at least two components. The state of the reduced system in this case is $\rho_S=\Sigma_m\rho_m$; we recall that Tr $\rho_m<1$.

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III. QUANTUM JUMP

For clarity, we define the jump operators $W^{\lambda}_{mn}=R^{\lambda}_{mn}$ and nonjump operators $W^{0}_{mm}=1-i\mathcal{H}_m dt$, where the non-Hermitian effective Hamiltonian is given by $\mathcal{H}_m=H_m-\frac{1}{2}i\Sigma_{n\lambda}R^{\lambda\dagger}_{nm}R^{\lambda}_{nm}$. There are two subscripts and one superscript for the operator W^{λ}_{mn}. The first subscript m denotes the index of the component corresponding to ρ_m, while the second subscript n denotes the index of the component for the operation acted on; the superscript λ represents the jump mode. Initially we assume that each operator $\rho_m(t_0)$ can be written as $\rho_m(t_0)=|\psi_m(t_0)\rangle\langle\psi_m(t_0)|$, where $|\psi_m(t_0)\rangle$ is a non-normalized wave function. After an infinitesimal time dt, it evolves into the state

$$\rho_m(t_0+dt)=\sum_{n\lambda}|\psi^{\lambda}_{mn}\rangle\langle\psi^{\lambda}_{mn}|dp^{\lambda}_{mn}+|\psi^{0}_{mm}\rangle\langle\psi^{0}_{mm}|dp^{0}_{mm}, \quad (2)$$

where the new states are defined by

$$|\psi^{\lambda}_{mn}\rangle=\frac{\sqrt{p_m}W^{\lambda}_{mn}|\psi_n(t)\rangle}{\|W^{\lambda}_{mn}|\psi_n(t)\rangle\|} \quad (3)$$

and

$$|\psi^{0}_{mm}\rangle=\frac{\sqrt{p_m}W^{0}_{mm}|\psi_m(t)\rangle}{\|W^{0}_{mm}|\psi_m(t)\rangle\|}, \quad (4)$$

with probabilities

$$dp^{\lambda}_{mn}=\frac{1}{p_m}\langle\psi_n(t_0)|W^{\lambda\dagger}_{mn}W^{\lambda}_{mn}|\psi_n(t_0)\rangle dt,$$

$$dp^{0}_{mm}=\frac{1}{p_m}\langle\psi_m(t_0)|W^{0\dagger}_{mm}W^{0}_{mm}|\psi_m(t_0)\rangle, \quad (5)$$

respectively. In Eqs. (3) and (4),

$$p_m=\sum_{n\lambda}\langle\psi_n(t_0)|W^{\lambda\dagger}_{mn}W^{\lambda}_{mn}|\psi_n(t_0)\rangle dt+\langle\psi_m(t_0)|W^{0\dagger}_{mm}W^{0}_{mm}|\psi_m(t_0)\rangle \quad (6)$$

is the weight for the component ρ_m that satisfies

$$p_m=\mathrm{Tr}\rho_m(t+dt). \quad (7)$$

Note that the jumps for ρ_m depend on the other components ρ_n $(n\neq m)$ of the reduced density matrix ρ. This makes our method different from the traditional quantum jump method.

We can prove this unraveling by putting the jump and nonjump states (3) and (4) and the probabilities (5) and (6) into Eq. (2),

$$\rho_m(t+dt)=\sum_{n\lambda}W^{\lambda}_{mn}|\psi_n(t)\rangle\langle\psi_n(t)|W^{\lambda\dagger}_{mn}dt+W^{0}_{mm}|\psi_m(t)\rangle\times\langle\psi_m(t)|W^{0\dagger}_{mm}. \quad (8)$$

