

Non-Markovian quantum-state diffusion: Perturbation approach

Ting Yu,¹ Lajos Diósi,^{2,3} Nicolas Gisin,¹ and Walter T. Strunz⁴

¹*Group of Applied Physics, University of Geneva, 1211 Geneva 4, Switzerland*

²*Research Institute for Particle and Nuclear Physics, 1525 Budapest 114, P.O.B. 49, Hungary*

³*Institute for Advanced Study, Wallotstrasse 19, D-14193 Berlin, Germany*

⁴*Fachbereich Physik, Universität GH Essen, 45117 Essen, Germany*

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We present a perturbation theory for non-Markovian quantum-state diffusion (QSD), the theory of diffusive quantum trajectories for open systems in a bosonic environment [Phys. Rev. A **58**, 1699 (1998)]. We establish a systematic expansion in the ratio between the environmental correlation time and the typical system time scale. The leading order recovers the Markov theory, so here we concentrate on the next-order correction corresponding to first-order non-Markovian master equations. These perturbative equations greatly simplify the general non-Markovian QSD approach, and allow for efficient numerical simulations beyond the Markov approximation. Furthermore, we show that each perturbative scheme for QSD naturally gives rise to a perturbative scheme for the master equation which we study in some detail. Analytical and numerical examples are presented, including the quantum Brownian motion model. [S1050-2947(99)03307-7]

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I. INTRODUCTION

Recently, a non-Markovian quantum trajectory theory—named non-Markovian quantum-state diffusion (QSD)—that describes the dynamics of a quantum “system” coupled to an “environment” of harmonic oscillators has been presented [1]. Many outstanding new experimental advances can be properly studied only if non-Markovian effects are taken into account. These include experiments with high- Q microwave cavities, quantum optics in materials with a photonic band gap, or output coupling from a Bose-Einstein condensate to create an atom laser [2–6], to name a few. Also, the important phenomenon of decoherence, which takes place on time scales that can be of the same order as the correlation time of the environment, requires theories beyond the standard Markov approximation. Further motivation are more fundamental questions about the proper description of individual open systems in quantum mechanics. Indeed, the infamous problem of the “Heisenberg cut” (understood here as the cut between the system and the environment) is intimately related to the non-Markovian evolution of the system when the environment is ignored.

In the Markov regime, quantum trajectory approaches using stochastic Schrödinger equations for pure states of the system play an important role in quantum optics, particularly for numerical simulations [7–13]. These Markov models also have many appealing features from a theoretical and conceptual point of view [8–10,14–16]. It is therefore desirable to generalize the powerful quantum trajectory approach from the Markov regime to the more general case of non-Markovian evolution. Several attempts have been made recently from different perspectives. The linear non-Markovian unraveling underlying our theory was developed in [18–20]—see also [17] for a related attempt. Alternatively, a non-Markovian theory based on pseudomodes and a non-Markovian jump approach have been developed recently [21–25].

In Ref. [1], the ultimate nonlinear non-Markovian QSD

equation relevant to this paper has been derived directly from a microscopic model. In this framework, the reduced density matrix of the subsystem obtained by tracing over the environmental degrees of freedom is unraveled into an ensemble of continuous trajectories which correspond to the various realizations of the driving complex Gaussian process. Non-Markovian QSD has been applied to interesting and physically relevant models where both computational power and many new features have been demonstrated [1]. However, many issues are still to be addressed. In particular, further applications of non-Markovian QSD to a variety of realistic problems are desirable. In addition, the theoretical implications of this new approach remain to be explored. Clearly, a full exploration of non-Markovian QSD is an extensive project. The purpose of the present paper is a step towards this extensive project.

So far, although being a general theory, it is difficult to implement non-Markovian QSD directly on a computer in all generality. It has been applied to a variety of model problems in [1]. However, in this paper we show how the non-Markovian QSD approach allows us to find a systematic expansion of the reduced system dynamics in powers of the ratio between the environmental correlation time and typical system time scales. Thus, in order for non-Markovian QSD to have more applications, we establish a useful and practically relevant perturbative approach that is directly amenable to computer simulations. Our first and most important motivation for this paper is to present a systematic perturbative approach for non-Markovian QSD around the Markov limit. This perturbative “post-Markovian” QSD scheme is a time-dependent approach which preserves the non-Markovian nature of the problem in each order of approximation.

The second purpose of the present paper is to establish the relationship between the non-Markovian QSD equation and non-Markovian master equations. Such a relation is well-known in the Markov regime, where one generally starts from the standard Lindblad Markov master equation to read off the Markov QSD equation [9,10]. For non-Markovian

dynamics, closed master equations are rare and, thus, the direct link between non-Markovian QSD and the corresponding master equation is of great interest. In order to obtain the master equation from its non-Markovian QSD counterpart, one has to take the ensemble mean over the stochastic process driving the QSD trajectories analytically (see also Ref. [1]). In general, this is only possible for simple models. In our perturbative scheme, however, we are able to derive master equations directly from non-Markovian QSD which turns out to be useful from both theoretical and practical points of view. It is important to note that a master equation derived in this way will necessarily preserve the positivity because such density matrices can be decomposed into pure states at all times. We thus also address the problem of how to ensure positivity for non-Markovian master equations—a difficult subject in itself.

The third motivation of the paper, therefore, is to present a perturbation approach to non-Markovian master equations. Using an example, we show that the resultant approximate master equation preserves positivity. We also analyze the approximations leading to the Caldeira-Leggett model [26]—which is known to violate positivity for certain initial conditions on short time scales.

The organization of this paper is as follows. In Sec. II we briefly review the basic concepts and equations of non-Markovian QSD. The aim of this section is twofold: first, to act as a brief introduction for readers not familiar with the subject; second, to serve as the natural starting point of our new development. In Sec. III we develop the formal time-dependent perturbation theory for non-Markovian QSD. In Sec. IV, we present a systematic method of deriving the master equation from non-Markovian QSD. We show that a perturbative QSD scheme naturally leads to a perturbative scheme for the master equation. We will apply the approximation schemes developed in this paper to some examples in Sec. V. In Sec. VI we take quantum Brownian motion as a typical model to illustrate the perturbative schemes based on QSD for the master equation. We conclude the paper in Sec. VII, while some useful material can be found in the Appendixes.

II. NON-MARKOVIAN QUANTUM-STATE DIFFUSION

Both Markov and non-Markovian QSD are based on two related stochastic dynamical equations, a linear one and a nonlinear one. The linear one is mathematically simpler. However, it does not preserve the norm of the state vector, which in general tends to zero. Hence, only the nonlinear equation, which preserves the norm, can be interpreted as a distribution of time-dependent pure states with given probabilities (i.e., as an unraveling): the density matrix is then given by the ensemble mean of the pure states, at all times. Moreover, only this nonlinear equation is suitable for numerical simulation [1,20]. Nevertheless, we start our presentation with the simpler linear equation, leaving the nonlinear one for the following subsection.

A. Linear non-Markovian quantum-state diffusion

Our quantum trajectory theory is based on a standard model of open system dynamics: a quantum system interacting with a bosonic environment with total Hamiltonian

$$H_{\text{tot}} = H + \sum_{\lambda} g_{\lambda} (L a_{\lambda}^{\dagger} + L^{\dagger} a_{\lambda}) + \sum_{\lambda} \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}, \quad (2.1)$$

where H is the Hamiltonian of the system of interest and L , a system operator coupling to environment, is called here the Lindblad operator (as it plays the role of a ‘‘Lindblad operator’’ in the Markov limit). The linear non-Markovian QSD equation [18–20] unravelling the reduced dynamics of model (2.1) takes the form¹

$$\frac{d}{dt} \psi_t = -iH \psi_t + L z_t \psi_t - L^{\dagger} \int_0^t \alpha(t,s) \frac{\delta \psi_t}{\delta z_s} ds, \quad (2.2)$$

where z_t is a colored complex Gaussian process with zero mean and correlations

$$M[z_t^* z_s] = \alpha(t,s), \quad M[z_t z_s] = 0. \quad (2.3)$$

The bath correlation function $\alpha(t,s)$ in Eq. (2.2) has to be a positive Hermitian kernel: $\alpha(t,s) = \alpha(s,t)^*$. This non-Markovian unraveling is ensured to be consistent with the reduced density operator approach since the ensemble mean of the solutions of Eq. (2.2) over the noise z_t will reproduce the density matrix of the system,

$$\begin{aligned} \rho_t &\equiv \text{Tr}_{\text{env}}(e^{-iH_{\text{tot}}t} |\psi_0\rangle \langle \psi_0| \otimes \rho_0^{\text{env}} e^{iH_{\text{tot}}t}) \\ &= M[|\psi_t(z)\rangle \langle \psi_t(z)|]. \end{aligned} \quad (2.4)$$

Here $M[\]$ denotes the *ensemble average* over the classical driving noise z_t .

