Stochastic simulation of dissipation and non-Markovian effects in open quantum systems

Denis Lacroix
GANIL, CEA, and IN2P3, Boîte Postale 5027, 14076 Caen Cedex, France

(Received 19 December 2007; revised manuscript received 14 February 2008; published 29 April 2008)

The exact dynamics of a system coupled to an environment can be described by an integro-differential stochastic equation for the reduced density. The influence of the environment is incorporated through a mean field which is both stochastic and nonlocal in time and where the standard two-time correlation functions of the environment appear naturally. Since no approximation is made, the presented theory incorporates exactly dissipative and non-Markovian effects. Applications to the spin-boson model coupled to a heat bath with various coupling regimes and temperature show that the presented stochastic theory can be a valuable tool to simulate exactly the dynamics of open quantum systems. Links with the stochastic Schrödinger equation method and possible extensions to "imaginary time" propagation are discussed.

DOI: 10.1103/PhysRevE.77.041126 PACS number(s): 05.70.Ln, 03.65.Yz, 05.10.Gg

I. INTRODUCTION

Numerous concepts in our understanding of quantum mechanics have emerged from the understanding and description of a system coupled to an environment: measurement, decoherence, appearance of classical world, irreversible processes, dissipation, and so on. All these phenomena, which are often encompassed in the "theory of open quantum systems," bridge different fields of physics and chemistry [1–3]. During the past decade, important advances have been made in the approximate and exact descriptions of system embedded in an environment using stochastic methods. Recently the description of open quantum systems by the stochastic Schrödinger equation (SSE) has received much attention [3–5]. Nowadays, Monte Carlo wave-function techniques are extensively used to treat master equations in the weak coupling and/or Markovian limit [3,4,6–12].

Great theoretical effort is actually devoted to the introduction of non-Markovian effects. Among the most recent approaches, one can mention either deterministic approaches like the projection operator techniques [13,14] or stochastic methods like quantum state diffusion [15–18] where non-Markovian effects are accounted for through nonlocal memory kernels and state vectors evolve according to integro-differential stochastic equations. In some cases, these methods have been shown to be exact [5,19].

Recently, alternative exact methods [20,21] have been developed to treat the system+environment problem that avoid evaluation of nonlocal memory kernels, although non-Markovian effects are accounted for exactly. However, up to now, only a few applications of these exact techniques exist [20–25]. In all cases, accurate description of the short-time dynamics is obtained but long-time evolution can hardly be described due to the large increase of statistical errors with time. Although the possibility of simulating exactly the dissipative dynamics of open quantum systems is already an important step, description of long-time evolution is highly desirable to make the techniques more powerful and versatile.

II. EXACT STOCHASTIC EQUATION FOR THE REDUCED SYSTEM DENSITY

A. Introduction

In the present work, starting from the exact stochastic formulation of Ref. [21] and projecting out the effect of the environment, an equation of motion for the reduced system dynamics is obtained where the environment effect is incorporated through a stochastic mean field which turns out to be nonlocal in time. Advantages of this stochastic theory for the description of long-time evolution of open quantum systems are underlined. We consider here a system (S) +environment (E) described by a Hamiltonian

$$H = h_S + h_E + h_I, \tag{1}$$

where h_S and h_E denote the system and environment Hamiltonians, respectively, while h_I is responsible for the coupling. Here we assume that the interaction is written

$$h_I = \mathbf{Q} \otimes \mathbf{B}, \tag{2}$$

where $\mathbf{Q} \equiv f(\{Q_i\}_{i=1,n_S})$ and $\mathbf{B} \equiv g(\{B_i\}_{i=1,n_B})$ correspond to functions of two sets of operators of the system and environment, respectively. In particular, this definition includes nonlinear couplings. For the sake of simplicity, we assume an initial separable density $D(t_0)=\rho_S(t_0)\otimes\rho_B(t_0)$. As will be discussed below, this assumption could be relaxed. The exact evolution of the system is described by the Liouville–von Neumann equation $i\hbar\dot{D}=[H,D]$. Due to the coupling, the simple separable structure of the initial condition is not preserved in time. It has, however, been realized recently in several works using either the SSE or path integral technique that the exact density of the total system $D(t)$ can be obtained as an average over simple separable densities, i.e., $D(t)=\rho_S(t)\otimes\rho_B(t)$. In its simplest version, the stochastic process takes the form [21]

$$\begin{aligned} d\rho_S &= \frac{dt}{i\hbar}[h_S,\rho_S] + d\xi_S \mathbf{Q}\rho_S + d\lambda_S \rho_S \mathbf{Q}, \\ d\rho_E &= \frac{dt}{i\hbar}[h_E,\rho_E] + d\xi_E \mathbf{B}\rho_E + d\lambda_E \rho_E \mathbf{B}, \end{aligned} \tag{3}$$

where the Ito convention for stochastic calculations is used [26]. $d\xi_{S/E}$ and $d\lambda_{S/E}$ denote Markovian Gaussian stochastic variables with zero means and variances,

$$\overline{d\xi_S d\xi_E} = \frac{dt}{i\hbar}, \quad \overline{d\lambda_S d\lambda_E} = -\frac{dt}{i\hbar}, \tag{4}$$

$$\overline{d\xi_S d\lambda_E} = \overline{d\lambda_S d\xi_E} = 0. \quad (5)$$

The average over stochastic paths described by Eqs. (3) matches the exact evolution. Indeed, assuming that at time t the total density is written $D(t)=\rho_S(t)\otimes\rho_B(t)$, the average evolution over a small time step dt is given by

$$\overline{dD} = \overline{d\rho_S \otimes \rho_E} + \overline{\rho_S \otimes d\rho_E} + \overline{d\rho_S \otimes d\rho_E}. \quad (6)$$

