Higher-order solutions to non-Markovian quantum dynamics via hierarchical functional derivative

Da-Wei Luo,1 Chi-Hang Lam,2 Lian-Ao Wu,3,4 Ting Yu,1,5 Hai-Qing Lin,1 and J. Q. You1
1Beijing Computational Science Research Center, Beijing 100084, China
2Department of Applied Physics, Hong Kong Polytechnic University, Hung Hom, Hong Kong, China
3Department of Theoretical Physics and History of Science, The Basque Country University (EHU/UPV), PO Box 644, 48080 Bilbao, Spain
4Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain
5Center for Controlled Quantum Systems and Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, New Jersey 07030, USA

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Solving realistic quantum systems coupled to an environment is a challenging task. Here we develop a hierarchical functional derivative (HFD) approach for efficiently solving the non-Markovian quantum trajectories of an open quantum system embedded in a bosonic bath. An explicit expression for arbitrary order HFD equation is derived systematically. Moreover, it is found that for an analytically solvable model, this hierarchical equation naturally terminates at a given order and thus becomes exactly solvable. This HFD approach provides a systematic method to study the non-Markovian quantum dynamics of an open system coupled to a bosonic environment.

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Introduction.—The theory of open quantum systems [1] has received great interest because environment-induced effects are important in a wide range of research topics such as quantum information [2] and quantum optics [3]. There were considerable studies involving environments modeled by either bosonic or fermionic baths (see, e.g., Refs. [1, 4–13]), as well as structured environments such as spin-chain baths [14]. Conventionally, Markov approximation has been extensively used because of its simplicity. Indeed, this is valid only when memory effects of the environment are negligible. However, this approximation becomes invalid when the system-environment coupling is strong or when the environment is structured [1, 15]. Therefore, non-Markovian environments have to be considered in explaining new experimental advances in quantum optics. Also, they must be considered in quantum information manipulations in which the environmental memory is utilized to control the entanglement dynamics [16]. Therefore, it is vital to have a non-Markovian description of the system’s dynamics under the influence of the memory effects and the backaction of the environment. Actually, this has long been a challenging task and many theoretical approaches have been developed (see, e.g., Refs. [1, 4–10, 17–21]). Among these approaches, the non-Markovian quantum state diffusion (QSD) [4–6] has been proven to be a powerful tool to study the quantum dynamics of the system and exact analytical results were derived for many interesting systems such as dissipative multi-level atoms [8] and quantum Brownian motion [4, 22] which was also analytically solved via a path-integral approach [17]. Quantum continuous measurement employing the QSD technique was also studied [23, 24].

For most realistic open quantum system problems, it is almost impossible to find any useful analytical solutions. Therefore, one has to develop numerical methods to study the quantum dynamics of the open systems. However, the application of the non-Markovian QSD is greatly hindered unless one can cast it to a numerically implementable time-local form. Recently, two hierarchical approaches have been proposed; one is the stochastic differential equation (SDE) method [9] based on a functional expansion of a system operator, and the other is an approach using a hierarchy of pure states (HOPS) [10] to calculate a related functional derivative. Apart from these two approaches, an earlier attempt at a perturbative solution of the non-Markovian QSD equation was based on hierarchical functional derivative (HFD) [7]. However, because of its apparent complexity, the hierarchical equations presented there were implemented only up to the second order where the higher-order terms were approximated by a simplified operator. Here we develop a systematic and efficient higher-order HFD approach to solving the non-Markovian quantum dynamics of an open system coupled to a bosonic environment. Remarkably, a compact explicit expression for an arbitrary order hierarchical equation is derived. Moreover, it is found that for an analytically solvable model, the hierarchical equation naturally terminates at a given order, so it becomes exactly solvable. As compared to the SDE and the HOPS approaches, our generalized HFD method has several distinct advantages. It provides not only an approach for efficiently solving the non-Markovian quantum dynamics of an open system, but also a systematic method for the exact solution of analytically tractable open systems.

