THE JOURNAL OF CHEMICAL PHYSICS **122**, 1 (2005)

Non-Markovian stochastic Schrödinger equations in different temperature regimes: A study of the spin-boson model

Inés de Vega
Departamento de Física Fundamental II, Universidad de La Laguna, La Laguna 38203, Tenerife, Spain

Daniel Alonso
Departamento de Física Fundamental y Experimental, Electrónica y Sistemas, Universidad de La Laguna, La Laguna 38203, Tenerife, Spain

Pierre Gaspard
Center for nonlinear phenomena and complex systems, Université Libre de Bruxelles, Bvd du Triomphe 1050-Bruxelles

Walter T. Strunz
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, 79104-Freibürg, Germany

(Received 30 September 2004; accepted 13 January 2005)

Stochastic Schrödinger equations are used to describe the dynamics of a quantum open system in contact with a large environment, as an alternative to the commonly used master equations. We present a study of the two main types of non-Markovian stochastic Schrödinger equations, linear and nonlinear ones. We compare them both analytically and numerically, the latter for the case of a spin-boson model. We show in this paper that two linear stochastic Schrödinger equations, derived from different perspectives by Diósi, Gisin, and Strunz [Phys. Rev. A **58**, 1699 (1998)], and Gaspard and Nagaoka [J. Chem. Phys. **13**, 5676 (1999)], respectively, are equivalent in the relevant order of perturbation theory. Nonlinear stochastic Schrödinger equations are in principle more efficient than linear ones, as they determine solutions with a higher weight in the ensemble average which recovers the reduced density matrix of the quantum open system. However, it will be shown in this paper that for the case of a spin-boson system and weak coupling, this improvement does only occur in the case of a bath at high temperature. For low temperatures, the sampling of realizations of the nonlinear equation is practically equivalent to the sampling of the linear ones. We study further this result by analyzing, for both temperature regimes, the driving noise of the linear equations in comparison to that of the nonlinear equations. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1867377]

I. INTRODUCTION

We consider a quantum system with a small number of degrees of freedom that interacts with an "environment." We denote with H_s the Hamiltonian of the small system, with H_{bath} the Hamiltonian of the environment, and with H_{int} the interaction Hamiltonian. A widely used model for describing the dynamics of such an open system is a large collection of harmonic oscillators for the bath, and an interaction Hamiltonian that linearly couples the bath with a system operator.[1] Thus, the Hamiltonian of our model of open quantum system dynamics takes the standard form

$$\begin{aligned} H_{\text{tot}} &= H_s + H_{\text{int}} + H_{\text{bath}} \\ &= H_s + g\sum_{\lambda} g_{\lambda}(L^{\dagger}a_{\lambda} + La_{\lambda}^{\dagger}) + \sum_{\lambda} w_{\lambda}a_{\lambda}^{\dagger}a_{\lambda}. \end{aligned} \tag{1}$$

Here, L is a system operator describing the coupling to the environmental degrees of freedom (operators $a_{\lambda}, a_{\lambda}^{\dagger}$) and the constants g_{λ} and ω_{λ} are, respectively, the coupling strengths and the frequencies corresponding to each of the environmental oscillators with index λ. One could easily consider sums of such interaction Hamiltonians with different coupling operators L_j, but we restrict ourselves in this paper to a single term.

Traditionally, the dynamics of an open system has been described in terms of the evolution of the reduced density operator $\rho_s(t) = \text{Tr}_{\text{bath}}[\rho_{\text{tot}}(t)]$ obtained from the total density operator by tracing over the environmental degrees of freedom. The theory of such open quantum system dynamics is well developed under the Markov hypothesis, assuming that the relaxation time of the bath is much smaller than any relevant time scale of the system. The general Markovian master equation takes the so-called Lindblad form,[2] which gives positive $\rho_s(t)$ for all initial conditions. However, in modern quantum technologies there are more and more situations in which the separation of time scales between the system and the bath does not apply, as for the case of atoms in contact with electromagnetic fields which are under spatial boundary conditions (quantum cavities),[3] or immersed in materials with a certain periodicity in the refraction index (photonic crystals).[4] For an application of non-Markovian stochastic Schrödinger equations to a photonic crystal, see Ref. 5. Non-Markovian effects also arise in the dynamics of an atomic "laser" beam extracted from a Bose–Einstein con-

densate where the beam plays the role of the environment.[6] Quite generally, non-Markovian effects are expected to be important at low temperatures.

For a general Hamiltonian of the form (1), the non-Markovian master equation, suitable for describing interactions with general baths in lowest relevant order of perturbation theory is presented in Ref. 7 and reads (here for temperature $T=0$)

$$\frac{d\rho_s(t)}{dt} = -i[H_s,\rho_s(t)] - g^2\int_0^t d\tau\alpha(\tau)L^\dagger L(-\tau)\rho_s(t) - g^2\int_0^t d\tau\alpha^*(\tau)\rho_s(t)L^\dagger(-\tau)L + g^2\int_0^t d\tau\alpha(\tau) \times L(-\tau)\rho_s(t)L^\dagger + g^2\int_0^t d\tau\alpha^*(\tau)L\rho_s(t)L^\dagger(-\tau). \tag{2}$$

In Eq. (2) we denote with

$$L(\tau) = e^{iH_s\tau}Le^{-iH_s\tau}, \tag{3}$$

the system part of the interaction Hamiltonian in the Heisenberg picture. In Ref. 7 it is also shown how the result (2) may be obtained from a stochastic Schrödinger equation. By redefining the operators L and $L^\dagger$ as explained in Sec. II, Eq. (2) is also equal to the master equation presented in Ref. 8, and leads to the so-called Redfield master equation[9] in the long-time limit when $\int_0^t$ can be replaced by $\int_0^\infty$. In this paper, we express the explicit dependence of the equations on the coupling parameter g, defined as $g[H_0]=[H_{\text{int}}]$, where $[A]$ denotes the magnitude of the operator A, and $H_0=H_s+H_{\text{bath}}$. The non-Markovian memory effects appear through the integrals over the correlation function $\alpha(\tau)$, which in the Markov approximation may be replaced by a δ function. In that limit, Eq. (2) turns indeed into a master equation of Lindblad form.