From Eq. (2.2), we see clearly that the evolution of the state ψ_t at t depends on the whole history of the noise z . Equation (2.2) can be written in the more appealing form

$$\frac{d}{dt} \psi_t = -iH \psi_t + L z_t \psi_t - L^{\dagger} \int_0^t \alpha(t,s) \hat{O}(t,s,z) ds \psi_t, \quad (2.5)$$

by defining an operator² $\hat{O}(t,s,z)$ in Eq. (2.5) such that

$$\hat{O}(t,s,z) \psi_t \equiv \frac{\delta \psi_t}{\delta z_s}. \quad (2.6)$$

It turns out that $\hat{O}(s,s,z) = L$. The t dependence of the operator $\hat{O}(t,s,z)$ can be determined by the consistency condition

$$\frac{d}{dt} \frac{\delta}{\delta z_s} \psi_t = \frac{\delta}{\delta z_s} \frac{d}{dt} \psi_t \quad (2.7)$$

together with the linear non-Markovian QSD equation (2.5).

The appeal of Eq. (2.5) [or Eq. (2.2)] is its linearity, which is often useful in the mathematical analysis of our

¹For simplicity, we choose $\hbar = 1$ throughout the paper.

²The notation $\hat{O}(t,s,z)$, rather than $\hat{O}(t,s,z_t)$, reflects that the operator $\hat{O}(t,s,z)$ contains the noise z in a nonlocal way, that is, it might be dependent on the whole histories of the noise $\{z_s : 0 \leq s \leq t\}$.

QSD approach (see Sec. IV). Its use as a simulation tool is severely undermined since, for an infinite heat bath, the norm $\|\psi_t\|$ of the solutions of Eq. (2.2) goes to zero with probability 1 and to infinity with probability zero. For this reason, an unraveling in terms of normalized states is crucial for non-Markovian QSD to be truly useful for numerical simulations.

B. Nonlinear non-Markovian quantum-state diffusion

The non-Markovian QSD unraveling based on normalized states

$$\tilde{\psi}_t(z) = \frac{\psi_t(z)}{\|\psi_t(z)\|} \quad (2.8)$$

has been derived recently [1] from the linear non-Markovian QSD equation (2.5) by making use of a Girsanov transformation of the noise. We get

$$\begin{aligned} \frac{d}{dt}\tilde{\psi}_t &= -iH\tilde{\psi}_t + (L - \langle L \rangle_t)\tilde{\psi}_t\tilde{z}_t \\ &\quad - \int_0^t \alpha(t,s)[(L^\dagger - \langle L^\dagger \rangle_t)\hat{O}(t,s,\tilde{z}) \\ &\quad - \langle (L^\dagger - \langle L^\dagger \rangle_t)\hat{O}(t,s,\tilde{z}) \rangle_t] ds \tilde{\psi}_t, \end{aligned} \quad (2.9)$$

where \tilde{z}_t is the shifted noise,

$$\tilde{z}_t = z_t + \int_0^t \alpha(t,s) * \langle L^\dagger \rangle_s ds, \quad (2.10)$$

and $\langle L \rangle_t \equiv \langle \tilde{\psi}_t | L | \tilde{\psi}_t \rangle$ denotes the *quantum average*. Again here, the *ensemble average* of the solution to Eq. (2.9) recovers the density matrix of the system,

$$\rho_t = M[\tilde{\psi}_t(z)\langle \tilde{\psi}_t(z) |]. \quad (2.11)$$

This nonlinear non-Markovian QSD equation can be rewritten in a more compact form:

$$\begin{aligned} \frac{d}{dt}\tilde{\psi}_t &= -iH\tilde{\psi}_t + \Delta_t(L)\tilde{\psi}_t\tilde{z}_t - \Delta_t(L^\dagger)\bar{O}(t,\tilde{z})\tilde{\psi}_t \\ &\quad + \langle \Delta_t(L^\dagger)\bar{O}(t,\tilde{z}) \rangle_t \tilde{\psi}_t, \end{aligned} \quad (2.12)$$

where $\Delta_t(A) \equiv A - \langle A \rangle_t$ for any operator A and

$$\bar{O}(t,z) = \int_0^t \alpha(t,s)\hat{O}(t,s,z)ds. \quad (2.13)$$

Equation (2.9) [or Eq. (2.12)] is the fundamental equation of non-Markovian QSD,³ and is our starting point for the perturbative approach in Sec. III. Numerical simulations of non-Markovian open system dynamics using this equation can be

found in Ref. [1]. Note that the non-Markovian QSD equation (2.9) reduced to the standard Markov QSD equation [10] for $\alpha(t,s) \rightarrow \delta(t-s)$.

To conclude this section, we would like to make two remarks about the non-Markovian QSD approach. First, the derivation of both the linear and nonlinear non-Markovian QSD equations are based on the assumptions that the environment is bosonic, and that initially the state of the total system+environment is factorable $\rho_0 = \rho_0^S \otimes \rho_0^{env}$, where the initial state of the system $\rho_0^S = |\psi_0\rangle\langle\psi_0|$ is independent of the noise z_t . In fact, if $L \neq L^\dagger$, Eq. (2.9) is valid for a zero temperature environment only and the equation for finite temperature gets two additional terms, see [1]. Second, since Eq. (2.2) and hence Eq. (2.9) are derived directly from the microscopic model, these QSD equations can be read off automatically from the total Hamiltonian (2.1). This suggests that the non-Markovian QSD approach also represents a brand new way to derive the quantum master equation of open quantum systems (see Sec. IV).

III. TIME-DEPENDENT PERTURBATION THEORY

The non-Markovian QSD approach offers a very promising method to handle quantum systems whenever non-Markovian effects are relevant. However, many interesting problems which arise in open quantum systems are such that the operator $\hat{O}(t,s,z)$ appearing in Eq. (2.9) cannot be determined exactly. Moreover, the nonlocal noise contained in the fundamental equation (2.12) might cause difficulties in numerical simulations. In this section, we aim for a formal perturbation scheme for the non-Markovian QSD equation (2.9). Applications of the general perturbative method developed here will be presented in Sec. V.

A. First-order approximation of the operator $\hat{O}(t,s,z)$

We need to know the operator $\hat{O}(t,s,z)$ from Eq. (2.6) in order to solve the non-Markovian QSD equation (2.9) on a computer. Notice that \hat{O} enters Eq. (2.9) under the memory integral $\int_0^t \alpha(t,s)\hat{O}(t,s,\tilde{z})ds$ only. Therefore, if the correlation time of the environment is not too long, only s values in the vicinity of the upper integration range are relevant, and thus we consider the expansion of the operator $\hat{O}(t,s,z)$ in Eq. (2.9) in powers of $(t-s)$,

$$\begin{aligned} \hat{O}(t,s,z) &= \hat{O}(s,s,z) + \left. \frac{\partial \hat{O}(t,s,z)}{\partial t} \right|_{t=s} (t-s) \\ &\quad + \frac{1}{2} \left. \frac{\partial^2 \hat{O}(t,s,z)}{\partial t^2} \right|_{t=s} (t-s)^2 + \dots \end{aligned} \quad (3.1)$$

Substituting Eq. (3.1) into Eq. (2.9) or Eq. (2.12), we get a hierarchy of approximate QSD equations by truncating the above expansion. The validity of the corresponding approximation depends on the environment correlation time τ determined by the correlation function $\alpha(t,s)$. In fact, it turns out that \hat{O} changes on *system* time scales as a function of $(t-s)$ and, thus, the expansion (3.1) corresponds to a systematic expansion of the non-Markovian QSD equation in pow-

³From now on, unless otherwise emphasized, non-Markovian QSD refers to Eq. (2.9) or Eq. (2.12), not to the linear equation (2.2).

ers of the number $\omega\tau$, where ω is a typical ‘‘system’’ frequency and τ the environmental correlation time. For example, the zeroth-order term leads to the standard Markov QSD, when $\tau \rightarrow 0$. The first-order term is the most important correction to the Markov dynamics. Therefore, in what follows we will work out the approximation up to the first order in some detail.