Using statistical properties of stochastic variables [Eqs. (4) and (5)], we obtain

$$\overline{d\rho_S \otimes \rho_E} + \overline{\rho_S \otimes d\rho_E} = \frac{dt}{i\hbar}[h_S + h_E, \rho_S \otimes \rho_E], \quad (7)$$

$$\overline{d\rho_S \otimes d\rho_E} = \frac{dt}{i\hbar}[\mathbf{Q}\otimes\mathbf{B}, \rho_S \otimes \rho_E]. \quad (8)$$

Therefore, the last term simulates the interaction Hamiltonian exactly and the average evolution of the total density over a time step dt reads

$$\overline{dD} = \frac{dt}{i\hbar}[H, D], \quad (9)$$

which is nothing but the exact evolution. Here, the exactness of the method is proved assuming that the density $D(t)$ is a single separable density. In practice, the total density at time t is already an average over separable densities obtained along each stochastic path, i.e., $\overline{D(t)}=\rho_S(t)\otimes\rho_E(t)$. Since Eq. (9) is valid for any density written as $\rho_S(t)\otimes\rho_E(t)$, by summing individual contributions, we deduce that the evolution of the total density obtained by averaging over different paths is given by $i\hbar d\bar{D}=dt[H,\overline{D(t)}]$ which is valid at any time and corresponds to the exact system+environment dynamics.

B. Stochastic mean-field dynamics

Here, a slightly modified version of the stochastic process is used. It incorporates part of the system-environment coupling using a "mean-field" approximation in the deterministic evolution. Following Ref. [21], we consider the coupled stochastic evolutions, called hereafter the stochastic mean field (SMF):

$$\begin{aligned} d\rho_S &= \frac{dt}{i\hbar}[h_S + \langle\mathbf{B}(t)\rangle_E\mathbf{Q}, \rho_S] + d\xi_S[\mathbf{Q} - \langle\mathbf{Q}(t)\rangle_S]\rho_S \\ &\quad + d\lambda_S\rho_S[\mathbf{Q} - \langle\mathbf{Q}(t)\rangle_S], \\ d\rho_E &= \frac{dt}{i\hbar}[h_E + \langle\mathbf{Q}(t)\rangle_S\mathbf{B}, \rho_E] + d\xi_E[\mathbf{B} - \langle\mathbf{B}(t)\rangle_E]\rho_E \\ &\quad + d\lambda_E\rho_E[\mathbf{B} - \langle\mathbf{B}(t)\rangle_E], \end{aligned} \quad (10)$$

where

$$\langle\mathbf{Q}(t)\rangle_S \equiv \mathrm{Tr}[\mathbf{Q}\rho_S(t)], \quad \langle\mathbf{B}(t)\rangle_E \equiv \mathrm{Tr}[\mathbf{B}\rho_E(t)]. \quad (11)$$

The SMF version also provides an exact reformulation of the system+environment problem. Indeed, the two terms in Eqs. (7) and (8) now read

$$\overline{d\rho_S \otimes \rho_E} + \overline{\rho_S \otimes d\rho_E} = \frac{dt}{i\hbar}[h_S + \langle\mathbf{B}(t)\rangle_E\mathbf{Q}, \rho_S \otimes \rho_E] + \frac{dt}{i\hbar}[h_E + \langle\mathbf{Q}(t)\rangle_S\mathbf{B}, \rho_S \otimes \rho_E],$$

$$\overline{d\rho_S \otimes d\rho_E} = \frac{dt}{i\hbar}[[\mathbf{Q} - \langle\mathbf{Q}(t)\rangle_S] \otimes [\mathbf{B} - \langle\mathbf{B}(t)\rangle_E], \rho_S \otimes \rho_E],$$

and properly recombine to recover Eq. (9).

1. Properties of the SMF theory

Equations (10) have several advantages compared to the simple version [Eqs. (3)]. First, this stochastic process automatically ensures that $\mathrm{Tr}(\rho_E)=\mathrm{Tr}(\rho_S)=1$ along the stochastic path. In addition, the inclusion of a mean-field term in the deterministic part will always reduce the statistical dispersion compared to the simple stochastic process given by Eqs. (3). This reduction could be significant if quantum fluctuations of the coupling operators $\mathbf{Q}$ and $\mathbf{B}$ remain small along each path [21,27]. Indeed, at any time, a measure of the statistical fluctuations is given by

$$\begin{aligned} \lambda_{\mathrm{stat}} &= \overline{\mathrm{Tr}\{[D^\dagger(t) - \overline{D^\dagger(t)}][D(t) - \overline{D(t)}]\}} \\ &= \overline{\mathrm{Tr}[D^\dagger D(t)]} - \mathrm{Tr}[\overline{D(t)}^2]. \end{aligned} \quad (12)$$