In recent years a new method has been developed to solve the dynamics of quantum open systems, based on so-called stochastic Schrödinger equations. These equations can take the form of a deterministic evolution interrupted by stochastic quantum jumps,[10] or they can be of continuous and diffusive type, that is, quantum state diffusion.[11–16] The latter class has recently been extended to treat non-Markovian situations[17,8,18–21]. In general, stochastic Schrödinger equations evolve wave functions $|\psi_t(z)\rangle$, which depend on a stochastic variable z_t [we will denote $|\psi_t(z)\rangle \equiv |\psi_t(z_t)\rangle$ throughout the paper]. The crucial property of any stochastic approach is that the ensemble average (denoted by $M[\cdots]$) of the projector composed by wave functions recovers the reduced density operator:

$$\rho_s = M[|\psi_t(z)\rangle\langle\psi_t(z)|]. \tag{4}$$

In principle, the theories we are going to develop preserve the norm of the reduced density operator, $1=\text{Tr}\,\rho_s = M[\langle\psi_t(z)|\psi_t(z)\rangle]$. In practice, however, due to approximations and due to only a finite number of realizations, the numerical ensemble mean $M[\langle\psi_t(z)|\psi_t(z)\rangle]$ may differ from unity. Therefore, in the applications discussed towards the end of this paper, we determine the reduced density operator through $\rho_s = M[|\psi_t(z)\rangle\langle\psi_t(z)|]/M[\langle\psi_t(z)|\psi_t(z)\rangle]$, a prescription that was seen to lead to stable results.

In all these considerations, $M[\cdots]$ denotes the average of solutions weighted by the distribution of the driving noise. The stochastic Schrödinger equation scheme may provide a significant numerical advantage over the master equation approach, in particular, as soon as the Hilbert space dimension N of the open system is large. In the stochastic approach, one only needs to integrate a state of dimension N for a certain number of realizations κ, in order to obtain ρ_s. In contrast, the solution of the master equation demands the integration of N^2 elements of the density operator. If the number of realizations of the stochastic scheme is not too large (which also depends on the accuracy one aims to achieve), then stochastic Schrödinger equations may be in practice more advantageous than master equations.

Moreover, to be numerically efficient (importance sampling), it may be very important to choose a stochastic equation which gives solutions with a significant weight in the average (4), providing the best possible sampling. The aim of this paper is to give some hints and criteria, based on the temperature of the bath, for making such a choice between different equations in the non-Markovian case. For this purpose, two particular kinds of non-Markovian stochastic Schrödinger equations will be studied: stochastic equations that are *linear* in the wave function, and *non-linear* stochastic equations. To be more concrete, two linear equations, which are characterized by having a constant noise distribution function, will be treated: the convolutionless linear equation derived by Diósi and Strunz in Ref. 19, and the convoluted equation derived by Gaspard and Nagaoka in Ref. 8.

As will be explained in more detail below, the probability distribution of the noise corresponds to a certain distribution function of the bath, and therefore it might be advantageous to take into account explicitly the dynamics of the bath. The nonlinear stochastic equation proposed by Diósi, Gisin, and Strunz in Ref. 17 considers such an evolution of the noise statistics, giving rise, in principle, to a more efficient sampling of the sum (4). However, we will show in this paper for the case of a spin-boson model that the temperature of the bath is a very important parameter to determine whether this improvement in the sampling is significant or not. This is very useful information: since nonlinear equations take a longer time to be integrated numerically compared to linear equations, they should only be used when it is needed or, to put it in another way, when the noise probability distribution (i.e., the environmental state) evolves considerably due to the interaction.

The paper is organized as follows: In Sec. II we briefly present the two non-Markovian linear equations already mentioned, and show analytically their equivalence in the relevant order of perturbation theory. In Sec. III we will study two nonlinear stochastic equations, both intimately related and characterized by having a dynamical probability distribution for the noise. Section IV will be devoted to the application of the different stochastic equations to a spin-boson system. In the first part of this section, we show the equivalence of the two linear equations. A study of the norm

of single trajectories, for high and low temperatures, is presented in the following section. The last sections are devoted to investigate the improvement in the sampling provided by nonlinear equations by comparing both linear and nonlinear equations in these two temperature regimes. In particular, the statistical significance of the solutions of the linear and nonlinear equations will be studied comparing their ensemble average with the solutions of the corresponding non-Markovian master equation (2). Finally, we draw conclusions.