By using the consistency condition (2.7), one can work out the following expressions for the operator $\hat{O}(t,s,z)$ at time point $t=s$, without knowing its explicit form (for details, see Appendix A):

$$\hat{O}(s,s,z) = L, \quad (3.2)$$

$$\left. \frac{\partial \hat{O}(t,s,z)}{\partial t} \right|_{t=s} = -i[H,L] - \int_0^s \alpha(s,u) du [L^\dagger, L]L, \quad (3.3)$$

where H is the Hamiltonian and L is the Lindblad operator, as specified in the preceding section. Now, we are in a position to write out the non-Markovian QSD equation up to the first order. Indeed, the first two terms in the expansion (3.1), substituted, respectively, by Eqs. (3.2) and (3.3), yield $\bar{O}(t)$ in Eq. (2.13) in the following form:

$$\bar{O}(t) = g_0(t)L - g_1(t)i[H,L] - g_2(t)[L^\dagger, L]L, \quad (3.4)$$

where

$$g_0(t) = \int_0^t \alpha(t,s) ds, \quad (3.5)$$

$$g_1(t) = \int_0^t \alpha(t,s)(t-s) ds, \quad (3.6)$$

$$g_2(t) = \int_0^t \int_0^s \alpha(t,s)\alpha(s,u)(t-s) du ds. \quad (3.7)$$

Note that g_0 is of the order 1, yet g_1 and g_2 are of the order of the environmental correlation time τ . Substituting Eq. (3.4) into Eq. (2.12), the first-order non-Markovian nonlinear QSD equation is obtained:

$$\begin{aligned} \frac{d}{dt} \tilde{\psi}_t &= -iH\tilde{\psi}_t + \Delta_t(L)\tilde{\psi}_t \tilde{z}_t \\ &- g_0(t)[\Delta_t(L^\dagger)L - \langle \Delta_t(L^\dagger)L \rangle_t] \tilde{\psi}_t \\ &+ i g_1(t)[\Delta_t(L^\dagger)[H,L] - \langle \Delta_t(L^\dagger)[H,L] \rangle_t] \tilde{\psi}_t \\ &+ g_2(t)[\Delta_t(L^\dagger)[L^\dagger, L]L \\ &- \langle \Delta_t(L^\dagger)[L^\dagger, L]L \rangle_t] \tilde{\psi}_t, \end{aligned} \quad (3.8)$$

where \tilde{z}_t is the shifted noise, $\Delta_t(L) = L - \langle L \rangle_t$, and $\langle L \rangle_t = \langle \tilde{\psi}_t | L | \tilde{\psi}_t \rangle$ is the quantum expectation value.

The Hamiltonian H defines a typical system frequency ω ; the combination $L^\dagger L$ defines a typical system relaxation rate Γ . We thus see that the zeroth-order term in Eq. (3.4) gives rise to a term of the order Γ [second line in Eq. (3.8)], whereas the two first-order terms in Eq. (3.4) lead to correc-

tions which are smaller by a factor $\omega\tau$ or $\Gamma\tau$, respectively [third and fourth lines in Eq. (3.8), where τ is again the environment correlation time. Therefore, we expect Eq. (3.8) to be valid for non-Markovian situations where the environmental correlation time may be finite but no larger than typical system time scales. The Markov case emerges for $\tau \rightarrow 0$, where the first-order correction becomes negligible and only the zeroth-order term remains. Then Eq. (3.8) reduces to the standard Markov QSD equation for $t > 0$.

We also see that non-Markovian properties are encoded in the time-dependent coefficients $g_i(t)$, which change on the very fast environmental correlation time scale τ . The absence of the noise z in the first-order expansion (3.4) is remarkable; the resulting first-order QSD equation (3.8) hence contains only local noise z_t [higher-order expansions contain the noise, consequently Eq. (3.8) will also contain the noise z in a nonlocal way]. Note that the approximate non-Markovian QSD equation (3.8) still preserves the norm of the wave function. Equation (3.8) is the main result of this section. As stated before, applicability of non-Markovian QSD lies in the determination of the operator $\hat{O}(t,s,z)$. As we have already pointed out, the difficulties in handling non-Markovian unravelings are often the nonlocal noise z appearing either in the functional derivative [see Eq. (2.2)] or in the integrand operator $\hat{O}(t,s,z)$ [see Eqs. (2.5) and (2.9)]. We see that the above approximate QSD equation greatly simplifies the non-Markovian QSD equation (2.12).

In addition, Eq. (3.8) is explicitly written in terms of the Hamiltonian of the system H , the Lindblad operator L , and their various commutators. All of these can be obtained automatically once the physical model is specified. The only work left is to calculate the coefficients $g_i(t)$ ($i=0,1,2$) from the environment correlation function $\alpha(t,s)$.

After working out the formal perturbative QSD equation, it is useful to see the concrete form of the coefficients $g_i(t)$. For simplicity, we assume here that the system is driven by Ornstein-Uhlenbeck noise, characterized by the exponential correlation function

$$\alpha(t,s) = \frac{\gamma}{2} e^{-\gamma|t-s|}, \quad (3.9)$$

where $\gamma^{-1} = \tau$ defines the finite environmental memory or correlation time. Note that this corresponds to a Lorentzian spectrum. In the limit $\gamma \rightarrow \infty$, the Ornstein-Uhlenbeck noise reduces to simple complex white noise:

$$\alpha(t,s) = \delta(t-s). \quad (3.10)$$

In the case of the Ornstein-Uhlenbeck process, the coefficients $g_i(t)$ can be easily obtained from Eqs. (3.5)–(3.7):

$$g_0(t) = \frac{1}{2}(1 - e^{-\gamma t}), \quad (3.11)$$

$$g_1(t) = \frac{1}{2\gamma}(1 - e^{-\gamma t} - \gamma t e^{-\gamma t}), \quad (3.12)$$

$$g_2(t) = \frac{1}{4\gamma} \left(1 - e^{-\gamma t} - \gamma t e^{-\gamma t} - \frac{1}{2} \gamma^2 t^2 e^{-\gamma t} \right). \quad (3.13)$$

In the long-time limit $t \gg \tau$, we see that the coefficients of the non-Markovian QSD (3.8) become constant: $g_0 = 1/2, g_1 = 1/2\gamma, g_2 = 1/4\gamma$, which also confirms that g_0 is of the order 1 whereas g_1 and g_2 are of the order of the environmental correlation time $\tau = \gamma^{-1}$.

In the Markov limit $\gamma \rightarrow \infty$, $g_0(t) \rightarrow 1/2$ and $g_1(t), g_2(t) \rightarrow 0$ for $t > 0$ and the non-Markovian QSD equation (3.8) reduces to the standard Markov QSD equation [10] (note here we write it in the Stratonovich form [27,28]):

$$\frac{d}{dt}\tilde{\psi}_t = -iH\tilde{\psi}_t + \Delta_t(L)\tilde{\psi}_t \circ (z_t + \langle L^\dagger \rangle_t) - \frac{1}{2}\Delta_t(L^\dagger L)\tilde{\psi}_t \quad (3.14)$$

with z_t the standard complex white noise, as expected.

Our formal perturbation approach can be carried out to any desired order of approximation. (For the details of the second-order expansion and the coefficients, see Appendix B.) It is important to note, however, that the higher-order derivatives of $\hat{O}(t,s,z)$ at $t=s$ may contain the noise z .

Since the linear non-Markovian QSD equation (2.2) is often simpler to use in deriving the corresponding master equation (see Sec. IV), we also give its first-order approximation:

$$\begin{aligned} \dot{\psi}_t = & -iH\psi_t + L\psi_t z_t - g_0(t)L^\dagger L\psi_t + ig_1(t)L^\dagger[H,L]\psi_t \\ & + g_2(t)L^\dagger[L^\dagger,L]L\psi_t, \end{aligned} \quad (3.15)$$

where the coefficients $g_0(t), g_1(t), g_2(t)$ are given by Eqs. (3.5), (3.6), and (3.7).

B. Functional expansion of $\hat{O}(t,s,z)$

In this subsection, we consider another kind of perturbative expansion, the functional expansion of the operator $\hat{O}(t,s,z)$ in terms of noise z_v :

$$\begin{aligned} \hat{O}(t,s,z) = & \hat{O}_0(t,s) + \int_0^t \hat{O}_1(t,s,v)z_v dv \\ & + \int_0^t \int_0^t \hat{O}_2(t,s,v_1,v_2)z_{v_1}z_{v_2} dv_1 dv_2 + \dots \\ & + \int_0^t \dots \int_0^t \hat{O}_n(t,s,v_1, \dots, v_n) \\ & \times z_{v_1} \dots z_{v_n} dv_1 \dots dv_n + \dots, \end{aligned} \quad (3.16)$$

where the operators $\hat{O}_n(t,s,v_1, \dots, v_n)$ are independent of the noise z and are symmetric in their n last variables [e.g., $\hat{O}_2(t,s,v_1,v_2) = \hat{O}_2(t,s,v_2,v_1)$]. The initial condition is $\hat{O}(t,t,z) = L$. The expansion (3.16) takes into account the generally nonlocal dependence of the operator $\hat{O}(t,s,z)$ on the noise z .

From the consistency condition (2.7) and the QSD equation (2.2), we get a hierarchy of equations for the operators $\hat{O}_n(t,s,v_1, \dots, v_n)$ (see Appendix A). Of particular interest is the zeroth-order term $\hat{O}_0(t,s)$, which satisfies the following equation (ignoring the first-order term):

$$\frac{\partial}{\partial t}\hat{O}_0(t,s) = [-iH, \hat{O}_0(t,s)] - [L^\dagger \bar{O}_0(t), \hat{O}_0(t,s)]. \quad (3.17)$$

For the approximation $\hat{O}(t,s,z) \approx \hat{O}_0(t,s)$, the approximate non-Markovian QSD equation then takes form:

$$\begin{aligned} \frac{d}{dt}\tilde{\psi}_t = & -iH\tilde{\psi}_t + \Delta_t(L)\tilde{\psi}_t z_t - \Delta_t(L^\dagger)\bar{O}_0(t)\tilde{\psi}_t \\ & + \langle \Delta_t(L^\dagger)\bar{O}_0(t) \rangle_t \tilde{\psi}_t. \end{aligned} \quad (3.18)$$

The justification of this approximation is that whenever the open quantum system deviates slightly from the Markov dynamics, then the first term $\hat{O}_0(t,s)$ of the expansion (3.16) plays the dominant role. This can be easily seen from the fact that all $\bar{O}_n(t,v_1, \dots, v_n) \equiv \int_0^t \alpha(t,s)\hat{O}_n(t,s,v_1, \dots, v_n)ds, n \geq 1$ go to zero in the Markov limit: $\alpha(t,s) \rightarrow \delta(t-s)$, except the first term $\bar{O}_0(t) \equiv \int_0^t \alpha(t,s)\hat{O}_0(t,s)ds$, which goes to $\frac{1}{2}L$. Physically this can be understood as follows. In the Markov case, the quanta coupled from the system to the environment never come back to the system, whereas in the non-Markovian case, the emitted quanta will re-couple from the environment to the system.