Starting from the total density associated with a pure state, the evolution of λ_{stat} over a small time step is directly connected to the average quantum fluctuations of $\mathbf{Q}$ and $\mathbf{B}$, i.e.,

$$d\lambda_{\mathrm{stat}} = \frac{2dt}{\hbar}[\overline{(\langle\mathbf{Q}^2\rangle_S - \overline{\langle\mathbf{Q}\rangle_S}^2)} + \overline{(\langle\mathbf{B}^2\rangle_S - \overline{\langle\mathbf{B}\rangle_S}^2)}], \quad (13)$$

where we have assumed implicitly that all second moments except those given in Eqs. (4) and (5) cancel out. For comparison, the growth of statistical fluctuations associated with the stochastic process without the mean field [Eqs. (3)] reads

$$d\lambda_{\mathrm{stat}} = \frac{2dt}{\hbar}(\overline{\langle\mathbf{Q}^2\rangle_S} + \overline{\langle\mathbf{B}^2\rangle_E}). \quad (14)$$

Equation (13) illustrates that the number of trajectories required to simulate the system dynamics will depend on the importance of the quantum fluctuations of the coupling operators along each path. In addition, a comparison between Eqs. (13) and (14) illustrates that the introduction of the mean field will always improve the numerical accuracy.

C. Reduced system evolution

In Eq. (10), the influence of the environment on the system enters only through $\langle\mathbf{B}(t)\rangle_E$. One expects in general to simplify the treatment by directly considering this observable evolution instead of the complete ρ_E evolution. To express $\langle\mathbf{B}(t)\rangle_E$, we introduce the environment evolution operator

$$U_E(t,t') \equiv \exp\left(\frac{1}{i\hbar}h_E(t-t')\right). \quad (15)$$

Defining the new set of stochastic variables dv_E and du_E through $d\xi_E=dv_E-idu_E$ and $d\lambda_E=dv_E+idu_E$, the evolution of $\rho_E(t)$ can be integrated as

$$\rho_E(t) = U_E(t,t_0)\rho_E(t_0)U_E^\dagger(t,t_0) + \int_0^t \frac{ds}{i\hbar}\langle \mathbf{Q}(s)\rangle_S U_E(t,s) \times[\mathbf{B},\rho_E(s)]U_E^\dagger(t,s) + \int_0^t dv_E(s)U_E(t,s) \times[\mathbf{B}-\langle \mathbf{B}(s)\rangle_E,\rho_E(s)]_+U_E^\dagger(t,s) - i\int_0^t du_E(s)U_E(t,s) \times[\mathbf{B}-\langle \mathbf{B}(s)\rangle_E,\rho_E(s)]U_E^\dagger(t,s). \quad (16)$$

Introducing also the new variables du_S and dv_S defined as $d\xi_S=du_S-idv_S$ and $d\lambda_S=du_S+idv_S$, the stochastic equation on the reduced density reads

$$d\rho_S = \frac{dt}{i\hbar}[\mathcal{H}_S(t),\rho_S] + du_S[\mathbf{Q}-\langle \mathbf{Q}(t)\rangle_S,\rho_S]_+ - idv_S[\mathbf{Q}-\langle \mathbf{Q}(t)\rangle_S,\rho_S] \quad (17)$$

with $\mathcal{H}_S(t)\equiv h_S+\langle \mathbf{B}(t)\rangle_E\mathbf{Q}$ and where the source term $\langle \mathbf{B}(t)\rangle_E$ takes the exact form

$$\langle \mathbf{B}(t)\rangle_E = \mathrm{Tr}[\mathbf{B}^I(t-t_0)\rho_E(t_0)] - \frac{1}{\hbar}\int_0^t D(t,s)\langle \mathbf{Q}(s)\rangle_S ds - \int_0^t D(t,s)du_E(s) + \int_0^t D_1(t,s)dv_E(s). \quad (18)$$

Here, $\mathbf{B}^I(t-s)\equiv U_E^\dagger(t,s)\mathbf{B}U_E(t,s)$ while D and D_1 are defined by

$$D(t,s) \equiv i\langle[\mathbf{B},\mathbf{B}^I(t-s)]\rangle_E, \quad (19)$$

$$D_1(t,s) \equiv \langle[\mathbf{B}-\langle \mathbf{B}(s)\rangle_E,\mathbf{B}^I(t-s)]_+\rangle_E, \quad (20)$$

where the environment expectation values are taken at time s, i.e., $\langle\cdots\rangle_S\equiv\mathrm{Tr}[\cdots\rho_E(s)]$. The two coupled equations (17) and (18) provide an exact reformulation of the system evolution if $du_{S/E}$ and $dv_{S/E}$ satisfy

$$\overline{du_S du_E} = \overline{dv_S dv_E} = \frac{dt}{2\hbar},$$

$$\overline{du_S dv_E} = \overline{dv_S du_E} = 0. \quad (21)$$

In the following, we simply assume that the first term in Eq. (18) cancels out. Substituting Eq. (18) into Eq. (17), we finally obtain an integro-differential stochastic equation for the exact system evolution where the environment effect has been incorporated through the two memory functions (19) and (20). The interesting aspect of replacing Eq. (10) by Eqs. (17) and (18) is that, in many physical situations, one can generally take advantage of specific commutation and anticommutation properties of $\mathbf{B}$ as well as flexibility in the noise to obtain an explicit form of the memory functions.