II. NON-MARKOVIAN *LINEAR EQUATION*

A. Linear convolutionless equation

The first Non-Markovian stochastic Schrödinger equation (linear) was derived by Diósi and Strunz[19] assuming that all the environmental oscillators are initially in the ground state (or analogously that the bath is at zero temperature). For the model Hamiltonian (1), the non-Markovian stochastic Schrödinger equation reads

$$\frac{d}{dt}|\psi_t\rangle = -iH_s|\psi_t\rangle + gLz_t|\psi_t\rangle - g^2L^\dagger\int_0^t d\tau\alpha(t-\tau)\frac{\delta|\psi_t\rangle}{\delta z_\tau}. \tag{5}$$

It should be clear that the states $|\psi_t\rangle = |\psi_t(z)\rangle$ are functionals of the driving noise z_t, which we do not always write out explicitly. The first term on the right-hand side of Eq. (5) represents the unitary free evolution of the system, whereas the other two terms correspond to the nonunitary and irreversible dynamics due to the interaction of the system with the bath. The second term (a stochastic driving term) may be interpreted as a stochastic forcing due to the action of the bath degrees of freedom on the system. The third term (a dissipative term) represents the energy damping or relaxation process of the system when interacting with the bath. The driving term depends on a colored complex Gaussian stochastic process z_t, which satisfies the following statistical properties:

$$M[z_t] = 0, \quad M[z_t z_\tau] = 0, \qquad M[z_t^* z_\tau] = \alpha(t-\tau), \tag{6}$$

where $\alpha(t-\tau)$ is the zero temperature correlation function of the bath (or response function in Refs. 22), which can be written as[23]

$$\alpha(t-\tau) = \sum_\lambda g_\lambda^2 e^{-i\omega_\lambda(t-\tau)}. \tag{7}$$

Equation (5) is exact, but its practical use is limited due to the functional derivative $\delta|\psi_t(z)\rangle/\delta z_\tau$ that appears in the dissipative term. This problem is tackled by Diósi, Gisin, and Strunz[17] by proposing the following replacement for it:

$$\frac{\delta|\psi_t\rangle}{\delta z_\tau} = O(t,\tau,z)|\psi_t\rangle, \tag{8}$$

where $O(t,\tau,z)$ is a linear operator that has to be constructed for each case under consideration. For instance, $O(t,\tau,z)$ may be obtained from a perturbation series,[24] which gives

$$O(t,\tau,z) = L(\tau-t) + \mathcal{O}(g), \tag{9}$$

where $L(\tau)$ is the Heisenberg operator from Eq. (3). It should be noted that the noise term is of order g, while the dissipative term is at least of order g^2 due to the presence of the correlation function of the noise. As a consequence, for a second-order linear stochastic equation, only the first term of the perturbative expansion of $O(t,\tau,z)$ in Eq. (9) is required. With the replacement of the form (8) for the functional derivative, there is no reference to the wave function at earlier times under the memory integral in the dissipative term of Eq. (5). The equation becomes time local in $|\psi_t\rangle$ and will be referred to as the *convolutionless* linear stochastic Schrödinger equation in this paper.

A possible derivation of the linear equation (5) may be found in Ref. 25, based on a (Bargmann) coherent state basis for the environmental degrees of freedom [in which $|z_\lambda\rangle = \exp(z_\lambda a_\lambda^\dagger)|0\rangle$]. In this basis, the state of the total system (quantum open system and environment) is expressed as

$$|\Psi_t\rangle = \int \frac{d^2z_\lambda}{\pi} e^{-|z|^2}|\psi_t(z)\rangle|z\rangle \tag{10}$$

with the notation $|z\rangle = |z_1\rangle|z_2\rangle\cdots|z_\lambda\rangle\cdots$ for the state of the environment, a product of coherent states of all the environmental oscillators. The quantity z_t that appears in the linear equation (5) has a simple microscopic expression. It is a combination of coherent state labels z_λ^*, given by

$$z_t = -i\sum_\lambda g_\lambda z_\lambda^* e^{i\omega_\lambda t}. \tag{11}$$

At first, there is no reason to refer to this z_t as a stochastic process. The latter meaning comes about as soon as we evaluate the reduced density operator ρ_t based on expression (10) of the total state. We find a a Gaussian mixture of states $|\psi_t(z)\rangle$,

$$\rho_t = \int \frac{d^2z}{\pi} e^{-|z|^2}|\psi_t(z)\rangle\langle\psi_t(z)| \tag{12}$$

and thus, an explicit construction of an ensemble mean of type (4).

The corresponding closed evolution equation (5) for the states of the system can now be seen as a stochastic equation. In a Monte Carlo sense, we have to choose a Gaussian random selection of coherent state labels z_λ to perform the integral over all of them in Eq. (12) which amounts to choosing realizations of the Gaussian noise z_t from Eq. (11) with statistics (7).

So far, the stochastic equation was derived from the zero-temperature expression (10) for the total state. A more general linear stochastic Schrödinger equation, valid for baths at finite temperature, can be derived by canonically mapping the nonzero temperature density operator of the heat bath onto the zero-temperature density operator of a larger hypothetical environment.[17] The resulting finite temperature linear equation is

$$\frac{d}{dt}|\psi_t\rangle = -iH_s|\psi_t\rangle + gLz_t^-|\psi_t\rangle + gL^\dagger z_t^+|\psi_t\rangle - g^2L^\dagger \times \int_0^t \alpha^-(t-\tau)\frac{\delta|\psi_t\rangle}{\delta z_\tau^-}d\tau - g^2L\int_0^t \alpha^+(t-\tau)\frac{\delta|\psi_t\rangle}{\delta z_\tau^+}d\tau. \tag{13}$$

For simplicity we have dropped the explicit dependence of the wave function on the two independent Gaussian noises z_t^- and z_t^+, which have zero means and the following correlations:

$$\begin{aligned} &M[z_t^- z_\tau^-] = 0, \\ &M[z_t^{-*} z_\tau^-] = \alpha^-(t-\tau) = \sum_\lambda g_\lambda^2(N(\omega_\lambda)+1)e^{-i\omega_\lambda(t-\tau)}, \\ &M[z_t^+ z_\tau^+] = 0, \\ &M[z_t^{+*} z_\tau^+] = \alpha^+(t-\tau) = \sum_\lambda g_\lambda^2 N(\omega_\lambda)e^{i\omega_\lambda(t-\tau)} \\ &M[z_t^{+*} z_\tau^-] = 0. \end{aligned} \tag{14}$$