Similarly, one can build the higher-order approximations which usually contain the noise z . One obtains then a series of approximate QSD equations. The master equation corresponding to the zeroth-order approximation (3.18) is derived in the next section.

IV. NON-MARKOVIAN QSD VERSUS NON-MARKOVIAN MASTER EQUATION

In this section, we discuss how to derive the master equation from the non-Markovian QSD equation. Our motivations are as follows. First, the master equation approach has a long tradition and is fundamental in open quantum system dynamics, and the reduced density operator contains all mean values of the ‘‘system’’ that can be directly observed and measured. Second, although it is clear in principle that each perturbative scheme for non-Markovian QSD gives rise to a perturbative scheme for the non-Markovian master equation, it is very difficult in practice to carry out this program without a systematic way to derive the non-Markovian master equation from its QSD counterpart. The aim of this section is to show how to derive the quantum master equation directly from the non-Markovian QSD. Based on this result, we establish explicitly the relation between the perturbative QSD equations and perturbative master equations.

A. General master equation

The starting point of the derivation of the general master equation is the unnormalized projection operator P_t ,

$$P_t = |\psi_t(z)\rangle\langle\psi_t(z)|. \quad (4.1)$$

Recall that the reduced density operator can be reproduced by taking the statistical means over the noise: $\rho_t = M[P_t]$

$=M[|\psi_t(z)\rangle\langle\psi_t(z)|]$. Accordingly, the temporal evolution equation for P_t can then be obtained from Eq. (2.5):

$$\begin{aligned} \frac{d}{dt}P_t &= -i[H, P_t] + LP_t z_t + P_t L^\dagger z_t^* \\ &\quad - L^\dagger \int_0^t \alpha(t, s) \hat{O}(t, s, z) ds P_t \\ &\quad - P_t \int_0^t \alpha(t, s) \hat{O}(t, s, z)^\dagger ds L. \end{aligned} \quad (4.2)$$

The above equation is, of course, a stochastic differential equation with time-dependent coefficients. Accordingly, the master equation corresponding to Eq. (2.2) may be obtained by taking statistical mean values of Eq. (4.2).

To this end, we note that for any complex Gaussian noise z_t , the following relations hold (see Appendix C):

$$M[P_t z_t] = \int_0^t ds M[z_t z_s^*] M\left[\frac{\delta P_t}{\delta z_s^*}\right], \quad (4.3)$$

$$M[P_t z_t^*] = \int_0^t ds M[z_t^* z_s] M\left[\frac{\delta P_t}{\delta z_s}\right]. \quad (4.4)$$

From Eqs. (4.3) and (4.4), the following identities are obtained:

$$M[LP_t z_t] = L \int_0^t \alpha(t, s) M[P_t \hat{O}(t, s, z)^\dagger] ds, \quad (4.5)$$

$$M[P_t L^\dagger z_t^*] = \int_0^t \alpha(t, s) M[\hat{O}(t, s, z) P_t] ds L^\dagger. \quad (4.6)$$

Here we used the following relations:

$$M\left[\frac{\delta}{\delta z_s} P_t\right] = M\left[\frac{\delta}{\delta z_s} |\psi_t\rangle\langle\psi_t|\right] = M[\hat{O}(t, s, z) P_t], \quad (4.7)$$

$$M\left[\frac{\delta}{\delta z_s^*} P_t\right] = M\left[|\psi_t\rangle\langle\psi_t| \frac{\delta}{\delta z_s^*}\right] = M[P_t \hat{O}(t, s, z)^\dagger], \quad (4.8)$$

and we take advantage of the definition of the \hat{O} operator (2.6). The validity of the above two identities (4.7) and (4.8) is ensured by the fact that the solution ψ_t of Eq. (2.2) is an analytic function of z and is thus independent of z^* . Accordingly, $\delta|\psi_t\rangle/\delta z_t^* = 0$, $\delta\langle\psi_t|/\delta z_t = 0$.

Hence, using Eqs. (4.5) and (4.6), the exact non-Markovian master equation corresponding to non-Markovian QSD (2.2) can be obtained:

$$\frac{d}{dt}\rho_t = -i[H, \rho_t] + [L, M[P_t \bar{O}(t, z)^\dagger]] - [L^\dagger, M[\bar{O}(t, z) P_t]], \quad (4.9)$$

where as before $M[\]$ stands for the ensemble average, and $\bar{O}(t, z)$ is defined in Eq. (2.13).

Equation (4.9) is the exact equation on which our perturbation approach is based. As an evolution equation, the above master equation does not look very nice since the last

two terms appearing in the equation have not yet been written in terms of ρ . It seems quite difficult to write this equation into a closed evolution equation in full generality, if not impossible. We shall see, however, that in many interesting and physically relevant situations, a closed form for this equation can be found (see below). Notably, the use of the relations (4.3) and (4.4) can make a tremendous simplification in deriving the master equation of an open quantum system from its QSD counterpart. In fact, it enables us to find out an exact or an approximate non-Markovian master equation by directly using the techniques of a stochastic process.

The non-Markovian master equation (4.9), by design, will always preserve the positivity, trace, and Hermiticity.

B. Approximate master equations

Since the master equation (4.9) cannot, in general, be written in a closed form, some kind of approximation has to be made to determine the operator $\hat{O}(t, s, z)$. The Markov approximation emerges for a vanishing environment correlation time, $\alpha(t, s) = \delta(t - s)$. In this case, from Eq. (3.4) $\bar{O}(t, z) = \frac{1}{2}L$, and Eq. (4.9) reduces to the Markov Lindblad master equation,

$$\frac{d}{dt}\rho_t = -i[H, \rho_t] + L\rho_t L^\dagger - \frac{1}{2}\{LL^\dagger, \rho_t\}. \quad (4.10)$$

where $\{, \}$ denotes the anticommutator. Another interesting case is when the dependence of the operator $\bar{O}(t, z)$ on the noise z_t is negligible, that is, $\bar{O}(t, z) \approx \bar{O}_0(t)$. Recall from Eq. (3.16) that this is indeed the case when the dynamics is not far from Markov or the driving noise is very small. Under this approximation, the master equation takes the following simple form:

$$\frac{d}{dt}\rho_t = -i[H, \rho_t] + [L, \rho_t \bar{O}_0(t)^\dagger] + [\bar{O}_0(t) \rho_t, L^\dagger]. \quad (4.11)$$

The notation $\bar{O}_0(t)$ is the same as before [see Eqs. (3.16) and (2.13)]. The master equation (4.11) will serve as a good approximation to the exact non-Markovian master equation (4.9) in many situations of interest. In particular, if the operator $\hat{O}(t, s, z)$ is independent of noise z_t , then Eq. (4.11) becomes exact. Interestingly, there are many physically relevant examples that satisfy this condition [1].

More importantly for this paper, this condition is always satisfied in the first-order perturbative approximation (3.4) developed in Sec. III A. Then the master equation (4.9) takes the following form:

$$\begin{aligned} \frac{d}{dt}\rho_t &= -i[H, \rho_t] + [g_0(t) + g_0^*(t)]L\rho_t L^\dagger - g_0(t)L^\dagger L\rho_t \\ &\quad - g_0^*(t)\rho_t L^\dagger L + ig_1(t)[L^\dagger, [H, L]\rho_t] \\ &\quad - ig_1^*(t)[\rho_t [L^\dagger, H], L] + g_2(t)[L^\dagger, [L^\dagger, L]L\rho_t] \\ &\quad + g_2^*(t)[\rho_t L^\dagger [L^\dagger, L], L]. \end{aligned} \quad (4.12)$$

This master equation is the main result of this subsection. It provides a systematic evolution for first-order non-Markovian systems. Hence it could be called the ‘‘post-

Markov” master equation. As for the first-order QSD equation (3.8), $g_1(t)$ and $g_2(t)$ terms are smaller by a factor $\omega\tau$ or $\Gamma\tau$ compared to the first line (recall that ω is the typical “system” frequency determined by H , Γ is a typical “system” relaxation time scale determined by $L^\dagger L$, and τ is the environmental correlation time).

Note that this “post-Markov” equation in general remains non-Markovian even when $g_1(t)=0, g_2(t)=0$, because of the $g_0(t)$ term. However, for long time $g_0(t)$ tends to a constant.