The HFD method for non-Markovian QSD.—We

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study a generic open system with the Hamiltonian [4, 5]

\[
H = H_s + \sum_k \left( g_k L b_k^\dagger + g_k^* L^\dagger b_k \right) + \sum_k \omega_k b_k^\dagger b_k,
\]

where \( H_s \) is the Hamiltonian of the system of interest, \( L \) is the coupling operator called Lindblad operator, \( b_k \) is the \( k \)th mode annihilation operator of the bosonic bath with a frequency \( \omega_k \), and \( g_k \) denotes the coupling strength between the system and the bosonic bath. The bath state can be specified by a set of complex numbers \( \{ z_k \} \) labeling the coherent state of all bath modes and the effect of the bath is characterized by the zero-temperature bath correlation function \( \alpha(t, s) = \sum_k |g_k|^2 e^{-i \omega_k (t-s)} \).

Defining \( z_i^* = -i \sum_k g_k z_k^2 e^{i \omega_k t} \), one can interpret \( z_k \) as a Gaussian random variable and \( z_i^* \) becomes a Gaussian process with its statistical mean given by the bath correlation function \( \alpha(t, s) = \langle \langle z_i z_i^* \rangle \rangle \).

Below we solve this problem by deriving an explicit expression of the coherent state of all bath modes and the effective operator except for a few simple models such as dissipative multi-level atoms [8], the quantum Brownian motion [4] and dissipative multiple qubits [25]. Owing to the importance of open systems, efforts [7, 9, 10] have been devoted to develop numerical methods for solving Eq. (3). In Ref. [7], an approach was proposed to calculate the functional derivative by defining a set of \( Q_k \) operators as

\[
Q_k(t, \tilde{z}^*) = \int_0^t \alpha(t, s) \frac{\delta}{\delta z_k} Q_{k-1}(t, \tilde{z}^*) ds,
\]

where \( Q_0(t, \tilde{z}^*) = \tilde{O}(t, \tilde{z}^*) \). For an environmental noise \( z_i \) characterized by the Ornstein-Uhlenbeck noise with autocorrelation \( \alpha(t, s) = \Gamma \exp(-|t-s|)/2 \), using the consistency condition \( \int_0^t \frac{\partial}{\partial t} \langle \langle \tilde{z} | \tilde{O} | z \rangle \rangle = \frac{\partial}{\partial t} \Gamma \langle \langle | \tilde{z} \rangle \rangle \), the equation of motion for \( Q_0(t, \tilde{z}^*) \) is obtained as

\[
\frac{\partial}{\partial t} Q_0(t, \tilde{z}^*) = \alpha(0) L - \gamma Q_0(t, \tilde{z}^*) - L^\dagger Q_1(t, \tilde{z}^*)
\]

\[
+ \left[ -i H_s + L z_t^\dagger - L^\dagger Q_0(t, \tilde{z}^*) \right] Q_0(t, \tilde{z}^*)
\]

which depends on \( Q_1(t, \tilde{z}^*) \). The evolution of \( Q_k \) follows a set of hierarchical equations which needs to be solved simultaneously to obtain the \( \tilde{O} \) operator. However, because of the complexity, the hierarchical equation of motion was obtained in Ref. [7] only up to the second-order \( Q_2 \) operator while the higher-order terms were approximated by a simplified operator so as to close the hierarchical equation.

Below we solve this problem by deriving an explicit compact expression for an arbitrary order of the hierarchical equation. Taking the time derivative of Eq. (4) and using the consistency condition, the equation of motion for the \( Q_k(t, \tilde{z}^*) \) operator with \( k \geq 1 \) can be formally obtained as

\[
\frac{\partial}{\partial t} Q_k(t, \tilde{z}^*) = \alpha(0) \frac{\delta}{\delta z_k} Q_{k-1}(t, \tilde{z}^*) - \gamma Q_k(t, \tilde{z}^*)
\]

\[
+ \int_0^t ds \alpha(t, s) \frac{\delta}{\delta z_k} \frac{\partial}{\partial t} Q_{k-1}(t, \tilde{z}^*).
\]