The function $N(\omega)=[\exp(\hbar\omega\beta)-1]^{-1}$, where we use the standard notation $\beta=(kT)^{-1}$ (with k the Boltzmann constant), is the average thermal number of quanta in the mode ω. Again one can try to replace the functional derivatives in Eq. (13) by an ansatz of type (8). Using a perturbative expansion for $O(t,\tau,z)$ we again find

$$\begin{aligned} \frac{\delta|\psi_t\rangle}{\delta z_\tau^-} &= O^-(t,\tau,z^\pm)|\psi_t\rangle = L(\tau-t)|\psi_t\rangle + \mathcal{O}(g), \\ \frac{\delta|\psi_t\rangle}{\delta z_\tau^+} &= O^+(t,\tau,z^\pm)|\psi_t\rangle = L^\dagger(\tau-t)|\psi_t\rangle + \mathcal{O}(g). \end{aligned} \tag{15}$$

Note that at zero temperature, the linear stochastic equation (5) is reobtained, since for this case $N(\omega)$, $\alpha^+(t-\tau)$, and z^+ are zero, while $\alpha^-(t-\tau)$ becomes equal to Eq. (7). For finite temperature and a Hermitian coupling operator $L=L^\dagger=K$, Eq. (13), is simplified as

$$\frac{d}{dt}|\psi_t\rangle = -iH_s|\psi_t\rangle + gKz_t|\psi_t\rangle - g^2K\int_0^t d\tau\alpha_T(t-\tau)K(\tau-t)|\psi_t\rangle + \mathcal{O}(g^3). \tag{16}$$

where now the noise is $z_t=z_t^+ + z_t^-$ and has the following statistical properties:

$$\begin{aligned} &M[z_t z_\tau] = 0, \\ &M[z_t^* z_\tau] = \alpha^-(t-\tau) + \alpha^+(t-\tau) = \alpha_T(t-\tau) \\ &\quad = \sum_\lambda g_\lambda^2\left[\coth\left(\frac{\omega_\lambda\beta}{2}\right)\cos[\omega_\lambda(t-\tau)] - i\sin[\omega_\lambda(t-\tau)]\right], \end{aligned} \tag{17}$$

this latter being the standard bath correlation function at nonzero temperature.[1,22] Clearly, as the temperature goes to zero, $\alpha_T(t-\tau)$ coincides with the zero-temperature expression (7).

B. Linear convoluted equation

A second linear non-Markovian stochastic Schrödinger equation has been proposed by Gaspard and Nagaoka.[8] In this section it will be shown that their equation is equivalent to Eq. (13) up to the relevant second order in the coupling parameter g, although its derivation is based on very different hypothesis. Following Ref. 8, let us start from a general Hamiltonian for a system and its environment in the form

$$H_{\text{tot}} = H_s + H_{\text{bath}} + H_{\text{int}} = H_0 + gV, \tag{18}$$

with $H_0=H_s+H_{\text{bath}}$ and an interaction potential V that we assume takes the form

$$V = V^\dagger = \sum_\beta S_\beta B_\beta. \tag{19}$$

The Hermitian subsystem and bath coupling operators are S_β and B_β, respectively. This form of the interaction Hamiltonian covers our earlier model (1) by choosing two contribution $\beta=1,2$ in the sum, with

$$S_1 = L + L^\dagger, \quad S_2 = i(L - L^\dagger) \tag{20}$$

and

$$B_1 = \frac{1}{2}\sum_\lambda g_\lambda(a_\lambda + a_\lambda^\dagger), \quad B_2 = \frac{i}{2}\sum_\lambda g_\lambda(a_\lambda - a_\lambda^\dagger). \tag{21}$$

In this approach to a stochastic equation the total wave function is again expanded, here, however, in the basis of eigenfunctions of the bath $\{|n\rangle\}$, to get

$$|\Psi_t\rangle = \sum_n |\psi_t^n\rangle|n\rangle. \tag{22}$$

As before, the ensemble of system states $|\psi_t^n\rangle$ recovers the mixed reduced density operator. The evolution of each of these states will depend on the evolution of others through a set of coupled differential equations. Due to this mutual interaction, and provided that the number of system states is sufficiently large, they will behave in a random way. This brings the idea of deriving a stochastic Schrödinger equation, which evolves only one member of the ensemble of system states $|\psi_t^n\rangle$, under the assumption that such a state is statistically representative of the rest. To decouple the evolution equation of such a state from the time evolution of the rest, the Feshbach projection-operator method is used. Using a perturbative expansion in the coupling strength, and for the special choice of operators (20) and (21), the following equation is obtained:

$$\frac{d}{dt}|\psi_t\rangle = -iH_s|\psi_t\rangle + g[L\eta_A(t) + L^\dagger \eta_B(t)]|\psi_t\rangle - 2g^2L^\dagger\int_0^t d\tau[C_{11}(\tau) - iC_{21}(\tau)] \times L(-\tau)e^{-iH_s\tau}|\psi_{t-\tau}\rangle - 2g^2L\int_0^t d\tau[C_{11}(\tau) + iC_{21}(\tau)]L^\dagger(-\tau)e^{-iH_s\tau}|\psi_{t-\tau}\rangle + \mathcal{O}(g^3), \tag{23}$$

where the selected system state $|\psi_t^l\rangle$ now represents the wave function $|\psi_t(\eta_A,\eta_B)\rangle \equiv |\psi_t\rangle$. The variables $\eta_A(t)$ and $\eta_B(t)$ are the combinations,

$$\eta_A(t) = \eta_2(t) - i\eta_1(t), \qquad \eta_B(t) = -\eta_2(t) - i\eta_1(t), \tag{24}$$

with

$$\eta_i(t) \equiv \sum_{m(\neq l)} \langle l|B_i(t)|m\rangle e^{-\beta(\epsilon_m-\epsilon_l)/2} e^{i(\theta_m-\theta_l)}. \tag{25}$$