Simple algebra shows that in the limit $dt\to 0$, Eq. (8) reveals Eq. (1). The evolution governed by Eq. (1) can be simulated numerically by the so-called Monte Carlo wave function approach according to the unraveling given above. We start the time evolution from the state $\rho(t_0)=\Sigma_m\rho_m(t_0)=\Sigma_m|\psi_m(t_0)\rangle\langle\psi_m(t_0)|$, where ρ_m $(m=1,2,3,\ldots)$ are the components for ρ. At time t_0+dt, where dt is much smaller than the time scale relevant for the evolution of the density matrix, a random number ϵ, which is randomly distributed in the unit interval $[0, 1]$, is used to determine the jump. Note that all the components are controlled by this random number. For each component $|\psi_m\rangle$, if $0\leqslant\epsilon\leqslant dp^{1}_{m1}$, it jumps to $|\psi^{1}_{m1}\rangle$, if $dp^{1}_{m1}<\epsilon\leqslant dp^{1}_{m1}+dp^{2}_{m1}$, it jumps to $|\psi^{2}_{m1}\rangle$, and so on. These jumps are all operated on the component ρ_1; if $\Sigma_\lambda dp^{\lambda}_{m1}<\epsilon\leqslant\Sigma_\lambda dp^{\lambda}_{m1}+dp^{1}_{m2}$, it jumps to the component 2—namely, $|\psi^{1}_{m2}\rangle$. Jumps to the other components can be established in a similar way. If $\epsilon>\Sigma_{n\lambda}dp^{\lambda}_{mn}$, a nonjump takes place and the state ends up in $|\psi^{0}_{mm}\rangle$. This operation is acted on the component ρ_m itself. We define a generalized jump superoperator $\mathcal{W}_i$, which denotes all jumps for all the components controlled by this random number. We repeat this process as many times as $n=\Delta t/dt$ for all components, where Δt is the total evolution time. We call this single evolution a generalized quantum trajectory. This trajectory contains all the components of the density matrix. Given an operator A, we can write its mean value $\langle A\rangle(t)=\mathrm{Tr}[A\rho(t)]$ as an average over $\mathcal{N}$ trajectories as

$$\langle A\rangle(t)=\lim_{N\to\infty}\sum_{j=1}^{\mathcal{N}}\sum_{m}\langle\psi_{m,j}(t)|A|\psi_{m,j}(t)\rangle. \quad (9)$$

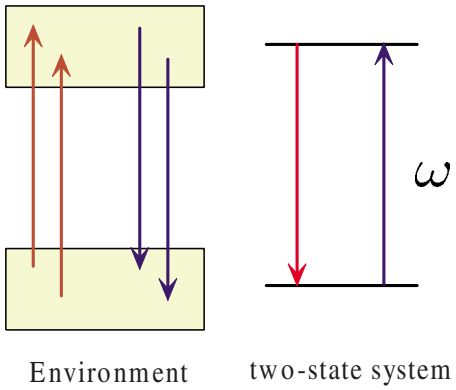

FIG. 1. (Color online) A two-state system coupled to an environment consisting of two energy bands with a finite number of levels.

IV. APPLICATION

In this section, we use the model and the generalized master equation given in Refs. [23,25] as two examples to illustrate our method. First consider a two-state system coupled to an environment. The environment consists of a large number of energy levels which are arranged into two energy bands with the same energy spacing (see Fig. 1). The lower-energy band contains N_1 levels, while the upper one N_2 levels. This model can be understood as a "many-level" environment or "container," of which only the relevant parts of the spectrum enter the model. For details of this model, we refer the reader to [26,27]. The total Hamiltonian for a qubit coupled to such an environment in the Schrödinger picture is $H=H_0+V$ [25] with (we set $\hbar=1$)

$$H_0 = \frac{1}{2}\omega\sigma_z + \sum_{n_1}\frac{\delta\epsilon}{N_1}n_1|n_1\rangle\langle n_1| + \sum_{n_2}\left(\omega + \frac{\delta\epsilon}{N_2}n_2\right)|n_2\rangle\langle n_2|,$$

$$V = \lambda\sum_{n_1 n_2} c(n_1,n_2)\sigma^+|n_1\rangle\langle n_2| + \text{H.c.},$$

where the index n_1 denotes the levels of the lower-energy band and n_2 denotes the levels of the upper band, and σ_z and $\sigma^\pm$ are Pauli operators. λ is the overall strength of the interaction, and $c(n_1,n_2)$ are coupling constants; they are independent of each other and are identically distributed, satisfying

$$\langle c(n_1,n_2)\rangle = 0,$$

$$\langle c(n_1,n_2)c(n_1',n_2')\rangle = 0,$$

$$\langle c(n_1,n_2)c^*(n_1',n_2')\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}.$$