III. APPLICATION TO A SYSTEM COUPLED TO A HEAT BATH

The method is illustrated for systems coupled to an environment of harmonic oscillators initially at thermal equilibrium and it shows that the present stochastic theory can be a valuable tool to simulate exactly open quantum systems. We take

$$h_E = \sum_n \left(\frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 x_n^2\right) \quad (22)$$

and $\mathbf{B}\equiv-\Sigma_n\kappa_n x_n$ [3]. The statistical properties of the stochastic variables $du_{S/E}$ and $dv_{S/E}$ specified above do not uniquely define the Wiener process. A simple prescription is to further assume

$$\overline{du_S du_S} = \overline{du_E du_E} = \overline{dv_S dv_S} = \overline{dv_E dv_E} = 0, \quad \overline{du_S dv_S} = \overline{du_E dv_E} = 0. \quad (23)$$

There are several advantages to this choice. First, stochastic calculations are greatly simplified. For instance, using standard techniques for a system coupled to a heat bath [28,29] and Ito stochastic rules, we can show that D and D_1 depend only on the time difference $\tau=(t-s)$ and are identified with the standard correlation functions [3] (see the Appendix)

$$D(\tau) = 2\hbar\int_0^{+\infty} d\omega\, J(\omega)\sin(\omega\tau), \quad (24)$$

$$D_1(\tau) = 2\hbar\int_0^{+\infty} d\omega\, J(\omega)\coth(\hbar\omega/2k_BT)\cos(\omega\tau), \quad (25)$$

where

$$J(\omega) \equiv \sum_n \frac{\kappa_n^2}{2m_n\omega_n}\delta(\omega-\omega_n) \quad (26)$$

denotes the spectral density. No approximation are made to obtain the above equations; therefore the average over different stochastic paths matches the exact evolution of the system, including all non-Markovian effects.

A. Equivalent stochastic Schrödinger equation formulation

Several works, based on the influence functional method [5,19,30] have led to similar stochastic equations for the reduced density. For instance, the authors of Refs. [19,30] use an evolution of $\langle \mathbf{B}(t)\rangle_E$ where the second term in Eq. (18) is absent. As demonstrated below, this term is of crucial importance for applications. In Ref. [5] and in Refs. [21–23] a stochastic formulation of the exact system+environment is given in terms of the stochastic Schrödinger equation technique. Thanks to the additional stochastic rules (23), Eq. (17) also has its SSE counterpart, where the system densities are replaced by $\rho_S=|\phi_1\rangle\langle\phi_2|$ and wave functions evolve according to

$$d|\phi_1\rangle = \left(\frac{dt}{i\hbar}\mathcal{H}_S(t) + d\xi_S[\mathbf{Q}-\langle \mathbf{Q}(t)\rangle_S]\right)|\phi_1\rangle, \quad d\langle\phi_2| = \langle\phi_2|\left(-\frac{dt}{i\hbar}\mathcal{H}_S(t) + d\lambda_S[\mathbf{Q}-\langle \mathbf{Q}(t)\rangle_S]\right), \quad (27)$$

where the bath effect is again incorporated through the mean-field kernel.

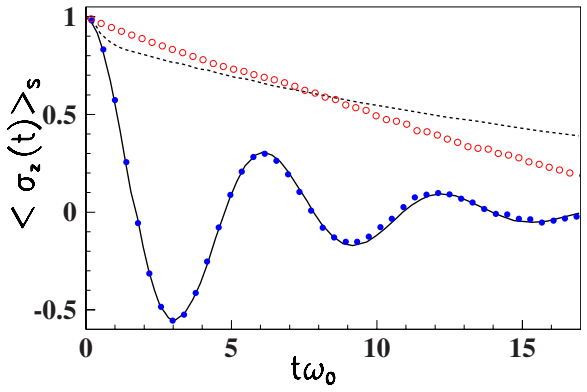

FIG. 1. (Color online) Evolution of $\langle \sigma_z(t) \rangle_S$ [assuming $\langle \sigma_z(0) \rangle_S = 1$] as a function of time obtained through the average of paths simulated with Eq. (17) with the Markovian process described by Eqs. (21) and (23) and memory functions given by Eqs. (24) and (25). We assume that $J(\omega) = \eta\omega\Delta_c^2/(\Delta_c^2+\omega^2)$. Two sets of parameters are used. In both cases, $\Delta_c = 5\omega_0$, $k_BT = 2\hbar\omega_0$, and $\hbar\varepsilon = 0$. The filled and open circles correspond, respectively, to $\pi\eta = 0.2\hbar\omega_0$ and $4\hbar\omega_0$ and are compared, respectively, with the solid and dashed lines obtained with the same set of parameters in Fig. 2 of Ref. [30]. Results are obtained with 2×10^4 trajectories.

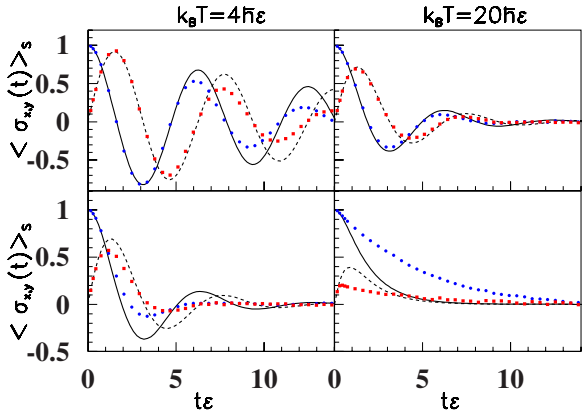

FIG. 2. (Color online) Average evolution of $\langle \sigma_x(t) \rangle_S$ (filled circles) and $\langle \sigma_y(t) \rangle_S$ (filled squares) as a function of time. The initial condition corresponds to $\langle \sigma_x(0) \rangle_S = 1$. In all cases, $\hbar\omega_0 = 0$ and $\Delta_c = 10\varepsilon$. $k_BT = 4\hbar\varepsilon$ and $20\hbar\varepsilon$ are used, respectively, for calculations presented in the left and right columns. In both cases, the upper panels present results for weak coupling ($\pi\eta = 0.2\hbar\varepsilon$) while in the lower panels a stronger coupling is considered ($\pi\eta = 1.0\hbar\varepsilon$). Simulations have been performed with 4×10^4 trajectories. For all cases, dynamical evolutions of the x and y spin components obtained with the TCL2 method [3,13] are displayed by solid and dashed lines, respectively.