In Eq. (6), the first term on the RHS is equal to \( \alpha(0) \left[ L, Q_{k-1}(t, \tilde{z}^*) \right] \). The third term can be calculated by substituting \( \tilde{O} = Q_{k-1}(t, \tilde{z}^*) \) with the equation of motion for \( Q_{k-1}(t, \tilde{z}^*) \), which depends on \( \frac{\partial}{\partial z_k} Q_{k-2}(t, \tilde{z}^*) \). Repeating this procedure, Eq. (6) can be rewritten as

\[
\frac{\partial}{\partial t} Q_k(t, \tilde{z}^*) = \sum_{i=0}^{k-1} \left( \mathcal{P}_i \right)^i \left\{ \alpha(0) \left[ L, Q_{k-1-i}(t, \tilde{z}^*) \right] - \gamma Q_{k-i}(t, \tilde{z}^*) \right\}
\]

\[
+ \left( \mathcal{P}_i \right)^k \frac{\partial Q_0(t, \tilde{z}^*)}{\partial t}
\]

\[
= k \alpha(0) \left[ L, Q_{k-1}(t, \tilde{z}^*) \right] - (k+1) \gamma Q_k(t, \tilde{z}^*)
\]

\[
+ \left[ -i H_s + L z_t^\dagger - L^\dagger Q_0(t, \tilde{z}^*) \right] L^\dagger Q_{k+1}(t, \tilde{z}^*)
\]

\[
- \left( \mathcal{P}_i \right)^k \left[ L^\dagger Q_0(t, \tilde{z}^*), Q_0(t, \tilde{z}^*) \right],
\]

where \( \mathcal{P}_i = \int_0^t ds \alpha(t, s) \frac{\delta}{\delta z_k} \). After some algebra, the last term on the RHS of Eq. (7) is found to be \( \sum_{i=0}^{k} C_i^k \left[ L^\dagger Q_i(t, \tilde{z}^*), Q_{k-i}(t, \tilde{z}^*) \right] \), where \( C_i^k \equiv \left\{ \alpha(0) \left[ L, Q_{k-1-i}(t, \tilde{z}^*) \right] - \gamma Q_{k-i}(t, \tilde{z}^*) \right\} \)
We obtain the central result in our HFD approach:

$$\frac{\partial}{\partial t} Q_k(t, \tilde{z}^*) = k\alpha(0) [L, Q_{k-1}(t, \tilde{z}^*)] + (k + 1) \gamma Q_k(t, \tilde{z}^*)$$

$$+ [\tau H_s + L\tilde{z}^*_t, Q_k(t, \tilde{z}^*)] - L Q_{k+1}(t, \tilde{z}^*)$$

$$- \sum_{i=0}^{k} C^k_i [L^i Q_i(t, \tilde{z}^*), Q_{k-i}(t, \tilde{z}^*)],$$  \hspace{1cm} (8)

where the initial conditions are $Q_k(0, \tilde{z}^*) = 0$ for $k \geq 0$, and the zeroth-order equation is given by Eq. (5). This set of hierarchical equations can always be numerically solved perturbatively if terminated at order $N + 1$ by putting either $Q_{N+1}(t, \tilde{z}^*) = 0$ or $Q_{N+1}(t, \tilde{z}^*) = \int_0^t ds \alpha(t, s) [L, Q_N(t, \tilde{z}^*)]$. \hspace{1cm} (7)

Now we also explore the use of this approach as a systematic method for models with exact solutions. For open systems that are known to be exactly soluble by QSD, the number of expansion terms is

$$\hat{O}(t, \tilde{z}^*) = \hat{O}^{(0)}(t) + \int_0^t \hat{O}^{(1)}(t, v_1) \tilde{z}^*_{v_1} dv_1$$

$$+ \int_0^t \int_0^t \hat{O}^{(2)}(t, v_1, v_2) \tilde{z}^*_{v_1} \tilde{z}^*_{v_2} dv_1 dv_2 + \ldots,$$  \hspace{1cm} (9)

must be finite \cite{6}. Thus, $\hat{O}^{(n)} = 0$ for all $n$ larger than a given finite integer $N_e$. In this case, we can readily show that

$$Q_{N_e}(t) = N_e! \int_0^t \ldots \int_0^{t_n} \alpha(t, v_1) \ldots \alpha(t, v_{N_e})$$

$$\times \hat{O}^{(N_e)}(t, v_1, \ldots, v_{N_e}) dv_1 \ldots dv_{N_e},$$  \hspace{1cm} (10)

which is independent of the noise $\tilde{z}^*_t$. Therefore, its functional derivative with respect to $\tilde{z}^*_t$ is zero. From Eq. (4), it follows that $Q_k = 0$ for all $k \geq N_e + 1$, so that the hierarchical equation naturally terminates and the approach becomes exact. This provides a useful and systematic method to deal with an open system with unknown properties by just implementing the hierarchical equation; if the hierarchical equation has a natural termination at a given order, the considered model is analytically solvable and our results will be essentially accurate.