According to H_0, one can transform the problem into the interaction picture and, with the help of the projection superoperator technique, obtain the non-Markovian evolution equation as

$$\frac{d}{dt}\rho_S^{(1)}(t) = \gamma_1\sigma^+\rho_S^{(2)}(t)\sigma^- - \frac{\gamma_2}{2}\{\sigma^+\sigma^-,\rho_S^{(1)}(t)\},$$

$$\frac{d}{dt}\rho_S^{(2)}(t) = \gamma_2\sigma^-\rho_S^{(1)}(t)\sigma^+ - \frac{\gamma_1}{2}\{\sigma^-\sigma^+,\rho_S^{(2)}(t)\}, \qquad (10)$$

where

$$\gamma_i = \frac{2\pi\lambda^2 N_i}{\delta\epsilon} \quad (i=1,2).$$

With the definitions of $\Pi_1=\Sigma_{n_1}|n_1\rangle\langle n_1|$ and $\Pi_2=\Sigma_{n_2}|n_2\rangle\langle n_2|$, $\Pi_1+\Pi_2=\mathbb{1}_E$, the two non-normalized density matrices can be obtained by $\rho_S^{(i)}=\mathrm{Tr}_E(\Pi_i\rho_T)$, $i=1,2$, where ρ_T is the total density matrix for the system and environment. The reduced density matrix for the system is then given by $\rho=\rho_S^{(1)}+\rho_S^{(2)}$. We note that in Eq. (10), there are no environment operators other than the two (c-number) parameters γ_1 and γ_2. The initial state of the environment is taken into account by means of the distribution of the initial $\rho_S^{(1)}$ and $\rho_S^{(2)}$; its effect on the system dynamics is plotted in Figs. 2 and 3. This equation can be written in the form of Eq. (1) by setting $H_i=0$, $R_{11}=R_{22}=0$, $R_{12}=\sqrt{\gamma_1}\sigma^+$, and $R_{21}=\sqrt{\gamma_2}\sigma^-$. In this model, there is only one jump operator for each component, i.e., $W_{12}^1=\sqrt{\gamma_1}\sigma^+$ and $W_{21}^1=\sqrt{\gamma_2}\sigma^-$, and nonjump operators $W_{mm}^0=\mathbb{1}-i\mathcal{H}_m dt$, with $\mathcal{H}_1=-\frac{1}{2}\gamma_2\sigma^+\sigma^-$ and $\mathcal{H}_2=-\frac{1}{2}\gamma_1\sigma^-\sigma^+$.

We consider two types of initial condition in the following simulation. First, only the lower band of the environment is populated—i.e., $\rho_S^{(2)}=0$. Under this condition, the reduced system can be solved analytically. Another case is where the two bands of the environment are all populated. With this initial condition, we solve the master equation numerically. In both cases, we choose initial states $|\phi(0)\rangle=|e\rangle$ and $|\phi(0)\rangle=\frac{1}{2}(|e\rangle+|g\rangle)$ for the system, where $|e\rangle$ and $|g\rangle$ denote the excited state and ground state, respectively. We compare the analytic solution and the numerical simulation (solve the equation by the Runge-Kutta method) to the results obtained from the quantum-jump–trajectory approach in Figs. 2 and 3. The trajectory number in this quantum jump approach is $\mathcal{N}=400$. We can see from the figures that the quantum trajectory approach correctly reproduces the system evolution. The errors are sufficiently small, although we choose a small number of trajectories, showing that this method is efficient.