It is assumed that the $\{\theta_i\}$ form a set of independent random phases, uniformly distributed in the interval $[0,2\pi]$, and ϵ_m and ϵ_l are eigenvalues corresponding to eigenfunctions $|m\rangle$ and $|l\rangle$ of the bath Hamiltonian, respectively. The stochastic nature of Eq. (23) is contained in the behavior of $\eta_i(t)$. If the number of states is large enough to perform the sum (25) over a large set of phases $\{\theta_m\}$, these quantities can be characterized as Gaussian random variables by the central limit theorem. As complex Gaussian variables, $\eta_i(t)$ satisfy similar conditions to Eq. (7),

$$M[\eta_i(t)] = 0, \quad M[\eta_i(t)\eta_j(\tau)] = 0, \qquad M[\eta_i(t)\eta_j^*(\tau)] = C_{ij}^*(t-\tau). \tag{26}$$

Following the definition (25) for the noise and since $M[\exp[i(\theta_m-\theta_n)]] = \delta_{mn}$, the noise correlation is given by

$$M[\eta_i(t)\eta_j^*(\tau)] = \sum_n e^{\beta(\epsilon_l-\epsilon_n)}\langle l|B_i(\tau)|n\rangle\langle n|B_j(t)|l\rangle, \tag{27}$$

or equivalently,

$$M[\eta_i(t)\eta_j^*(\tau)]|_l = \frac{Z_b}{e^{-\beta\epsilon_l}}\langle l|B_i(t)\rho_b^{eq}B_j(\tau)|l\rangle, \tag{28}$$

where $\rho_b^{eq} = Z_b^{-1}\exp(-H_b\beta)$ is the bath density matrix in equilibrium. In order to obtain the typical value of this correlation function, a thermal average is performed (see Ref. 8, and references therein for further details), so that

$$\sum_l \frac{e^{-\beta\epsilon_l}}{Z_b} M[\eta_i(t)\eta_j^*(\tau)]|_l = \mathrm{Tr}_b[\rho_b^{eq}B_j(\tau)B_i(t)] = C_{ij}^*(t-\tau). \tag{29}$$

With the choice (21) for the bath coupling operators B_1 and B_2 we find

$$C_{12}(t) = -C_{21}(t) = \frac{i}{4}\sum_\lambda g_\lambda^2\{N(\omega_\lambda)e^{i\omega_\lambda t} - [N(\omega_\lambda)+1]e^{-i\omega_\lambda t}\},$$
$$C_{11}(t) = C_{22}(t) = \frac{1}{4}\sum_\lambda g_\lambda^2\{N(\omega_\lambda)e^{i\omega_\lambda t} + [N(\omega_\lambda)+1]e^{-i\omega_\lambda t}\}, \tag{30}$$

where the thermal averages of a_λ, $a_\lambda^\dagger$, are[26]

$$\mathrm{Tr}_b[\rho_b^{eq}a_\lambda(0)a_\lambda(0)] = 0, \qquad \mathrm{Tr}_b[\rho_b^{eq}a_\lambda^\dagger(0)a_{\lambda'}(0)] = \delta_{\lambda\lambda'}N(\omega_\lambda), \tag{31}$$

and $N(\omega_\lambda)$ is again the average thermal number of quanta in the mode ω_λ. With expressions (31), the combinations $2[C_{11}(t) \pm iC_{21}(t)]$ appearing in Eq. (23) are equal to the correlation functions $\alpha^\pm(t)$ of Eq. (14), and the noise combinations η_A and η_B are equal, respectively, to the noises z^- and z^+ of that equation. As in the previous approach, when we consider the case of a system coupling operator L that is Hermitian $L = L^\dagger = K$, we find

$$\frac{d}{dt}|\psi_t\rangle = -iH_s|\psi_t\rangle + gKz_t|\psi_t\rangle - g^2K\int_0^t d\tau\alpha_T(t-\tau) \times K(\tau-t)e^{-iH_s(t-\tau)}|\psi_\tau\rangle + \mathcal{O}(g^3), \tag{32}$$

where we have already changed the notation for the noise, $\eta_B(t) + \eta_A(t) \equiv z_t$.

Let us now show how Eq. (16) derived by Diósi and Strunz[19] and Eq. (32) obtained by Gaspard and Nagaoka[8] are equivalent up to order g^2. Indeed, it is consistent with the second-order approximation to substitute the wave function $|\psi_\tau\rangle$ appearing in the dissipative term of Eq. (32) by its expansion up to order g^0 only. For that it is enough to see that $|\psi_\tau\rangle = [e^{-iH_s\tau} + \mathcal{O}(g)]|\psi_0\rangle$ and furthermore, $|\psi_0\rangle = [e^{iH_st} + \mathcal{O}(g)]|\psi_t\rangle$. Replacing this expression for $|\psi_0\rangle$ in the expression for $|\psi_\tau\rangle$, we conclude that

$$|\psi_\tau\rangle = [e^{iH_s(t-\tau)} + \mathcal{O}(g)]|\psi_t\rangle. \tag{33}$$

Therefore, within second order in the coupling strength g, Eq. (32) becomes equal to convolutionless Eq. (16). The same holds true for its non-Hermitian version (23), which becomes equal to Eq. (13). Clearly, this equivalence also extends to the zero temperature equations.