B. Application to the spin-boson model

We illustrate the proposed technique using the spin-boson model. This model can be regarded as one of the simplest quantum open system coupled to a heat bath [31] that could not be integrated exactly. In addition, it has often been used as a benchmark for theories of open quantum systems [1,5,14,16,19,31,32]. The system and coupling Hamiltonians are respectively chosen as

$$h_S = \hbar\omega_0\sigma_x + \hbar\varepsilon\sigma_z, \quad h_I = \sigma_x \otimes \mathbf{B},$$

where the $\{\sigma_i\}_{i=x,y,z}$ are the standard Pauli matrices. In the spin-boson model, the numerical solution of Eq. (17) for the system density, is equivalent to solving three nonlinear coupled equations for the $\langle \sigma_i \rangle_S$. Figure 1 shows examples of the dynamical evolution of $\langle \sigma_z(t) \rangle_S$ obtained using Eq. (17) and averaging over stochastic trajectories both for weak (filled circles) and strong (open circles) coupling. Results are compared with the hierarchical approach proposed in Ref. [30]. This deterministic approach provides an alternative *a priori* exact formulation of open quantum system dynamics and was originally motivated by numerical difficulties encountered in the stochastic theory proposed in Ref. [19]. Such difficulties do not occur in the present simulation and many fewer stochastic trajectories seem to be needed to accurately describe the dynamical evolution. Only 2×10^4 trajectories have been used to obtained Fig. 1, leading to statistical errors close to zero (for comparison, see the discussion in [24]). The computer time for the two figures was less than an hour for the weak-coupling case up to several hours for the strong-coupling case on a standard personal computer. The difference in computing time comes from the fact that a smaller numerical time step should be used as the coupling strength increases to achieve good numerical accuracy, the main difficulty being to properly evaluate the time integrals in Eq. (18). Denoting the time step by Δt, $\Delta t\,\omega_0 = 1.2\times10^{-3}$ and 2.2×10^{-4} have been used for weak and strong coupling, respectively.

In the weak-coupling case, the results of our stochastic scheme displayed in Fig. 1 (filled circles) perfectly match the result of Ref. [30] (solid line). In contrast to Ref. [24], statistical errors remain small even for long-time evolution. The difference in numerical accuracy can be assigned to the second term in Eq. (18) which turns out to be crucial for numerical implementation. Stochastic simulations for strong-coupling parameters (open circles) slightly differ from the results obtained with the hierarchical approach in Ref. [30]. The numerical convergence of the stochastic simulation presented in Fig. 1 has been checked. Therefore, the difference might be due to the fact that the numerical accuracy depends on the truncation scheme used in the hierarchy, even though the method of Ref. [30] is exact.

C. Comparison with the time-convolutionless method

The possibility of simulating exactly the system dynamics can also serve as a benchmark for other methods. For instance, we compared the exact stochastic scheme with the approximate time-convolutionless (TCL) projection operator method of Refs. [3,13]. Figure 2 presents the results of the exact stochastic simulation compared with the TCL2 method applied to the spin-boson model in Ref. [13]. Here, TCL2 (or more generally TCLx) refers to the TCL technique with a second order ("x" order) truncation in terms of the interaction **B**. In this figure different cases corresponding to either the low- or high-temperature regime and weak or strong coupling are presented. We see that the best agreement is obtained in the weak-coupling and high-temperature case. In

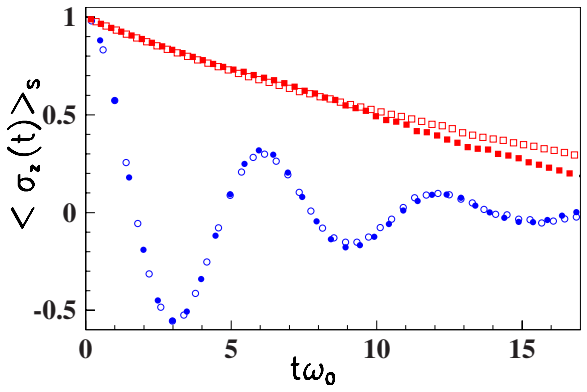

FIG. 3. (Color online) Results obtained in the weak- and strong-coupling cases with the exact stochastic simulation using complex noises and non-Hermitian (filled circles) are compared with the approximate simulation (open circles) using real noise and Hermitian densities along each path. In this figure, the values of the parameters are the same as in Fig. 1.