As an illustrative example, we consider an analytically solvable three-level system \cite{8}, with $H_{sys} = \omega J_z$, and $L = J_z$. The functional expansion of its $O$ operator is only up to the first-order term, i.e., $N_e = 1$. Thus, only $Q_0(t, \tilde{z}^*)$ and $Q_1(t)$ are involved in the hierarchical equation, and $Q_k \equiv 0$ for $k \geq 2$. We numerically solve the hierarchical equation up to order $N = 10$. From Fig. 1(a), it can be seen that the numerically calculated ensemble averages $\langle J_i \rangle$, $i = x, y$ and $z$, agree well with the exactly solved results. Also, the trace norms $||Q_k|| \equiv \text{Tr} \left( \sqrt{Q_k^* Q_k} \right)$ are calculated in Fig. 1(b), which shows that for $k \geq 2$, the $Q_k$ operators remain zero and the hierarchical equation naturally terminates at order $k = 2$ (i.e., $N_e = 1$), in full consistency with the analytical derivations.

The relationship to the SDE method.— Recently, a numerical approach \cite{9} was developed to solve the non-Markovian QSD equation via a set of stochastic differential equations (SDE). A key part of the SDE formulation is the introduction of a $Q$ operator

$$Q_m(t, \tilde{z}^*) = \int_0^t \ldots \int_0^{t_n} \alpha(t, v_1) \ldots \alpha(t, v_n) \tilde{z}^*_{v_n+1}$$

$$\ldots \tilde{z}^*_{v_n} \hat{O}^{(n)}(t, v_1, \ldots, v_n) dv_1 \ldots dv_n,$$  \hspace{1cm} (11)

where $\hat{O}^{(n)}(t, v_1, \ldots, v_n)$ corresponds to the $n$th-order functional expansion term in Eq. (9) and $\hat{O}(t, \tilde{z}^*) = \sum_{n=0}^\infty Q_m^{(n)}(t, \tilde{z}^*).$ For $m \neq 0$, $Q_m^{(n)}$ do not directly contribute to $\hat{O}(t, \tilde{z}^*)$ but form a set of hierarchical equations with $Q_0^{(n)}$ and need to be solved simultaneously. Within this framework, one can calculate the quantum trajectory up to an arbitrary order of the environmental noise.

The spin-boson model without the rotating-wave approximation (RWA) was studied using this approach (see \cite{9}). This is a typical example where the explicit form of the $O$ operator is unknown and the hierarchical approach can serve as a powerful numerical tool. In Fig. 2(a), we display the expectation value of the angular momentum $\langle \sigma_x \rangle$ as a function of time using both the SDE and our HFD approaches. An excellent agreement is reached for the numerical results obtained by them. As a matter of fact, these two hierarchical methods are very closely related mathematically because it can be proved that the operators $Q_k$ and $Q_m$ are related by \cite{26}

$$Q_k(t, \tilde{z}^*) = \sum_{n=k}^N \frac{n!}{(n-k)!} Q_m^{(n)}(t, \tilde{z}^*).$$  \hspace{1cm} (12)

The key advantage of the HFD method over the SDE approach is that the HFD equation (8) effectively groups
the $Q_{m}^{(n)}$ operator according to Eq. (12) and sums up their contributions. This makes the HFD method much more efficient than the SDE approach. In fact, for a given termination order $N$, the SDE approach needs to simultaneously solve coupled equations for $Q_{m}^{(n)}$ where $n + m \leq N$, resulting in a total number of $\frac{1}{2}(N+2)(N+1)$ equations. On the other hand, the HFD approach greatly reduces the total number of equations to $N + 1$. Figure 2(b) shows the total number of coupled differential equations that should be solved in both the HFD and the SDE approaches. The very high efficiency of the HFD method over the SDE approach is clearly seen when increasing $N$.