III. NON-MARKOVIAN *NONLINEAR EQUATIONS*

As noted by Diósi, Gisin, and Strunz,[17] the linear equation has an important drawback. During the evolution of the trajectories, which is driven by an input noise governed by the initial state of the bath, the solutions $|\psi_t\rangle$ may lose their norm and therefore statistical relevance. This problem comes from not having considered that the interaction between the system and the bath not only affects the system, but also the bath itself. To see this more clearly (see Ref. 25 for further details) let us follow the coherent state basis derivation of Sec. II A to define the Husimi function (or Q function) of the bath as

$$Q_t(z,z^*) = \frac{e^{-|z|^2}}{\pi}\langle z|\mathrm{Tr}_s[|\Psi_t\rangle\langle\Psi_t|]|z\rangle, \tag{34}$$

where $|z\rangle$ denotes a coherent state of the bath in the Bargmann basis. Since each of these states corresponds to a certain value of the noise the function $Q_t(z,z^*)$ may be interpreted as the probability distribution of the noise. The substitution of Eq. (10) in Eq. (34) gives the following expression for the Husimi function:

$$Q_t(z,z^*) = \langle\psi_t(z)|\psi_t(z)\rangle Q_0(z,z^*) \tag{35}$$

with $Q_0(z,z^*)$ the initial Gaussian distribution of coherent states $Q_0(z,z^*)=e^{-|z|^2}/\pi$. In terms of Eq. (35), the density operator (12) can be defined as a mixture of pure normalized states weighted by $Q_t(z,z^*)$,

$$\rho_t = \int d^2z Q_t(z,z^*)\frac{|\psi_t(z)\rangle\langle\psi_t(z)|}{\langle\psi_t(z)|\psi_t(z)\rangle}. \tag{36}$$

With this expression it is clearer to see that, once the interaction is "switched on" and the environmental oscillators start to move away from the origin according to the distribution $Q_t(z,z^*)$, the states $|\psi_t(z)/\langle\psi_t(z)|\psi_t(z)\rangle^{1/2}$, which according to $Q_0(z,z^*)$ correspond to small z, will have a decreasing weight in the sum (36).

The Husimi function shows a closed time evolution of Liouville form for the set of oscillators z_λ composing the quantity z, corresponding to the following phase space flow:[17]

$$\dot{z}_\lambda^* = ig_\lambda e^{-i\omega_\lambda t}\langle L^\dagger\rangle_t. \tag{37}$$

In terms of the trajectories $z(t)$ that follow this flow, the Husimi function $Q_t(z,z^*)$ at time t can be expressed as

$$Q_t(z,z^*) = \int d^2z_0 Q_0(z_0,z_0^*)\delta^2[z-z(t)], \tag{38}$$

where somewhat symbolically, $z(t)$ represents the set of solutions of the different trajectories of the oscillators starting from the set of initial values $\{z_\lambda^*(0)=z_{\lambda,0}^*\}$. In that way, we can now replace Eq. (36) by an integral of wave functions evaluated in the dynamical states $z(t)\equiv\{z_\lambda(t)\}$ as

$$\rho_t = \int d^2z_0 Q_0(z_0,z_0^*)\frac{|\psi_t[z(t)]\rangle\langle\psi_t[z(t)]|}{\langle\psi_t[z(t)]|\psi_t[z(t)]\rangle}$$
$$= \int \frac{d^2z_0}{\pi}e^{-|z_0|^2}\frac{|\psi_t[z(t)]\rangle\langle\psi_t[z(t)]|}{\langle\psi_t[z(t)]|\psi_t[z(t)]\rangle}. \tag{39}$$

Now, to perform the integral (39) with a Monte Carlo method, a new stochastic variable $\tilde{z}_t^*$ is defined, which corresponds to $z(t)$ with a random selection of the initial values for the environmental oscillators $\{z_\lambda^*(0)\}$. From the flow equation (37), one obtains

$$\tilde{z}_t = z_t + g\int d\tau\alpha^*(t-\tau)\langle L^\dagger\rangle_\tau. \tag{40}$$

Here, the variable z_t is the noise as it appears in the linear stochastic Schrödinger equation, which corresponds to the stationary statistics with distribution function $Q_0(z,z^*)$. The last term represents a dynamical shift or displacement of each z_t which depends on the history of the interaction with the system. The stochastic equation for the wave function $|\psi(\tilde{z}_t)\rangle$ with a shifted noise in the driving term is[17]

$$\frac{|\psi_t(\tilde{z}_t)\rangle}{dt} = -iH_s|\psi_t(\tilde{z}_t)\rangle + gL\tilde{z}_t|\psi_t(\tilde{z}_t)\rangle$$
$$- g^2(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{z}_t)|\psi_t(\tilde{z}_t)\rangle, \tag{41}$$

with $\bar{O}=\int_0^t d\tau\alpha(t-\tau)O(t,\tau,\tilde{z}_t)$. In order to make clear that the wave function now depends on the shifted noise, we show this dependency explicitly through the notation $|\psi_t(\tilde{z}_t)\rangle$. By evolving (41) we ensure that the wave functions $|\psi_t(\tilde{z}_t)\rangle$ correspond to those realizations that contribute with a significant probability (importance sampling), which according to Eq. (40) is ensured by the shift term. It is important to note that the difference between the original and the shifted noise is of the order of the coupling strength parameter g. Thus, the contribution of the shift turns out to be of the relevant order g^2 in the evolution of the wave functions.

