Stochastic wave-function approach to non-Markovian systems

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We extend the quantum Monte Carlo wave-function method of quantum optics to non-Markovian system-reservoir interactions. The finite correlation time of the reservoir and the associated memory effects are incorporated into the dynamics by expanding the initial system using fictitious harmonic-oscillator modes, which have Markovian dissipative interactions. The underlying principle is the fact that a class of reservoir spectral functions can be approximated by a finite superposition of Lorentzian functions with positive coefficients.

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Recently, there has been considerable interest in stochastic wave-function methods in quantum optics [1–4]. The new approach, which is limited to Markovian system-reservoir interactions, leads to considerable simplification in the numerical simulations of quantum systems, due to a reduction of the number of variables from N^2 to N, as compared to simulations based on a master equation. The direct correspondance of the Monte Carlo wave-function (MCWF) description of dissipative dynamics to the experiments currently conducted in the field of quantum optics has also contributed to the growing interest in the new approach. Even though the MCWF method is applicable to a very wide variety of problems in atomic and optical physics [5–7], its application to other dissipative systems is rather limited, as a result of the Born-Markov approximation used in its derivation [8].

In this paper, we propose an extension of the stochastic wave-function method that can be used to analyze a large class of non-Markovian system-reservoir interactions. To eliminate the *memory effects* associated with non-Markovian dynamics, we expand (enlarge) the original system by adding fictitious harmonic-oscillator modes. These fictitious modes interact both with the original system (by a Hermitian $\mathbf{r}\cdot\mathbf{p}$-type coupling), and with an independent reservoir which has a vanishing correlation time (i.e., reservoir spectral function independent of frequency). In the case of dissipative electron-phonon interaction [9], for example, we could think of the expanded system as the electron *dressed* by a few strongly interacting phonon modes: This effective *polaron* system now has Markovian dynamics and can be analyzed using the MCWF method. The true dynamics of the original (bare electron) system is recovered by an eventual trace over the fictitious (phonon) modes. Here, we prove that the master equation that corresponds to the original system-reservoir interaction is identical to that obtained for the model expanded system after the tracing operation, in the Born approximation. We also discuss some of the possible applications of the new method.

It is known that a given non-Markovian process can be embedded in a larger Markovian process [10]. The method presented in this paper realizes this embedding by expanding the original system by the fictitious harmonic-oscillator modes. Let us consider a system interacting with a single harmonic-oscillator mode, which in turn interacts with a zero-correlation-time reservoir. It can be shown that the effective spectral function seen (after tracing over the fictitious mode) is a Lorentzian, given by

$$L_i(\omega) = \frac{\Gamma_i}{\frac{\Gamma_i^2}{4} + (\omega-\omega_i)^2} \quad .$$

In the case of N fictitious modes, the effective reservoir spectral function is a sum over Lorentzians contributed by each mode. The method we propose is based on the fact that a given reservoir spectral function can be approximately represented by a superposition of Lorentzians with non-negative expansion coefficients. By expanding the original system using fictitious modes that "correspond" to these Lorentzians, we show that a class of non-Markovian system-reservoir interactions can be represented by the Markovian expanded-system dynamics. For a given (fixed) number of fictitious modes, this representation will only be good in a finite frequency interval: One should first determine the required *time accuracy* in the problem and then choose the fictitious modes accordingly.

We shall assume for generality that we have a harmonic-oscillator mode (annihilation operator $\hat{a}_s$) that interacts with a bath of harmonic oscillators (annihilation operator $\hat{b}_{\mathbf{k}}$) which has a given (non-Markovian) spectral function $R(\omega)$. Since extension to finite temperatures is straightforward, we only deal with the zero-temperature case here. The original Hamiltonian in the rotating-wave approximation (RWA) is then

$$\hat{H}_{s\text{-}r} = \hbar\omega_s \hat{a}_s^\dagger \hat{a}_s + \frac{\hbar V}{(2\pi)^3}\int d\mathbf{k}\,\omega_{\mathbf{k}}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}} + i\frac{\hbar V}{(2\pi)^3}\int d\mathbf{k}\,\mathbf{g}_{\mathbf{k}}(\hat{b}_{\mathbf{k}}^\dagger\hat{a}_s - \hat{a}_s^\dagger\hat{b}_{\mathbf{k}}) \quad , \tag{1}$$