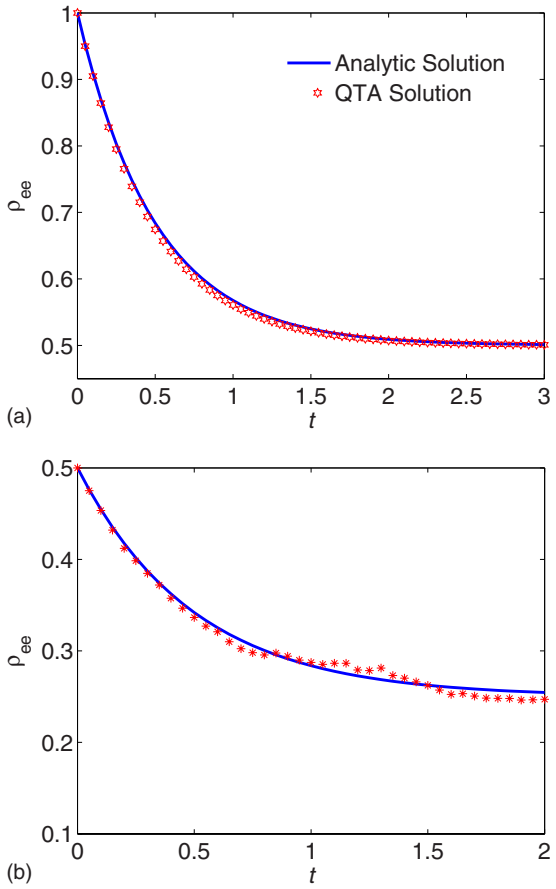

FIG. 2. (Color online) Comparisons of the analytic solution to Eq. (10) to the results given by the quantum trajectory approach. The initial state of the system is chosen as $|\phi(0)\rangle=|e\rangle$ in the top figure, while $|\phi(0)\rangle=\frac{1}{\sqrt{2}}(|e\rangle+|g\rangle)$ in the bottom one. Initially only the lower band of the environment is populated. The other parameters chosen are $\gamma_1=\gamma_2=1$. The time t is plotted in units of $1/\hbar$.

Another example is a qubit coupled to a spin bath [23]. The full system consists of a central spin interacting with a bath of N spins. Such a system can be described by

$$H = \frac{\omega}{2}\sigma_z + \sum_{k=1}^{N}\alpha_k\vec{\sigma}\cdot\vec{\sigma}_k, \qquad (11)$$

where $\vec{\sigma}$ denotes the Pauli matrix for the central spin, which is the system we are interested in, and $\vec{\sigma}_k$ stands for the kth spin in the bath. After defining an unperturbed part $H_0=\frac{\omega}{2}\sigma_z+2\sigma_z K_z$, where $K_z=\frac{1}{2}\Sigma_{k=1}^N\alpha_k\sigma_z^k$, the Hamiltonian can be transformed into the interaction picture. Assuming the parameters are real and time independent, the master equation reads

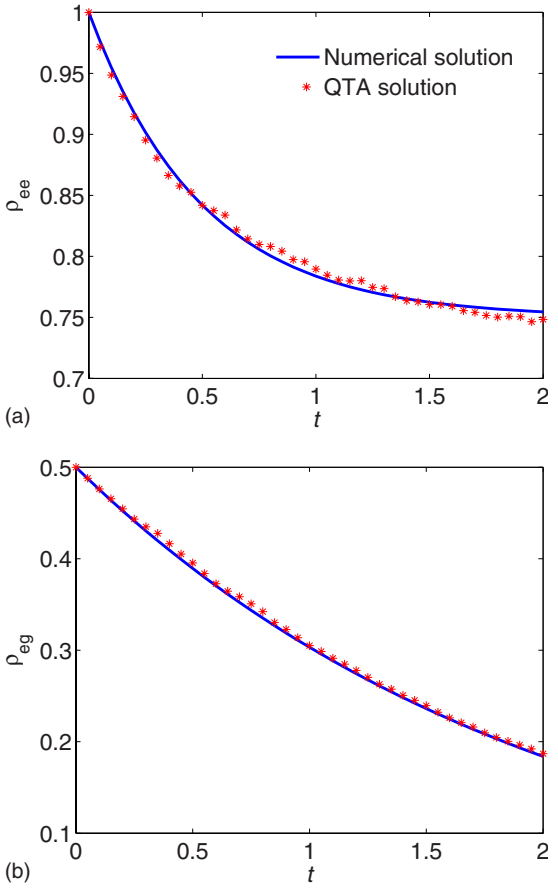

FIG. 3. (Color online) Comparisons of the numerical solution to Eq. (10) to the results given by the quantum trajectory approach. The initial state of the system is chosen as $|\phi(0)\rangle=|e\rangle$ in the top figure, while $|\phi(0)\rangle=\frac{1}{\sqrt{2}}(|e\rangle+|g\rangle)$ in the bottom one. Initially the two bands of the environment are populated. The two parameters are $\gamma_1=\gamma_2=1$. The time t is plotted in units of $1/\hbar$. Note that in the bottom figure we plot the off-diagonal element ρ_{eg} of the reduced system.