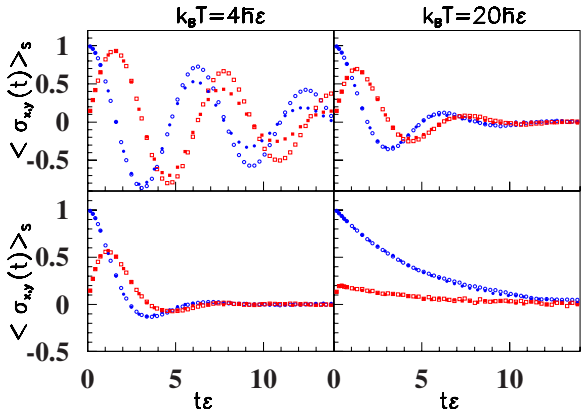

FIG. 4. (Color online) Average evolution of $\langle \sigma_x(t) \rangle_S$ (filled circles) and $\langle \sigma_y(t) \rangle_S$ (filled squares) as a function of time obtained with the exact stochastic scheme using the same sets of parameters as in Fig. 2. In each case, dynamical evolutions of the x and y spin components obtained with the approximate stochastic simulation using real noise are displayed with open circles and open squares, respectively.

general, the TCL2 method compares well with the exact simulation if the coupling is rather small. As the coupling increases (lower panels of Fig. 2), the difference between the TCL technique and the exact method increases. Note that the TCL method seems to systematically underestimate the damping. Note finally that the use of higher order truncation in the interaction, for instance TCL4 instead of TCL2, does not improve the comparison.

D. Discussion of approximate system evolution obtained with real noise and Hermitian system densities in stochastic evolution

The applications presented above use specific constraints on the Markovian process given by Eqs. (23). This prescription greatly simplifies the stochastic calculus. For instance, simple exact expressions have been obtained for $D(t,s)$ and $D_1(t,s)$ when the system is coupled to a heat bath of harmonic oscillators [Eqs. (24) and (25)]. The main consequence of Eqs. (23) is that $du_{S/E}$ and $dv_{S/E}$ should be *complex* stochastic variables leading to non-Hermitian densities along the paths. As illustrated above, such a stochastic process could be used to simulate exactly the reduced density evolution. The main disadvantage of non-Hermitian densities is, however, that system observables could hardly be interpreted. We discuss here the possibility of performing stochastic evolution of reduced Hermitian densities.

Relaxing the constraints given by Eqs. (23) authorizes us to choose $du_{S/E}$ and $dv_{S/E}$ as real stochastic variables, which automatically ensures that $\rho_S(t)$ and $\rho_E(t)$ remain Hermitian. This alternative has, however, two major drawbacks. First, one can no longer have an equivalent SSE picture. Second, while $D(t,s)$ still identifies with Eq. (24), no simple exact expression can be worked out for $D_1(t,s)$. However, since this kernel is a functional of $\rho_E(s)$, a hierarchy of more and more accurate approximations could be obtained by successive replacements of $\rho_E(s)$ into Eq. (19) by its integral expression, Eq. (16). In the present work, we concentrate on the simplest case where $\rho_E(s)$ is replaced by $\rho_E(s) \simeq U_E(t,t_0)\rho_E(t_0)U_E^\dagger(t,t_0)$ in the time integral of the memory kernel. In this limit, $D_1(s,t)$ also reduces to Eq. (25). Because of this approximation, the stochastic process is no longer exact. Figure 3 presents a comparison of the exact stochastic simulation obtain with complex noise (filled circles) and the approximate case with real noise (open circles). The parameters of the spin-boson model are the same as in Fig. 1. This figure shows that the approximate scheme with real noise is very close to the exact simulation even in the strong-coupling limit. In the latter case, only at very large time do the two simulations start to deviate slightly from one another. For completeness, approximate stochastic simulations obtained for the cases presented in Fig. 2 are compared to the exact scheme in Fig. 4. We see that, except for the weak-coupling and low-temperature case, the approximate simulation is very close to the exact result. It is worth mentioning that the approximate simulation presented here uses the simplest prescription for $D_1(s,t)$. Therefore, improved description could *a priori* be obtained using better approximations of $D_1(s,t)$ with the method described above. This example is very encouraging and provides a method to simulate open systems with a stochastic process that preserves the Hermitian properties of the system density.

IV. CONCLUSION

The results obtained with the stochastic theory for the spin-boson model are very encouraging. The theory turns out to be accurate to simulate not only short- but also long-time dynamics and does not seem to suffer from the numerical instability quoted in Ref. [24]. It is worth mentioning that optimization techniques proposed in Ref. [21], which are not used here, can be implemented to further reduce the number of stochastic paths. Besides the numerical aspects, a link with classical dissipation dynamics could be easily made, as in Ref. [5].

Our stochastic approach could be generalized to any initial conditions that can be written as a mixture of separable

densities, i.e., $D(t_0)=\Sigma_n W_n D^{(n)}(t_0)$ with $D^n=\rho_S^n\otimes\rho_E^n$ where the W_n are complex coefficients. Then the complete exact dynamics is recovered by both averaging over trajectories starting from each $D^{(n)}(t=0)$ individually and averaging over the initial conditions. The theory is also not restricted to real time evolution. Statistical properties of the system +environment can be studied by considering imaginary time propagation, i.e., $idt/\hbar\rightarrow\beta$. Imaginary time propagation leads naturally to densities written as a mixture of separable densities and can then serve as initial conditions for real time evolution. By combining both imaginary and real time propagation, general physical problems similar to those depicted in Ref. [5] can be addressed. The main limitation of the technique is clearly the choice of coupling operator **B**, which should give simple memory functions [Eqs. (19) and (20)]. It is, however, worth mentioning that most of the coupling operators used in the context of open quantum systems are already in this category [1,3,9,12]. We believe that the stochastic theory presented in this paper can be a valuable tool to access exactly the dynamics of more complex open quantum systems. We presented here specific applications to systems coupled to a heat bath. The approach can, however, be applied to various types of environments and couplings, which might be of great interest in addressing dissipation, measurement, and/or decoherence problems in quantum systems.