where $\mathbf{g}_{\mathbf{k}}$ is the sytem-reservoir-mode coupling strength and V is the quantization volume. $\hbar\omega_s$ and $\hbar\omega_{\mathbf{k}}$ are the energies of the system and reservoir harmonic-oscillator modes, respectively. $R(\omega)$ is determined by the Fourier transform of the correlation function of the reservoir op-

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erator $\int d\mathbf{k}\, \mathbf{g}_{\mathbf{k}} \hat{b}_{\mathbf{k}} e^{-i\omega_{\mathbf{k}} t}$ and its Hermitian conjugate. [11] The master equation obtained from the Liouville–von Neumann equation after tracing over the reservoir parameters is an integrodifferential equation: Due to the finite correlation time $\tau_{\rm corr}$ of the reservoir, the dynamics of the reduced-system density operator depends on its earlier values.

We want to prove that the system-reservoir interaction of Eq. (1) can be equivalently described by the same harmonic-oscillator (system) mode now interacting with finitely many harmonic-oscillator modes, each of which couples to an independent (Markovian) reservoir. The dynamics of the equivalent expanded system can be represented by the quantum MCWF method since the reservoir couplings in this case are assumed to be Markovian. The effective Hamiltonian of the new dressed system is [2]

$$\hat{H}_{\rm eff} = \hbar\omega_s \hat{a}_s^\dagger \hat{a}_s + \hbar \sum_i \omega_i \hat{c}_i^\dagger \hat{c}_i + i\hbar \sum_i \mathbf{g}_i (\hat{c}_i^\dagger \hat{a}_s - \hat{a}_s^\dagger \hat{c}_i) - \frac{i\hbar}{2} \sum_i \Gamma_i \hat{c}_i^\dagger \hat{c}_i \quad , \tag{2}$$

where $\hat{c}_i$ ($\hat{c}_i^\dagger$) is the annihilation (creation) operator for the ith fictitious harmonic-oscillator (FHO) mode, which has energy $\hbar\omega_i$. $\mathbf{g}_i$ is the system-mode coupling strength and Γ_i is the decay rate to an independent Markovian reservoir. The quantum MCWF description of this system is complete with the independent collapse operators

$$\hat{\mathrm{C}}_i = \sqrt{\Gamma_i}\hat{c}_i \quad , \tag{3}$$

which are used to determine the *post-measurement* wave function in the case of a quantum-jump event. The details of the quantum MCWF method can be found elsewhere [1–3]. As shown in Ref. [2], the single-quantum system stochastic wave-function description is equivalent to the master equation that describes the dynamics of an ensemble of identical systems. We remark that we can also add a direct decay term of the form $-i\hbar\Gamma_s \hat{a}_s^\dagger \hat{a}_s /2$ to the effective Hamiltonian of Eq. (2): Γ_s in that case would not be the actual decay rate of the system mode.

We now show the equivalence of the master equations obtained from the Hamiltonians of Eq. (1) and Eq. (2), in the first Born approximation. The interaction-picture system master equation that follows Eq. (1) is [11,10]

$$\frac{d\hat{\sigma}_s(t)}{dt} = -\int_0^t d\tau \Gamma(\tau)[\hat{a}_s^\dagger \hat{a}_s \hat{\sigma}_s(t-\tau) + \hat{\sigma}_s(t-\tau)\hat{a}_s^\dagger \hat{a}_s - 2\hat{a}_s \hat{\sigma}_s(t-\tau)\hat{a}_s^\dagger] \, . \tag{4}$$

Here $\hat{\sigma}_s(t)$ is the reduced-system density operator and the (complex) kernel $\Gamma(\tau)$ is given by

$$\Gamma(\tau) = \int d\mathbf{k}\, |\mathbf{g}_{\mathbf{k}}|^2 e^{-i(\omega_{\mathbf{k}} - \omega_s)\tau} = \int_0^\infty d\omega R(\omega)\, e^{-i(\omega-\omega_s)\tau} \quad . \tag{5}$$