$$\frac{d}{dt}\rho_m = g_{m+1}\sigma^+\rho_{m+1}\sigma^- + f_{m-1}\sigma^-\rho_{m-1}\sigma^+ - \frac{1}{2}f_m\{\sigma^+\sigma^-,\rho_m\} - \frac{1}{2}g_m\{\sigma^-\sigma^+,\rho_m\}, \tag{12}$$

where $\rho_m=\mathrm{Tr}_B(\rho_T\Pi_m)$, ρ_T is the density matrix for the total system (the central spin plus the bath), and Π_m is a projection superoperator that projects the z component of the bath angular momentum into an eigenvector with eigenvalue m. We take $N=2$ as an example; then, the density matrix of the central spin has three components, denoted by ρ_1, ρ_0, and ρ_{-1}, respectively. Each component has two jump operators, which act on the other two components, and a nonjump operator, which acts on itself. The comparison between direct numerical simulations (by the Runge-Kutta method) and the quantum trajectory method is shown in Fig. 4. Here the trajectory number is chosen to be $\mathcal{N}=4000$. We can find that as the number of jump operators and components increases, the number of quantum trajectories with which we can obtain a correct result increases.

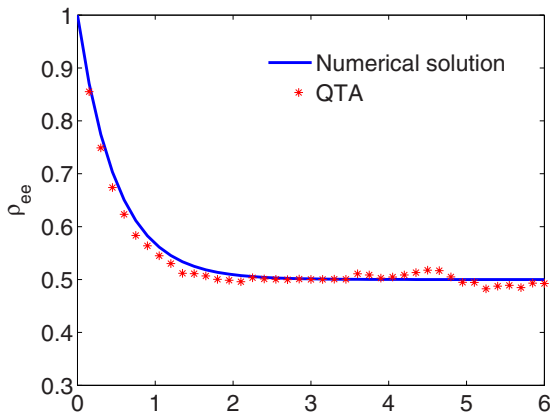

FIG. 4. (Color online) Comparisons of the numerical solution to Eq. (12) to the results given by the quantum trajectory approach. The initial state of the system is chosen as $\rho_1=\rho_0=\rho_{-1}=\frac{1}{3}|e\rangle\langle e|$. All parameters in the equation are set to be equal. The time t is plotted in units of $1/\hbar$.

V. CONCLUSION AND DISCUSSION

In this paper, we have developed an efficient unraveling for the generalized Lindblad master equation. Based on this unraveling, a generalized Monte Carlo wave function method is presented. It is worth addressing the fact that in this Monte Carlo wave function method, we need only to store M non-normalized wave functions—i.e., M length-N vectors (M denotes the number of the components for the reduced density matrix and N stands for the dimension of the Hilbert space) instead of the density operator, which are M $N\times N$ matrices—hence this method saves the computer time and space. The difference between the ordinary quantum jump method and the present one is that the latter describes a non-Markovian dynamics. In addition, the point that each component ρ_i of the density matrix is non-normalized and jumps along the component ρ_i depends on a component other than ρ_i, which is also different. By successfully simulating the coupling among those components, this method can simulate the non-Markovian dynamics efficiently. Further examination shows that the computational complexity increases with the number of the components. The increased complexity due to the increase of the components and jump operators can by analyzed as follows. Assume the jump operators and the number of jump operators are restricted to be the same for each component; the possible jump mode for $\varrho=(\rho_1,\rho_2,\ldots)$ or the number of generalized jump superoperators $\mathcal{W}$ is

$$\Delta = M(J-1)+1. \tag{13}$$

Here J is the number of jump operators for each component (including the nonjump operator). The role that Δ plays is similar to the number of jump operators in the ordinary Markovian master equation. It is well known that one downside of the quantum jump approach is the complexity growth as the jump operators proliferate. From Eq. (13), we can find

that this downside still exists in the presented method. Still, our method is effective when one simulates the decoherence governed by the non-Markovian master equation, as well as for a system with Hilbert space of high dimension.

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