Equations (3.8) and (4.12) will be applied to some examples in Sec. V. In addition, Sec. VI presents a perturbation analysis of the quantum Brownian motion model.

Finally, it should be noted that we have not addressed issues such as mathematical conditions for the convergence of the expansions (3.1) and (3.16). Also, we are not able to prove, in full generality, that Eq. (4.12) always yields a positive density operator. However, in this paper, we shall illustrate in several examples that the resulting approximate QSD and master equations around the Markov limit (i.e., τ is not too large) are mathematically consistent. We will come back to these issues in future publications.

V. EXAMPLES AND APPLICATIONS

The perturbative approach developed in the previous sections allows us to apply first-order non-Markovian QSD to any open quantum system once the Hamiltonian of the system H , the Lindblad operator L , and the environment correlation function $\alpha(t,s)$ are specified. All of these are determined by the physical model itself, as illustrated in this section using some typical models. For simplicity, we assume that the complex process z_t entering the non-Markovian QSD equation (3.8) has a Lorentzian spectrum, i.e., is of the Ornstein-Uhlenbeck type with the correlation function $\alpha(t,s)=(\gamma/2)e^{-\gamma|t-s|}$, where $\gamma^{-1}=\tau$ is the environmental correlation time, unless otherwise stated.

A. Dissipative model

In this subsection, we consider a dissipative two-level model characterized by

$$H = \frac{\omega}{2} \sigma_z, \quad L = \lambda \sigma_- . \quad (5.1)$$

Since this model can be solved exactly [1], we are able to compare the perturbation approach with the exact non-Markovian QSD and master equations. Note that the model defines two “system” time scales through the parameters by ω (oscillation) and λ^2 (damping). Here we assume that they are of the same order of magnitude.

The first-order non-Markovian QSD equation can be obtained from Eq. (3.8):

$$\begin{aligned} \frac{d}{dt} \tilde{\psi}_t = & -i \frac{\omega}{2} \sigma_z \tilde{\psi}_t + \lambda (\sigma_- - \langle \sigma_- \rangle_t) \tilde{\psi}_t \tilde{z}_t \\ & - [\lambda^2 g_0(t) + i\lambda^2 \omega g_1(t) + \lambda^4 g_2(t)] \\ & \times (\sigma_+ \sigma_- - \langle \sigma_+ \rangle_t \sigma_- - \langle \sigma_+ \sigma_- \rangle_t + \langle \sigma_+ \rangle_t \langle \sigma_- \rangle_t) \tilde{\psi}_t \end{aligned} \quad (5.2)$$

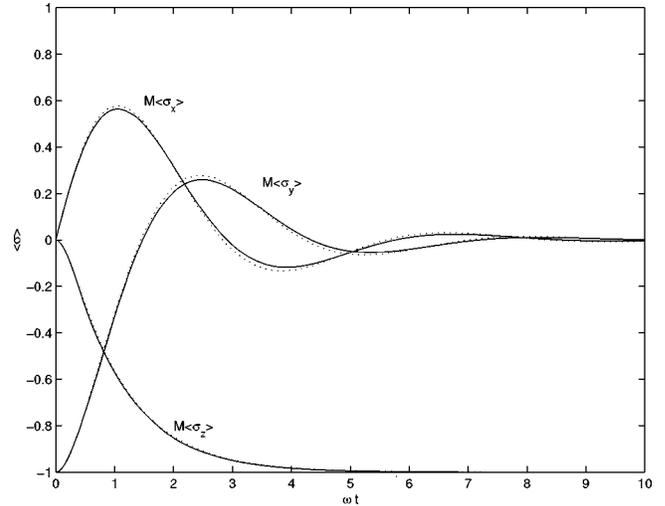


FIG. 1. Ensemble average of the Bloch vector $\langle \vec{\sigma} \rangle$ over 2000 trajectories of the first-order QSD (solid curve), and by the exact master equation (dotted curve) with Hamiltonian $H = (\omega/2) \sigma_z$, $L = \lambda \sigma_-$, and $\alpha(t,s) = (\gamma/2) e^{-\gamma|t-s|}$. Here we choose $\omega = \lambda = 1$ and $\gamma = 10$. The initial state is chosen as $|\psi_0\rangle = |-\rangle + i|+\rangle$.

and the first-order non-Markovian master equation can be obtained from Eq. (4.12):

$$\begin{aligned} \frac{d}{dt} \rho_t = & -i \frac{\omega}{2} [\sigma_z, \rho_t] + \lambda^2 g_0(t) (2\sigma_- \rho_t \sigma_+ - \{\sigma_+ \sigma_-, \rho_t\}) \\ & - i\lambda^2 \omega g_1(t) [\sigma_+ \sigma_-, \rho_t] - \lambda^4 g_2(t) \{\sigma_+ \sigma_-, \rho_t\} \\ & + 2\lambda^4 g_2(t) \sigma_- \rho_t \sigma_+ , \end{aligned} \quad (5.3)$$

where $g_1(t)$ gives the time-dependent frequency shift. Thus the master equation is of the Lindblad form with time-dependent coefficients. As seen in the next subsection, this property cannot be regarded as a generic feature of a non-Markovian master equation. Note that the first-order master equation (5.3) respects the Hermiticity, normalization, and positivity for any initial states and time scales. We can easily identify the first-order non-Markovian correction terms of the order ω/γ and λ^2/γ in Eqs. (5.2) and (5.3). We expect these equations to be a good approximation for the exact solution as long as terms of the order $(\omega/\gamma)^2$ and $(\lambda^2/\gamma)^2$ are negligible.

In Fig. 1, the average of $\langle \vec{\sigma} \rangle$ for $\omega = \lambda = 1$ and $\gamma = 10$ is plotted. The results given by the perturbation QSD equation over 2000 realizations (solid curve) are in remarkable agreement with the exact master equation (dotted curve).

To illustrate the limits of the Markov approximation, Fig. 2 presents the ensemble average $\langle \sigma_x \rangle$ for the first-order QSD (solid curve) for the same parameters as Fig. 1 except for the memory time $\gamma = 1$, and compares this with the Markov master equation (dotted curve) and the exact master equation (dashed curve). Clearly, the ensemble average of σ_x over 1000 trajectories still gives a good approximation to the exact master equation. The result is fully in accordance with our expectation as for relatively long memory times the Markov approximation is no longer valid. It should be noted that, in general, the accuracy of the first-order QSD is also limited to relatively short memory times, but not as severely as the

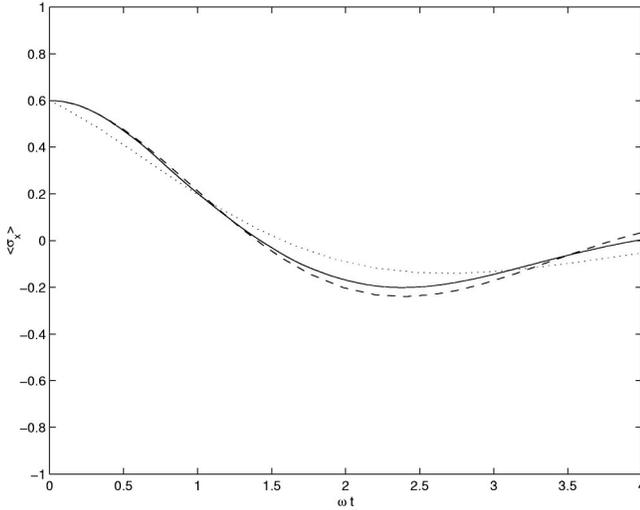


FIG. 2. Ensemble average of $\langle \sigma_x \rangle$ over 1000 realizations by using the first-order non-Markovian QSD (solid curve) for the same model as Fig. 3. Here, $\gamma=1$, $\omega=\lambda=1$, and $|\psi_0\rangle=|-\rangle+3|+\rangle$. The dashed curve is the exact master equation for the same choice of parameters, and the dotted curve is the master equation in the Markov limit.

Markov approximation. Then the higher-order approximations or an alternative expansion such as Eq. (3.16) should be used.

B. Two-level model

Let us consider a driven two-level atomic system interacting with a dissipative environment. The Hamiltonian of the system, H , and the Lindblad operator, L , which represents the influence of the environment are given by

$$H = \frac{\omega}{2} \sigma_x, \quad L = \lambda \sigma_z, \quad (5.4)$$

respectively, where the parameter λ is a coupling constant. For this model, it can be shown that the expansion (3.16) will not terminate at any finite order. The application of the perturbative approach is thus necessary. The first-order non-Markovian QSD equation can be readily obtained from Eq. (3.8):

$$\begin{aligned} \frac{d}{dt} \tilde{\psi}_t = & -i \frac{\omega}{2} \sigma_x \tilde{\psi}_t + \lambda (\sigma_z - \langle \sigma_z \rangle_t) \tilde{\psi}_t + \lambda^2 g_0(t) (\langle \sigma_z \rangle_t \sigma_z \\ & - \langle \sigma_z \rangle_t^2) \tilde{\psi}_t - \omega \lambda^2 g_1(t) (i \sigma_x + \langle \sigma_z \rangle_t \sigma_y - i \langle \sigma_x \rangle_t \\ & - \langle \sigma_z \rangle_t \langle \sigma_y \rangle_t) \tilde{\psi}_t, \end{aligned} \quad (5.5)$$

where the coefficients $g_0(t), g_1(t)$ are given by Eqs. (3.11) and (3.12), respectively. $g_0(t)$ terms in the above equation are expected from the Markov QSD picture. $g_1(t)$ terms represent the non-Markovian correction and are smaller by a factor $\omega\tau = \omega/\gamma$.