The master equation for the system-FHO reduced density matrix that follows the quantum MCWF formulation is

$$\frac{d\hat{\sigma}_{s\text{-}m}(t)}{dt} = \left[\sum_i \mathbf{g}_i (\hat{c}_i^\dagger \hat{a}_s\, e^{i(\omega_i-\omega_s)\tau} - \hat{a}_s^\dagger \hat{c}_i\, e^{-i(\omega_i-\omega_s)\tau}) \, , \, \hat{\sigma}_{s-m}(t) \right] - \frac{1}{2} \sum_i \Gamma_i [\hat{c}_i^\dagger \hat{c}_i \hat{\sigma}_{s-m}(t) + \hat{\sigma}_{s-m}(t) \hat{c}_i^\dagger \hat{c}_i - 2\hat{c}_i \hat{\sigma}_{s-m}(t) \hat{c}_i^\dagger] \quad . \tag{6}$$

We note that Eq. (6) is valid to all orders in the interaction of the system-FHO modes (within the RWA: $\omega_i, \omega_s \gg \mathbf{g}_i$). It can alternatively be derived from first principles using the Born-Markov approximation for the FHO-mode–reservoir interactions [11]. To make the first Born approximation for the system-FHO interaction, we formally integrate Eq. (6) and substitute the resulting expression for $\hat{\sigma}_{s\text{-}m}(t)$ back in the right-hand side of Eq. (6). After making the Born approximation and performing a trace over the fictitious modes, we obtain a master equation for the *approximate* reduced-system density operator $\hat{\sigma}_{\rm app}(t)$ of exactly the same form as Eq. (4), but with a different kernel

$$\Gamma_{\rm app}(\tau) = \sum_i |\mathbf{g}_i|^2 e^{-\Gamma_i \tau - i(\omega_i - \omega_s)\tau} \simeq \int_0^\infty d\omega \left(\sum_i \frac{|\mathbf{g}_i|^2 \Gamma_i}{\frac{\Gamma_i^2}{4} + (\omega - \omega_i)^2} \right) e^{-i(\omega-\omega_s)\tau} \quad , \tag{7}$$

provided that $\forall i$, $|\omega_i| \gg \Gamma_i$. We note that this approximation is consistent with the RWA and the fact that for practically all reservoir spectral functions of interest $R(\omega = 0) = 0$. Comparing Eqs. (5) and (7), we see that provided we can approximate $R(\omega)$ by the superposition of Lorentzians that appear in (the second line of) Eq. (7), we can describe the non-Markovian (memory) effects associated with the original system-reservoir interaction by simply expanding the system by a few fictitious harmonic-oscillator modes.

Going beyond the first Born approximation in the master equation formalism is rather difficult. We have, however, obtained a general proof of equivalence between the expanded-system modeling and the actual interaction for arbitrary coupling strengths using Heisenberg equations of motion, assuming Gaussian density matrix operators for the reservoirs. This approach utilizes the fact that higher order correlation functions of the noise operators that appear in the Langevin equation for $\hat{a}_s(t)$ (for both the actual and model systems) are the same, provided that their second-order correlation function is identical [10]. The details will be published elsewhere [12].

The next important question is whether we can obtain an arbitrarily good approximation to $R(\omega)$ using the superposition of Lorentzians. One line of argument could be to prove the completeness (or overcompleteness) of Lorentzians over a finite frequency interval. Even though this seems plausible, the fact that the coefficients of the superposition have to be non-negative (i.e., $|\mathbf{g}_i|^2\Gamma_i \geq 0$) hinders us from making a general statement.