The relationship to the HOPS method.— Previously, almost all QSD approaches are focused on how to calculate the functional derivative associated with the $O$ operator. Recently, a hierarchy of pure states (HOPS) approach [10] was developed as a numerical tool which, instead of using the $O$ operator, introduces a set of pure states

$$|\psi_k(t)\rangle = \int_0^t \alpha(t,s) \frac{\delta}{\delta z_k} ds |\psi_{k-1}(t)\rangle,$$

where $|\psi_0(t)\rangle \equiv |\psi(t)\rangle$. In this approach, a set of hierarchical equations of motion was found for $|\psi_k(t)\rangle$. Its advantage is that the hierarchical equations deal with state vectors of size $\text{dim}(H_s) \times 1$ rather than the operators of size $\text{dim}(H_s) \times \text{dim}(H_a)$, where $\text{dim}(H_a)$ is the dimension of the system’s Hilbert space. From the definition, it is easy to see that

$$|\psi_1(t)\rangle = Q_0(t, z^*) |\psi_0(t)\rangle,$$
$$|\psi_2(t)\rangle = Q_2(t, z^*) |\psi_0(t)\rangle + Q_0(t, z^*) |\psi_1(t)\rangle,$$
$$|\psi_3(t)\rangle = Q_2(t, z^*) |\psi_0(t)\rangle + 2Q_1(t, z^*) |\psi_1(t)\rangle + Q_0(t, z^*) |\psi_2(t)\rangle,$$
$$\ldots$$

and in general,

$$|\psi_k(t)\rangle = \sum_{i=0}^{k-1} C_i^k Q_i(t, z^*) |\psi_{k-i-1}\rangle.$$

Therefore, it is also possible to formulate the HOPS approach using the $Q_i$ operators in Eq. (4). However, this set of equations does not naturally terminate as expected for some analytically solvable models. To see this, we consider a simple subset of these models where the $O$ operator itself is independent of the noise, i.e., $Q_k \equiv 0$ for $k \geq 1$. In this case, $|\psi_k(t)\rangle = (Q_0)^k |\psi_0(t)\rangle$. For example, the analytically solvable dephasing spin-boson model with $H_{\text{sys}} = \omega \sigma_z / 2$, and $L = \lambda \sigma_z$ belongs to this subset. It has been derived [4] that the $O$ operator for this model is $\tilde{O} = Q_0 = A(t) \sigma_z$, where $A(t) = \lambda \int_0^t \alpha(t,s) ds$. Therefore, the hierarchical equation in the HFD approach naturally terminates at the first order for this model. However, in the HOPS approach, one has

$$|\psi_k(t)\rangle = (Q_0)^k |\psi_0(t)\rangle = \begin{cases} A^k(t) |\psi_0(t)\rangle, & \text{for even } k, \\ A^k(t) \sigma_z |\psi_0(t)\rangle, & \text{for odd } k. \end{cases}$$

In general, it does not vanish because $\lambda \neq 0$. As a result, unlike the HFD approach, the HOPS equations for this analytically solvable example do not naturally terminate and a large set of hierarchical equations must then be solved so as to obtain arbitrarily accurate results.

Discussion and Conclusion.— Solving non-Markovian dynamics of an open quantum system has long been a challenge. The conventional master equation for the system’s reduced density matrix is driven by a superoperator $\mathbb{K}$, which is given by the perturbation expansion with respect to the strength of system-bath interaction [1]. Whereas the expansion could be done manually up to the orders beyond 2, it is difficult to find an automatic numerical way to obtain the higher-order $\mathbb{K}$ operator. As such, the conventional master equation is used in the weakly-coupled scenario. Likewise, the quantum state diffusion equation driven by an $O$ operator (which plays a role similar to $\mathbb{K}$) encounters the same problem. As a breakthrough, this work develops a systematic and efficient higher-order HFD approach for solving the non-Markovian quantum trajectories of an open system coupled to a bosonic environment. A compact explicit expression for an arbitrary order hierarchical equation of motion is derived and it can be efficiently implemented numerically. As a distinctive advantage of this method, while this hierarchical equation naturally terminates at a given order and becomes exactly solvable for an analytically solvable model, it provides a systematic perturbation for a generic open system irrespective of the existence of the time-local $O$ operator. For simplicity, zero temperature is taken for the environment, but this
can be generalized to the finite-temperature case by using thermal vacuum states [27]. Also, it is known [7, 28] that more generic noise type can be decomposed using a linear combination of a set of Ornstein-Uhlenbeck noises. Thus, the HFD method developed here can in principle be extended to solving the non-Markovian open system dynamics for other types of environmental noise.

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