We see from Eq. (39) that the reduced density operator can now be written as a mixture of normalized stochastic states,

$$\rho_t = \int \frac{d^2z_0}{\pi}e^{-|z_0|^2}|\tilde{\psi}_t[z(t)]\rangle\langle\tilde{\psi}_t[z(t)]| \tag{42}$$

with $|\tilde{\psi}_t\rangle=|\psi_t(\tilde{z}_t)\rangle/\sqrt{\langle\psi_t(\tilde{z}_t)|\psi_t(\tilde{z}_t)\rangle}$. From Eq. (41) one obtains an evolution equation for these normalized states,[17] giving

$$\frac{d|\tilde{\psi}_t(\tilde{z}_t)\rangle}{dt} = -iH_s|\tilde{\psi}_t(\tilde{z}_t)\rangle + g(L-\langle L^\dagger\rangle)\tilde{z}_t|\tilde{\psi}_t(\tilde{z}_t)\rangle$$
$$- g^2[(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{z}_t) - \langle(L^\dagger - \langle L^\dagger\rangle_t)\bar{O}(t,\tilde{z}_t)\rangle]$$
$$\times|\tilde{\psi}_t(\tilde{z}_t)\rangle. \tag{43}$$

Let us now investigate the three equations described above, the linear equation (5), the shifted equation (41) and the nonlinear equation (43) by applying them to a spin-boson model. We are interested in studying the numerical equivalence of both linear equations that has been already proved analytically. Finally, we will focus on the problem of sampling, and the convenience of using a linear or a nonlinear stochastic Schrödinger equation.

IV. THE SPIN-BOSON MODEL

A spin-boson model consists of a two-level system (or a spin $s=1/2$) coupled to a thermal bath of bosonic harmonic oscillators. Defining the Pauli matrices σ_z and σ_x as usual,

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

the spin-boson model takes the form of the total Hamiltonian (1),

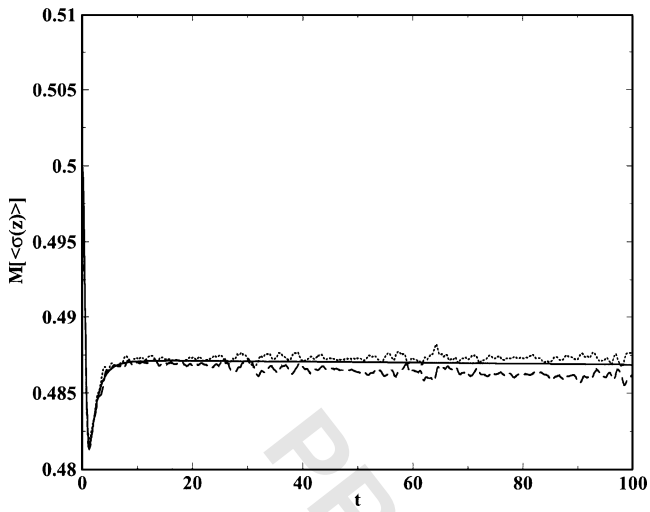

FIG. 1. Comparison of the convolutionless linear equation (16) (dotted line) and the convoluted linear equation (32) (long dashed line) for the same number of trajectories ($\kappa=10\,000$). It can be observed that both equations present the same degree of approximation to the non-Markovian master equation (2) (solid line). The difference between each other increases with time as the second-order approximation becomes less accurate.

$$H_{\text{tot}} = -\frac{\Delta}{2}\sigma_z + g\sum_{\lambda} g_{\lambda}\sigma_x(a_{\lambda} + a_{\lambda}^{\dagger}) + \sum_{\lambda} \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}, \tag{44}$$

where Δ is the energy splitting between the two levels, g is the coupling parameter, and σ_x is the coupling operator of the system with the bath. Here we have chosen $\Delta=0.1$ and $g=0.1$. In the continuum limit, the correlation function (17) that characterizes the bath, reads as follows:

$$\alpha_T(t) = \int_0^{\infty} d\omega J(\omega)\left[\coth\left(\frac{\omega\beta}{2}\right)\cos(\omega t) - i\sin(\omega t)\right]. \tag{45}$$

Here, $J(\omega)$ is the spectral strength,

$$J(\omega) = \frac{\omega^3}{\omega_c^2}\exp(-\omega/\omega_c), \tag{46}$$

where ω_c is a cutoff frequency,[8] here chosen as $\omega_c=1$.

A. Comparison of the linear equations

It has been shown in Sec. II B that the linear equation (13) with the perturbative replacement (15) of the functional derivative is equivalent to Eq. (23) up to second order in g. Figure 1 confirms this expectation where we compare the ensemble averaged result of both equations obtained with the same number of trajectories, with that of the master equation. Indeed, the difference between each result and the master equation is approximately equal, and the discrepancy between both results increases with time as the effects of the perturbation becomes more important and the second-order approximation less accurate.

B. Norm of the wave function

We first study the norm of the linear equation (5) and the shifted equation (41) for a single trajectory representative of the rest. As we see in Fig. 2, norm preservation is lost after very few time steps for high temperatures. In the lower temperature case (Fig. 3), the norm of the solutions of either equation is clearly more stable than for the high temperature $\beta=0.01$, and remains approximately bounded in the time interval studied. Finally, the nonlinear normalized equation (43) properly maintains the norm provided that the time step of the numerical integration of the equations is small enough to avoid the problems derived from its discretization. In practice, one keeps the states properly normalized numerically.