In the limit of vanishing widths ($\Gamma_i \to 0$), Lorentzians converge to δ functions, which do form a complete set and can be used to represent any non-negative function [such as $R(\omega)$] by a superposition with non-negative coefficients. In other words, by definition,

$$R(\omega) = \lim_{\kappa\to 0}\sum_i R(\omega_i)\,\frac{1}{\pi}\,\frac{\kappa}{\kappa^2+(\omega-\omega_i)^2}$$

$$= \lim_{\kappa\to 0}\sum_i R(\omega_i)\,\tilde{L}_{2\kappa}(\omega) \quad . \tag{8}$$

Note that $\tilde{L}_\kappa(\omega) = L_i(\omega)/(2\pi)$, with $\Gamma_i = \kappa$. Therefore, for any given $\epsilon > 0$, we can choose a finite set of Lorentzians with a non zero (identical) width Γ that represents the original function with an accuracy better than ϵ in a given finite frequency interval (we use the metric of the L_2 space) [13]. This *proof-of-principle* equivalence statement, unfortunately, is not very useful from a practical viewpoint.

The fact that we can independently vary the width (Γ_i) of each Lorentzian gives us an additional degree of freedom and could in principle enable us to reduce the number of fictitious harmonic modes we need to include to satisfy the given accuracy requirement. The determination of the center frequency (ω_i), width (Γ_i), and the coupling strength ($|\mathbf{g}_i|^2$) of the Lorentzians that would optimize the representation of $R(\omega)$ (in a given frequency interval) for a given number of fictitious modes is a nonlinear-programming (optimization) problem.

To illustrate the usefulness of the new method, we first consider the simplest possible extension of Markovian dynamics; that is, a reservoir spectral function which is linearly proportional to frequency [$R(\omega) = A\,\omega$]. We shall assume for simplicity that the center frequency of the oscillator (ω_i) satisfies $\omega_s \gg \omega_r = 2\pi/\tau_r$, where τ_r is the desired time accuracy. The Markov approximation in such a problem would replace ω by ω_s. To go beyond the Markov approximation we consider a single fictitious harmonic-oscillator mode centered at $\omega_1 = \omega_s + 10\omega_r$ with a width $\Gamma_1 = \omega_r$. Around $\omega \simeq \omega_s$, we can represent the Lorentzian associated with the mode as

$$L_1(\omega) \simeq \frac{|\mathbf{g}_1|^2\Gamma_1}{(\omega_1-\omega_s)^2}\left(1+2\frac{\omega-\omega_s}{\omega_1-\omega_s}\right) \quad . \tag{9}$$

Therefore the choice of $R_{\rm app}(\omega) = B + L_1(\omega)$ is a good approximation to $R(\omega)$ in the frequency interval $(\omega_s-\omega_r, \omega_s+\omega_r)$ of interest, provided we choose $|\mathbf{g}_1|^2$ such that $A = 2|\mathbf{g}_1|^2\Gamma_1/(\omega_1-\omega_s)^3$ and set $B = |\mathbf{g}_1|^2\Gamma_1(3\omega_s-\omega_1)/(\omega_1-\omega_s)^3$. We see that, by adding a single fictitious harmonic-oscillator mode, we can get an arbitrarily good representation of the actual spectral function in this simple non-Markovian reservoir interaction. In this case, however, we had to keep a direct decay channel for the system mode as well. Note that this direct decay channel practically gives the decay rate obtained in the Markov approximation, provided we choose $|\omega_1-\omega_s| \ll \omega_s, \omega_1$, since in this limit $B \simeq A$. Alternatively, we can eliminate the direct decay channel by introducing coupling to another fictitious mode centered at $\omega_2 = \omega_s$ and with a width $\Gamma_s \gg \omega_1$. Finally, for a weak quadratic dependence of $R(\omega)$ on ω, we could use two fictitious modes with $\omega_1 > \omega_s > \omega_2$, in addition to the direct (Markovian) decay channel.

Recent developments in photonic band-gap structures [14] and microcavities [15] could enable us to tailor the reservoir spectral function and observe its effects on the dissipative dynamics of the atoms embedded in these structures. The method that we present here would be ideal in simulating the *effective cavity modes* introduced by the photonic band-gap structures and their effect on the atom or exciton dynamics.