Similarly, the first-order non-Markovian master equation can be obtained directly from Eq. (4.12):

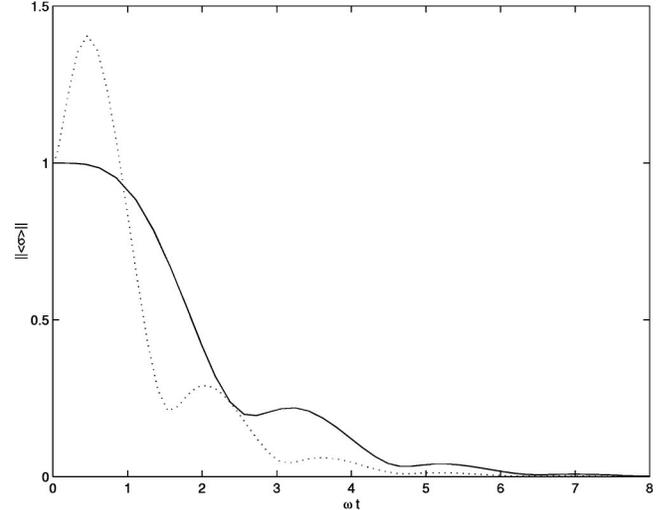


FIG. 3. Illustration of the norm of the Bloch vector of a two-level system with $H = (\omega/2) \sigma_x$, $L = \lambda \sigma_z$ and exponentially decaying correlation function $\alpha(t, s) = (\gamma/2) e^{-\gamma|t-s|}$. The initial state is chosen as the excited state $|\psi_0\rangle = |+\rangle$. The parameters are chosen as $\omega = \lambda = 1$, $\gamma = \frac{1}{2}$. The solid curve represents the norm of the Bloch vector by the master equation, and the dotted line represents the norm of Bloch vector from the long-time limit master equation (LME). We see $\|\langle \vec{\sigma} \rangle\| > 1$ for the Bloch vector by LME for the chosen initial state at short times. Accordingly, LME loses the positivity at short times for some initial states.

$$\begin{aligned} \frac{d}{dt} \rho_t = & -i \frac{\omega}{2} [\sigma_x, \rho_t] + 2\lambda^2 g_0(t) \sigma_z \rho_t \sigma_z - 2\lambda^2 g_0(t) \rho_t \\ & - i\lambda^2 \omega g_1(t) [\sigma_x, \rho_t] - \lambda^2 \omega g_1(t) \sigma_z \rho_t \sigma_y \\ & - \lambda^2 \omega g_1(t) \sigma_y \rho_t \sigma_z. \end{aligned} \quad (5.6)$$

There are some new features about the master equation (5.6). First, it is obviously not in the Lindblad form due to the presence of the cross term $\sigma_z \rho \sigma_y$ and its conjugate. Second, the master equation derived in this way naturally preserves the Hermiticity, trace, and positivity. The preservation of trace and Hermiticity is obvious. It is known that positivity of any two-dimensional density matrix is equivalent to the condition $\|\langle \vec{\sigma} \rangle\| \leq 1$, where $\langle \vec{\sigma} \rangle = \text{Tr}(\vec{\sigma} \rho)$ is the Bloch vector [29,30]. In Fig. 3 we have plotted the norms of the Bloch vector using the time-dependent master equation (5.6) (solid curve) and the long-time limit master equation (LME) (dotted curve), in which the coefficients of the master equation become constant: $g_0(t) = 1/2, g_1(t) = 1/2\gamma$. Clearly, LME loses positivity for some initial states at short time scales, whereas the time-dependent master equation (5.6) preserves positivity at all times (provided τ is not too large). Note that this simple model is the two-level analog of the Caldeira-Leggett master equation studied in Sec. VI below.

We also solved numerically the first-order QSD equation (5.5). The average of $\vec{\sigma}$ obtained through many realizations of Eq. (5.5) (solid line) and through the first-order master equation (5.6) (dotted curve) is plotted in Fig. 4. Taking the ensemble mean over 500 realizations, we see from Fig. 4 that the first-order QSD equation is in good agreement with the first-order master equation, for the short memory time ($\gamma = 10$).

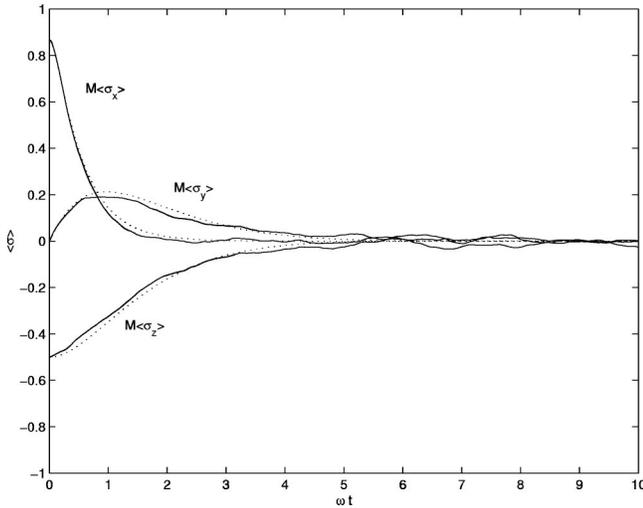


FIG. 4. Ensemble average of $\langle \vec{\sigma} \rangle$ over 500 realizations (solid curve) for the same model as Fig. 3. Here we choose $\omega = \lambda = 1$, $\gamma = 10$, and the initial state $|\psi_0\rangle = |-\rangle + \sqrt{3}|+\rangle$. The dotted curve is an average by the first-order master equation for the same choice of parameters.

VI. QUANTUM BROWNIAN MOTION: PERTURBATIVE ANALYSIS

The transition from non-Markovian to Markov processes is an outstanding problem. It is debated how to take the correct Markov limit for a non-Markovian process. Certain approximations of the exact dynamics can lead to master equations with bad properties such as nonpositivity. A notorious example is the Caldeira-Leggett master equation [26,31,32], which may violate positivity of the density operator at short time scale [33–36]. Consequently, it is impossible to simulate friction in the manner of Caldeira-Leggett with stochastic Schrödinger equations. The aim of this section is to apply the time-dependent perturbation approach for the master equation developed in the previous sections to the quantum Brownian motion (QBM) model [26,31,32,37]. In particular, we shall show that our first-order non-Markovian master equation recovers the Caldeira-Leggett master equation in the Fokker-Planck and long-time ($t \gg \tau$) limit. The Hamiltonian of the system and the Lindblad operator are as follows:

$$H = \frac{1}{2}p^2 + V(q), \quad L = q, \quad (6.1)$$

where we choose a unit mass particle moving in a general potential $V(q)$. For the sake of simplicity, we consider the case of the Ohmic heat bath, $I(\omega) \sim \omega$. The bath correlation function is then given by

$$\alpha(t, s) = \frac{\eta}{\pi} \int_0^\Lambda d\omega \omega \left[\coth\left(\frac{\omega}{2kT}\right) \cos[\omega(t-s)] - i \sin[\omega(t-s)] \right], \quad (6.2)$$

where Λ is the cutoff frequency of the bath which characterizes the correlation time $\tau = \Lambda^{-1}$ and η is the friction coefficient.

From Eq. (3.4), we get

$$\bar{O}(t) = g_0(t)q - g_1(t)p, \quad (6.3)$$

where the coefficients $g_0(t), g_1(t)$ are defined as before Eqs. (3.5) and (3.6).

The zeroth-order master equation can be obtained from Eq. (4.12) by setting $g_1(t) = g_2(t) = 0$:

$$\frac{d}{dt}\rho_t = -i[H, \rho_t] - g_{0R}(t)[q, [q, \rho_t]] - i g_{0I}(t)[q^2, \rho_t]. \quad (6.4)$$

This master equation preserves positivity for all times, regardless of the initial states, as it is of the standard Lindblad form with time-dependent coefficients. (This is of course not a generic feature for non-Markovian master equations.) However, Eq. (6.4) does not take the energy dissipation into account. More relevant is therefore the first-order approximation. The master equation in this case can be obtained from Eq. (4.12),

$$\begin{aligned} \frac{d}{dt}\rho_t = & -i[H, \rho_t] - g_{0R}(t)[q, [q, \rho_t]] - i g_{0I}(t)[q^2, \rho_t] \\ & + g_{1R}(t)[q, [p, \rho_t]] + i g_{1I}(t)[q, \{p, \rho_t\}], \end{aligned} \quad (6.5)$$

where the coefficients $g_{iR}(t), g_{iI}(t)$ ($i=0,1$) are the real and imaginary parts of $g_i(t)$ ($i=0,1$), respectively. The coefficient $g_{0R}(t)$ induces diffusion and the decoherence in position q while $g_{0I}(t)$ gives rise to a time-dependent frequency shift. The coefficient $g_{1R}(t)$ is responsible for further diffusion, and the last coefficient $g_{1I}(t)$ gives the friction. All of these time-dependent coefficients vanish at $t=0$ due to the assumption that initially the state of bath+system is factorable. In the special case when $V(q)$ is a quadratic potential, it is reassuring that our non-Markovian master equations (6.4) and (6.5) coincide with the zeroth- and, respectively, first-order expansions of the exact Hu-Paz-Zhang master equation [32].