ACKNOWLEDGMENTS

The author thanks G. Adamian, N. Antonenko, S. Ayik, and B. Yilmaz for valuable discussions and C. Simenel and G. Hupin for careful reading of the manuscript.

APPENDIX: PROOF OF EQ. (18) FOR A HEAT BATH OF HARMONIC OSCILLATORS

We give here a proof of Eq. (18) where D and D_1 are identified with Eqs. (24) and (25). The environment is assumed to be a set of harmonic oscillators, labeled by n, associated with creation and annihilation $(a_n^\dagger,a_n)$, i.e.,

$$H=\sum_n \hbar\omega_n\left(a_n^\dagger a_n+\frac{1}{2}\right). \tag{A1}$$

If thermal equilibrium is initially assumed, the environment density is written as a product of densities of each oscillator, $\rho_E=\Pi_n\rho_n$, where each density can be written as Gaussian operators (see, for instance, [12]) determined by the first and second moments of $(a_n^\dagger,a_n)$. The time evolution of the environment is given by Eq. (10) where $\mathbf{B}\equiv-\Sigma_n\kappa_n x_n$ and where the fluctuating variables satisfy [according to Eq. (23)]

$$\overline{d\lambda_E d\lambda_E}=\overline{d\xi_E d\xi_E}=\overline{d\lambda_E d\xi_E}=0. \tag{A2}$$

The above prescription and the specific form of **B** induce important simplifications listed below. First, the initial product form of the environment density is preserved along the stochastic paths where each oscillator density satisfies $\mathrm{Tr}(\rho_n)=1$ and where for each pair of densities $d(\rho_n\rho_m)=\rho_n d\rho_m+d\rho_n\rho_m$. Second, due to the linear coupling operator, the Gaussian nature of the initial densities is also preserved along the paths. Therefore, we can equivalently solve the density equation of motion or follow the first and second moments of each $(a_n^\dagger,a_n)$ in time. Here we consider the second strategy.

From the ρ_E evolution, the equation of motion of each pair $\langle a_n^\dagger\rangle=\mathrm{Tr}(\rho_E a_n^\dagger)$ and $\langle a_n\rangle=\mathrm{Tr}(\rho_E a_n)$ reads

$$\begin{aligned}
d\langle a_n\rangle &= -i\omega_n dt\langle a_n\rangle+\frac{dt}{i\hbar}c_n\langle\mathbf{Q}\rangle+c_n\{d\xi_E[\sigma_{+-}^{(n)}(t)+\sigma_{--}^{(n)}(t)+1]\\
&\quad+d\lambda_E[\sigma_{+-}^{(n)}(t)+\sigma_{--}^{(n)}(t)]\},\\
d\langle a_n^\dagger\rangle &= +i\omega_n dt\langle a_n^\dagger\rangle-\frac{dt}{i\hbar}c_n\langle\mathbf{Q}\rangle+c_n\{d\xi_E[\sigma_{+-}^{(n)}(t)+\sigma_{++}^{(n)}(t)]\\
&\quad+d\lambda_E[\sigma_{+-}^{(n)}(t)+\sigma_{++}^{(n)}(t)+1]\},
\end{aligned} \tag{A3}$$

where we have introduced the notation $c_n\equiv-\kappa_n/\sqrt{2\eta_n}$ and $\eta_n=m_n\omega_n/\hbar$. Here, $\sigma_{++}^{(n)}$, $\sigma_{--}^{(n)}$, and $\sigma_{+-}^{(n)}$ denote the second moments of the $a_n^\dagger,a_n$ operators:

$$\begin{aligned}
\sigma_{+-}^{(n)} &\equiv \langle a_n^\dagger a_n\rangle-\langle a_n\rangle\langle a_n^\dagger\rangle=\sigma_{-+}^{(n)}-1,\\
\sigma_{--}^{(n)} &\equiv \langle a_n a_n\rangle-\langle a_n\rangle\langle a_n\rangle,\\
\sigma_{++}^{(n)} &\equiv \langle a_n^\dagger a_n^\dagger\rangle-\langle a_n^\dagger\rangle\langle a_n^\dagger\rangle.
\end{aligned}$$

According to the stochastic environment dynamics, we can show that these moments simply evolve as

$$\begin{aligned}
d\sigma_{--}^{(n)} &= -2i\omega_n dt\sigma_{--}^{(n)},\\
d\sigma_{++}^{(n)} &= +2i\omega_n dt\sigma_{++}^{(n)},\\
d\sigma_{+-}^{(n)} &= 0.
\end{aligned} \tag{A4}$$