As a somewhat straightforward but illustrative example, we can consider the dissipative dynamics in a nested-cavity configuration (similar to an external-cavity laser structure). The internal-cavity mode in this case, experiences a Lorentzian reservoir spectral function and its non-Markovian decay dynamics can be modeled by considering the Hermitian coupling to a single external-cavity mode (which has Markovian dynamics). Figure 1 shows the MCWF simulation of the time dependence of the first excited state population $|a_{n=1}|^2(t)$ of the internal-cavity mode (obtained by tracing over the external-cavity mode parameters), for the initial condition $|a_{n=1}|^2(t=0) = 1$ (i.e., one photon in the internal cavity). For the assumed coupling parameter $|\mathbf{g}_{i\text{-}e}|^2 = \Gamma_e$ (external-cavity decay rate), we see that the *memory effects* associated with the external cavity show up as a slower decay for short

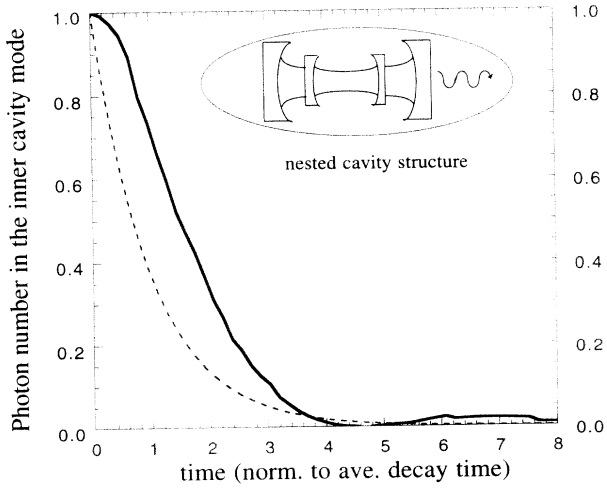

FIG. 1. The time dependence of the first excited state population of the internal-cavity mode in a nested-cavity structure. The assumed cavity-coupling coefficient satisfies $|\mathbf{g}_{i\text{-}e}|^2 = \Gamma_e$ and the plot refers to an average over 100 stochastic wave functions. The dashed curve gives the exponential decay that would be obtained from a Markov approximation.

times than is predicted by the long-time (Markovian) decay rate $4|g_{i-e}|^2/\Gamma_e$ (shown in dashed lines). "Ringing" effects are also observed in the simulations, due to the relatively strong coupling strength. We note that the problem of short-time dissipative dynamics of an atom embedded in an ideal single-mode microcavity structure is equivalent to the nested-cavity problem.

In the author's opinion, one of the most important applications of the non-Markovian stochastic wave-function approach developed in this paper would be in the MCWF modeling of dissipative electron-phonon interactions [9]. In this context, we note the recent article by Register and Hess [16] where they consider stochastic coupling of an electron to a single phonon mode, to model the electron-phonon interaction in the weak-coupling limit. The model that we describe here should be related to theirs, at least from a conceptual point of view.

From the computational viewpoint, the memory effects associated with the non-Markovian dynamics are eliminated in the new formalism by introducing new degrees of freedom associated with the fictitious modes. Whether or not the new method would increase or decrease the speed of simulations would depend on the number of modes introduced and their coupling strengths. Independent of the speed issue, however, the simple quantum MCWF formalism, which uses nonunitary (Schrödinger-like) time evolution and instantenous quantum jumps, would be simpler to deal with numerically as it is based on a first-order (in time) differential equation.

In summary, we have presented a method to extend the quantum MCWF formalism to the analysis of non-Markovian system-reservoir interactions. Given a non-Markovian dissipative *electron* system, the underlying idea is to find the *effective-polaron* (or polariton) system that has Markovian dynamics, simulate the dynamics of the polaron using the MCWF method described by Eqs. (2) and (3), and eventually perform a trace over the *phonon* modes to obtain the relevant *electronic* quantities. Possible extensions of the proposed method would include the treatment of the dissipative electron-phonon interactions (using the actual second-quantized interaction Hamiltonian [9]) and the harmonic-oscillator–reservoir coupling without the RWA. As discussed, the method should find applications in quantum optics and mesoscopic physics.

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