In the Ohmic case (6.2), there exists a special high-temperature limit (Fokker-Planck limit) which results in a Markov master equation. We take the high-temperature limit in such a way that $kT \gg \Lambda$. For times $t \gg \tau = \Lambda^{-1}$, the time-dependent coefficients in Eq. (6.5) approach constant values and we get the Markov ‘‘Caldeira-Leggett’’ master equation for Brownian motion:

$$\frac{d}{dt}\rho_t = -i[H', \rho_t] - i \frac{\eta}{2}[q, \{p, \rho_t\}] - \eta kT [q, [q, \rho_t]], \quad (6.6)$$

where H' is the cutoff-dependent renormalized Hamiltonian. This is a Markov master equation with constant coefficients. It does not belong to the Lindblad class and it may violate the positivity of the density operator. We mention casually that a next-order high-temperature expansion improves this situation and replaces the Caldeira-Leggett equation (6.6) by a proper Markov Lindblad equation [36]. This $1/T$

asymptotic expansion has nothing to do with the perturbative approach in our present work. Note that the Fokker-Planck limit of the zeroth-order non-Markovian equation (6.4) does not contain the dissipative (friction) term on the right-hand side so it is a Lindblad master equation.

It is instructive to look at the nonpositivity of the Caldeira-Leggett master equation (6.6) from the QSD point of view. It is clear from the derivation that the QSD master equation (6.5) differs from the standard Caldeira-Leggett master equation (6.6) for short times of the order of the environmental correlation time. During this short time, an arbitrary initial condition, which might lead to positivity violation when propagated with the non-Lindblad master equation (6.6), evolves towards an effective, modified “initial” density operator for the long time master equation (6.6) [35].

Our QSD master equation (6.5) is also a non-Lindblad equation but with time-dependent coefficients. As in the case of the spin model in Sec. V B, their time dependence can assure the preservation of the state’s positivity. In the master equation (6.5), the coefficient $g_{1I}(t)$ of the dissipative term is zero at $t=0$ and its time derivative vanishes, too. The diffusion coefficient $g_{0R}(t)$ also vanishes but its initial derivative is positive. Thus the initial phase of the evolution is dominated by diffusion. This mechanism may, as is well known in the exact model of Ref. [32], guarantee the positivity of the density matrix at short times as well as at later times when the dissipation enters. In contrast, in the Caldeira-Leggett master equation (6.6) the constant dissipative term will immediately violate the positivity of a distinguished class of initial density matrices.

In summary, we have presented the zeroth-order master equation (6.4) and the first-order non-Markovian master equations (6.5) based on the QBM model. After an initial “slip” time, of the order of the environmental correlation time, we recover the standard QBM master equation. We note that both decoherent histories and environment-induced decoherence are discussed using the QBM model, but mainly in the Markov regimes [15,38–40]. It would be interesting to study these approaches with a non-Markovian master equation like Eq. (6.5). We shall discuss these topics elsewhere.

VII. CONCLUSIONS

Non-Markovian QSD offers a brand new avenue to explore non-Markovian dynamics of open quantum systems. Such situations appear in a variety of practical problems, such as, e.g., materials with photonic band gaps or output coupling from a Bose-Einstein condensate. In this paper we present a systematic perturbation approach to non-Markovian QSD.

Our perturbation approach makes non-Markovian QSD more amenable to computer simulations. In particular, a detailed analysis of first-order “post-Markov” QSD equations and the corresponding “post-Markov” master equations are presented in Secs. III and IV. It is noteworthy that these equations depend only on the system Hamiltonian, the Lindblad operator, and the environment correlation function. The equations can thus be read off directly from the total system + environment Hamiltonian. We have illustrated the pertur-

bation approach with some typical examples.

In the Markov regime, it is well-known that each Lindblad master equation can be unraveled by either continuous or jump trajectories which decompose the density matrix into pure states at all times. The reverse is also true; each stochastic unraveling uniquely yields a positive density matrix. In the present paper, we have shown that this correspondence is even more fruitful in the non-Markovian regime. We show explicitly how the non-Markovian QSD equation gives rise to the corresponding non-Markovian master equation. As the most important application, we have shown that each perturbative QSD equation naturally gives rise to a perturbative master equation. We have shown numerically that the resulting master equation naturally respects the properties of hermiticity, normalization, and, more importantly, positivity.

Admittedly, many issues remain to be solved in this subject. In this paper we have exclusively discussed the first-order “post-Markov” perturbation theory for QSD without touching the perturbative QSD based on the functional expansion (3.16). It is important to note that these two expansions (3.1) and (3.16) are of rather different physical meaning. The former expansion, on which we concentrate in this paper, is an expansion in the environmental correlation time, whereas the latter is the expansion for the “small noise.” Clearly, the comparison of these two expansions will be interesting. Another important project in the next step is to apply the non-Markovian QSD to some realistic physical problems, such as non-Markovian atom-field interaction and, in particular, the superradiance near a photonic band gap, in which the non-Markovian interaction is essential (e.g., see [5]). Also, it is known in the Markov regime [41,42] that localization of quantum trajectories—typically in phase space—is of great significance in accelerating the numerical simulations. Therefore, investigations into localization in non-Markovian QSD would be useful in both theoretical and practical respects.

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APPENDIX A: PERTURBATION EXPANSION OF THE OPERATOR $\hat{O}(t,s,z)$

Let us consider the following expansion of the operator $\hat{O}(t,s,z)$:

$$\begin{aligned} \hat{O}(t,s,z) = & \hat{O}_0(t,s) + \int_0^t \hat{O}_1(t,s,v) z_v dv \\ & + \int_0^t \int_0^t \hat{O}_2(t,s,v_1,v_2) z_{v_1} z_{v_2} dv_1 dv_2 + \dots \\ & + \int_0^t \dots \int_0^t \hat{O}_n(t,s,v_1, \dots, v_n) \\ & \times z_{v_1} \dots z_{v_n} dv_1 \dots dv_n + \dots, \end{aligned} \quad (\text{A1})$$

where the operators $\hat{O}_n(t,s,v_1, \dots, v_n)$ are independent of the noise z and are symmetric in their n last variables [e.g., $\hat{O}_2(t,s,v_1,v_2) = \hat{O}_2(t,s,v_2,v_1)$]. The initial condition is $\hat{O}(t,t,z) = L$.
Accordingly, we get

$$\begin{aligned} \frac{d}{dt} \frac{\delta \psi_t}{\delta z_s} = & \partial_t \hat{O}_0(t,s) \psi_t + \left(\hat{O}_1(t,s,t) z_t + \int_0^t \partial_t \hat{O}_1(t,s,v) z_v dv \right) \psi_t + \left(2 \int_0^t \hat{O}(t,s,t,v_2) z_t z_{v_2} dv_2 \right. \\ & + \int_0^t \int_0^t \partial_t \hat{O}_2(t,s,v_1,v_2) z_{v_1} z_{v_2} dv_1 dv_2 \left. \right) \psi_t + \dots + \left(n \int_0^t \dots \int_0^t \hat{O}(t,s,t,v_2, \dots, v_n) z_t z_{v_2} \dots z_{v_n} dv_2 \dots dv_n \right. \\ & \left. + \int_0^t \dots \int_0^t \partial_t \hat{O}_n(t,s,v_1, \dots, v_n) z_{v_1} \dots z_{v_n} dv_1 \dots dv_n \right) \psi_t + \dots + \hat{O}(t,s,z) \frac{d}{dt} \psi_t \end{aligned} \quad (\text{A2})$$

and

$$\begin{aligned} \frac{\delta}{\delta z_s} \frac{d}{dt} \psi_t = & (-iH + L z_t) \frac{\delta \psi_t}{\delta z_s} - L^\dagger \bar{O}(t,z) \frac{\delta \psi_t}{\delta z_s} \\ & - L^\dagger \left(\bar{O}_1(t,s) + 2 \int_0^t \bar{O}_2(t,s,v_2) z_{v_2} dv_2 + \dots \right. \\ & + n \int_0^t \dots \int_0^t \bar{O}_n(t,s,v_2, \dots, v_n) \\ & \left. \times z_{v_2} \dots z_{v_n} dv_2 \dots dv_n \right) \psi_t + \dots, \end{aligned} \quad (\text{A3})$$

where $\bar{O}_n(t,v_1, \dots, v_n) \equiv \int_0^t \alpha(t,s) \hat{O}_n(t,s,v_1, \dots, v_n) ds$.
Consequently, from the consistency condition