Since we assume that each oscillator is initially at thermal equilibrium, we deduce that the second moments are constant in time with $\sigma_{--}^{(n)}(t)=\sigma_{++}^{(n)}(t)=0$, while $\sigma_{-+}^{(n)}(t)=\sigma_{+-}^{(n)}+1=[\bar{N}(\omega_n)+1]$. Here, we have introduced the standard function [12] $[2\bar{N}(\omega_n)+1]=\coth[\hbar\omega_n/(2k_BT)]$. Substituting in Eqs. (A3) and (A4) and using standard integration techniques [3] we finally obtain

$$\begin{aligned}
\langle a_n(t)\rangle &= e^{-i\omega_n t}\langle a_n(0)\rangle+\frac{c_n}{i\hbar}\int_0^t e^{-i\omega_n(t-s)}\langle\mathbf{Q}(s)\rangle ds\\
&\quad+c_n\int_0^t e^{-i\omega_n(t-s)}\{d\xi_E(s)[\bar{N}(\omega_n)+1]+d\lambda_E(s)\bar{N}(\omega_n)\},\\
\langle a_n^\dagger(t)\rangle &= e^{+i\omega_n t}\langle a_n^\dagger(0)\rangle-\frac{c_n}{i\hbar}\int_0^t e^{+i\omega_n(t-s)}\langle\mathbf{Q}(s)\rangle ds\\
&\quad+c_n\int_0^t e^{+i\omega_n(t-s)}\{d\xi_E(s)\bar{N}(\omega_n)+d\lambda_E(s)[\bar{N}(\omega_n)+1]\}.
\end{aligned} \tag{A5}$$

Accordingly, each position operator entering in $\langle\mathbf{B}(t)\rangle$ reads

$$\langle x_n(t)\rangle = \frac{1}{\sqrt{2\eta_n}}[\langle a_n(0)\rangle e^{-i\omega_n t} + \langle a_n^\dagger(0)\rangle e^{+i\omega_n t}] + \frac{\kappa_n}{\hbar\eta_n}\int_0^t \sin[\omega_n(t-s)]\langle \mathbf{Q}(s)\rangle ds,$$

$$-\frac{\kappa_n}{2\eta_n}\int_0^t \{\cos[\omega_n(t-s)][2\bar{N}(\omega_n)+1][d\xi_E(s)+d\lambda_E(s)] - i\sin[\omega_n(t-s)][d\xi_E(s)-d\lambda_E(s)]\}.$$

Assuming the initial conditions $\langle a_n(0)\rangle = \langle a_n^\dagger(0)\rangle = 0$, substituting in the expression of $\langle \mathbf{B}(t)\rangle = -\Sigma_n \kappa_n \langle x_n(t)\rangle$, and introducing the spectral density [Eq. (26)], we finally recover Eq. (18) where D and D_1 are, respectively, given by Eqs. (24) and (25).

[1] U. Weiss, *Quantum Dissipative Systems*, 2nd ed. (World Scientific, Singapore, 1999).
[2] E. Joos, H. Zeh, C. Kiefer, D. Giulini, J. Kupsch, and I.-O. Stamatescu, *Decoherence and the Appearance of a Classical World in Quantum Theory* (Springer, New York, 2003).
[3] H. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
[4] M. B. Plenio and P. L. Knight, Rev. Mod. Phys. **70**, 101 (1998).
[5] J. T. Stockburger and H. Grabert, Phys. Rev. Lett. **88**, 170407 (2002).
[6] J. Dalibard, Y. Castin, and K. Mølmer, Phys. Rev. Lett. **68**, 580 (1992).
[7] R. Dum, P. Zoller, and H. Ritsch, Phys. Rev. A **45**, 4879 (1992).
[8] N. Gisin and I. Percival, J. Math. Phys. **A25**, 5677 (1992).
[9] H. Carmichael, *An Open Systems Approach to Quantum Optics*, Lecture Notes in Physics Vol. 18 (Springer-Verlag, Berlin, 1993).
[10] Y. Castin and K. Mølmer, Phys. Rev. A **54**, 5275 (1996).
[11] M. Rigo and N. Gisin, Quantum Semiclassic. Opt. **8**, 255 (1996).
[12] W. Gardiner and P. Zoller, *Quantum Noise* (Springer-Verlag, Berlin, 2000).
[13] H.-P. Breuer, B. Kappler, and F. Petruccione, Phys. Rev. A **59**, 1633 (1999).
[14] H.-P. Breuer, B. Kappler, and F. Petruccione, Ann. Phys. (N.Y.) **291**, 36 (2001).
[15] W. T. Strunz, Phys. Lett. A **224**, 25 (1996).
[16] L. Diósi, N. Gisin, and W. T. Strunz, Phys. Rev. A **58**, 1699 (1998).
[17] W. T. Strunz, L. Diósi, and N. Gisin, Phys. Rev. Lett. **82**, 1801 (1999).
[18] W. T. Strunz, New J. Phys. **7**, 91 (2005).
[19] J. Shao, J. Chem. Phys. **120**, 5053 (2004).
[20] H.-P. Breuer, Eur. Phys. J. D **29**, 105 (2004).
[21] D. Lacroix, Phys. Rev. A **72**, 013805 (2005).
[22] H.-P. Breuer, D. Burgarth, and F. Petruccione, Phys. Rev. B **70**, 045323 (2004).
[23] H.-P. Breuer, Phys. Rev. A **69**, 022115 (2004).
[24] Y. Zhou, Y. Yan, and J. Shao, Europhys. Lett. **72**, 334 (2005).
[25] H.-P. Breuer and F. Petruccione, Phys. Rev. E **76**, 016701 (2007).
[26] W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, Berlin, 1985).
[27] D. Lacroix, Ann. Phys. (N.Y.) **322**, 2055 (2007).
[28] R. P. Feynman and F. L. Vernon, Jr., Ann. Phys. (N.Y.) **24**, 118 (1963).
[29] A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983).
[30] Y. Yan, F. Yang, Y. Liu, and J. Shao, Chem. Phys. Lett. **395**, 216 (2004).
[31] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[32] R. Egger and C. H. Mak, Phys. Rev. B **50**, 15210 (1994).