$$\frac{d}{dt} \frac{\delta}{\delta z_s} \psi_t = \frac{\delta}{\delta z_s} \frac{d}{dt} \psi_t \quad (\text{A4})$$

one obtains the following hierarchy of equations:

$$\begin{aligned} \frac{\partial}{\partial t} \hat{O}_n(t,s,v_1, \dots, v_n) = & [-iH, \hat{O}_n(t,s,v_1, \dots, v_n)] - \frac{1}{n!} \sum_{P_n \in S_n} \sum_{k=0}^n \\ & \times [L^\dagger \bar{O}_k(t, v_{P_n(1)}, \dots, v_{P_n(k)}), \\ & \times \hat{O}_{n-k}(t, s, v_{P_n(k+1)}, \dots, v_{P_n(n)})] \\ & - (n+1) L^\dagger \bar{O}_{n+1}(t, s, v_1, \dots, v_n) \end{aligned} \quad (\text{A5})$$

with initial conditions

$$\hat{O}_0(t,t) = L, \quad (\text{A6})$$

$$\hat{O}_n(t,t,v_1, \dots, v_n) = 0 \quad \text{for all } n \geq 1, \quad (\text{A7})$$

$$n \hat{O}_n(t,s,t,v_2, \dots, v_n) = [L, \hat{O}_{n-1}(t,s,v_2, \dots, v_n)], \quad (\text{A8})$$

where S_n is the permutation group and P_n is the permutation operators acting on the indices v_1, v_2, \dots, v_n .

Of particular interest is $n=0$. We get

$$\begin{aligned} \frac{\partial}{\partial t} \hat{O}_0(t,s) = & [-iH, \hat{O}_0(t,s)] - [L^\dagger \bar{O}_0(t), \hat{O}_0(t,s)] \\ & - L^\dagger \bar{O}_1(t,s). \end{aligned} \quad (\text{A9})$$

From this the derivative of \hat{O}_0 can be easily worked out.

For simplicity, we assume here exponentially decaying correlations:

$$\alpha(t,s) = \frac{\gamma}{2} e^{-\gamma|t-s|}. \quad (\text{A10})$$

The evolution equations for the $\bar{O}_n(t,v_1, \dots, v_n)$ read

$$\begin{aligned}
& \frac{\partial}{\partial t} \bar{O}_n(t, v_1, \dots, v_n) \\
&= \frac{\gamma}{2} \hat{O}_n(t, t, v_1, \dots, v_n) - \gamma \bar{O}_n(t, v_1, \dots, v_n) \\
&+ [-iH, \bar{O}_n(t, v_1, \dots, v_n)] - \frac{1}{n!} \sum_{P_n \in S_n} \sum_{k=0}^n \\
&\times [L^\dagger \bar{O}_k(t, v_{P_n(1)}, \dots, v_{P_n(k)}), \\
&\times \bar{O}_{n-k}(t, v_{P_n(k+1)}, \dots, v_{P_n(n)})] - (n+1)L^\dagger \\
&\times \int_0^t \alpha(t, s) \bar{O}_{n+1}(t, s, v_1, \dots, v_n) ds, \quad (\text{A11})
\end{aligned}$$

where $n\bar{O}_n(t, t, v_2, \dots, v_n) = [L, \bar{O}_{n-1}(t, v_2, \dots, v_n)]$ for $n \geq 1$ and $\bar{O}_n(0, v_1, \dots, v_n) = 0$ for all n .

Equations (A5) and (A11) are very useful in the determination of the operator $\hat{O}(t, s, z)$.

APPENDIX B: SECOND-ORDER QSD EQUATION

In this appendix, we present the second-order non-Markovian QSD equation.

By using the functional expansion of $\hat{O}(t, s, z)$ and the consistency condition (See Appendix A), we can work out an expansion of the operator $\hat{O}(t, s, z)$ at point s to any desired order. In what follows, for simplicity, we only give the second-order expansion of the operator $\hat{O}_0(t, s)$, which contains no nonlocal noise z .

$$\hat{O}_0(s, s) = L, \quad (\text{B1})$$

$$\partial_1 \hat{O}_0(s, s) = -i[H, L] - g_0(s)[L^\dagger, L]L, \quad (\text{B2})$$

$$\begin{aligned}
\partial_1^2 \hat{O}_0(s, s) &= -[H, [H, L]] + i g_0(s)[H, [L^\dagger, L]L] \\
&- \alpha(s, s)[L^\dagger, L]L + i g_0(s)[L^\dagger[H, L], L] \\
&+ g_0^2(s)[L^\dagger[L^\dagger, L]L, L] + i g_0(s)[L^\dagger L, [H, L]] \\
&+ g_0^2(s)[L^\dagger L, [L^\dagger, L]L]. \quad (\text{B3})
\end{aligned}$$

Note that all derivatives above are kinds of approximations, in particular, the second-order derivative might contain more terms. Taking the first three terms of the expansion (3.1), and making the approximation $\hat{O}(t, s, z) \approx \hat{O}_0(t, s)$, one obtains

$$\begin{aligned}
\bar{O}_0(t) &= g_0(t)L - i g_1(t)[H, L] - g_2(t)[L^\dagger, L]L \\
&- g_3(t)[H, [H, L]] - g_4(t)[L^\dagger, L]L \\
&+ i g_5(t)([H, [L^\dagger, L]L] + [L^\dagger[H, L], L] \\
&+ [L^\dagger L, [H, L]]) + g_6(t)([L^\dagger[L^\dagger, L]L, L] \\
&+ [L^\dagger L, [L^\dagger, L]L]), \quad (\text{B4})
\end{aligned}$$

where the coefficients are as follows:

$$g_0(t) = \int_0^t \alpha(t, s) ds, \quad (\text{B5})$$

$$g_1(t) = \int_0^t \alpha(t, s)(t-s) ds, \quad (\text{B6})$$

$$g_2(t) = \int_0^t \int_0^s \alpha(t, s) \alpha(s-u)(t-s) ds du, \quad (\text{B7})$$

$$g_3(t) = \frac{1}{2} \int_0^t \alpha(t, s)(t-s)^2 ds, \quad (\text{B8})$$

$$g_4(t) = \frac{1}{2} \int_0^t \alpha(t, s) \alpha(s, s)(t-s)^2 ds, \quad (\text{B9})$$

$$g_5(t) = \frac{1}{2} \int_0^t \int_0^s \alpha(t, s) \alpha(s-u)(t-s)^2 du ds, \quad (\text{B10})$$

$$g_6(t) = \int_0^t \int_0^s \int_0^u \alpha(t, s) \alpha(s, u) \alpha(s, v)(t-s)^2 dv du ds. \quad (\text{B11})$$

Then the second-order QSD equations can be obtained by substituting Eq. (B4) into Eq. (2.12). Notice that, in principle, we could obtain any order approximate QSD equations by directly using the consistency condition and the functional expansion of $\hat{O}(t, s, z)$.

APPENDIX C: DERIVATION OF THE RELATIONS (4.3) AND (4.4)

In this appendix, we shall prove the relations (4.3) and (4.4). We take Eq. (4.3), for instance,

$$M[P_t z_t] = \int ds M[z_t z_s^*] M \left[\frac{\delta P_t}{\delta z_s^*} \right]. \quad (\text{C1})$$

Suppose the complex Gaussian measure takes the form

$$P(z) d\mu = N \exp \left[- \int d\sigma \int d\tau z_\sigma^* z_\tau \beta(\sigma, \tau) \right] d\mu, \quad (\text{C2})$$

where N is the normalization constant and $\beta(\sigma, \tau)$ is a kernel reciprocal to the correlation function $\alpha(\lambda, \tau)$, which is defined by

$$M[z_t^* z_s] = \alpha(t, s). \quad (\text{C3})$$

Note that the correlation function $\alpha(t, s)$ satisfies $\alpha(t, s) = \alpha(s, t)^*$. We then have the following relation:

$$\int \alpha(t, \tau)^* \beta(\tau, s) d\tau = \delta(t-s). \quad (\text{C4})$$

Now, we consider the right-hand side of Eq. (C1):

$$\begin{aligned}
& \int ds M[z_t z_s^*] M \left[\frac{\delta P_t}{\delta z_s^*} \right] \\
&= N \int d\mu \int ds \alpha(t, s)^* \frac{\delta P_t}{\delta z_s^*} P(z) \\
&= -N \int d\mu \int ds \alpha(t, s)^* P_t \frac{\delta}{\delta z_s^*} P(z). \tag{C5}
\end{aligned}$$

Here, integration by parts has been used from the second line to the third line. Note that

$$\frac{\delta}{\delta z_s^*} P(z) = - \int d\tau z_\tau \beta(s, \tau) P(z). \tag{C6}$$

Inserting Eq. (C6) into Eq. (C5), changing the integration order $\int ds$ and $\int d\tau$, and using the relation (C4), we obtain Eq. (C1). The relation (4.4) can be obtained by taking the Hermitian conjugate of Eq. (C1).

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