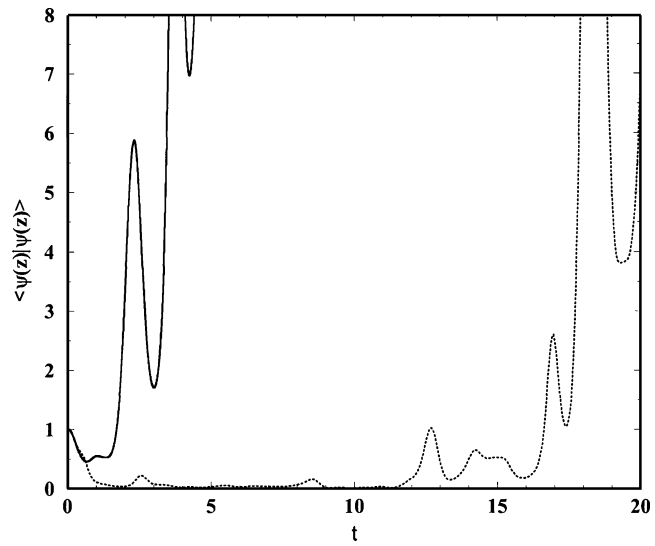

FIG. 2. Evolution of the norm of a single trajectory for high temperature $\beta=0.01$, using the linear equation (5) (dotted line) and the shifted equation (41) (solid line).

C. Ensemble averaged results at different temperatures

We have seen in the last section that norm preservation is rapidly lost at high temperatures. However, the important aspect is that despite of this problem, the shifted equation (41) gives good averaged results. Averaging with the same

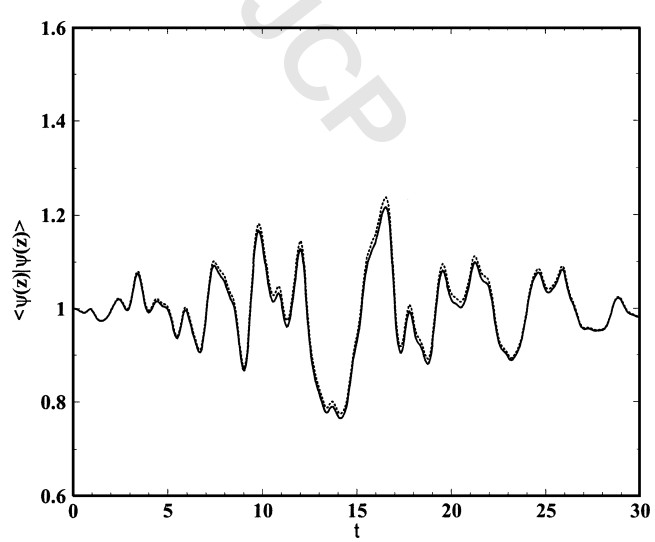

FIG. 3. Same as Fig. 2 but for low temperature $\beta=10$.

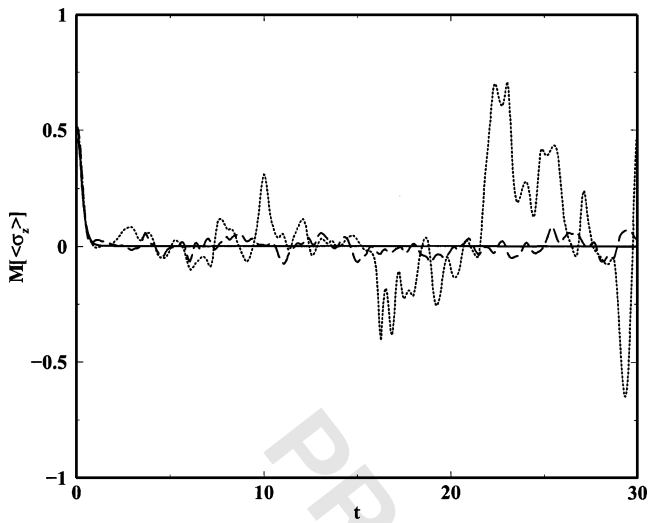

FIG. 4. Solutions of the linear equation (5) (dashed line) and the shifted equation (41) (long dashed line) for $\beta=0.01$ (high temperatures), using an ensemble of $\kappa=100$ trajectories. Results are compared to the master equation (thick line).

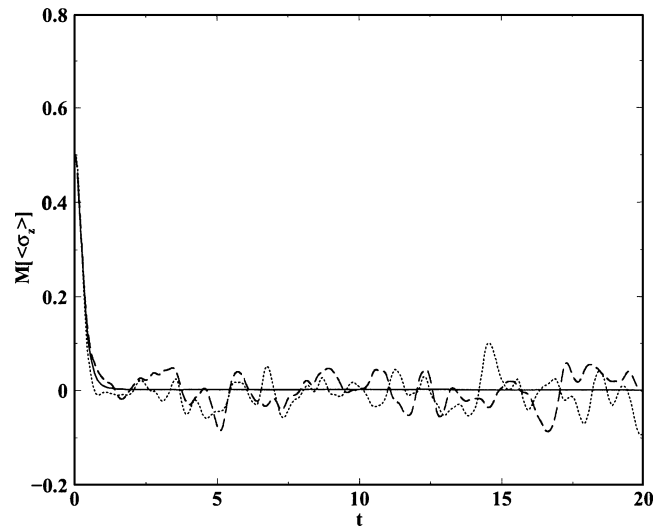

FIG. 6. Solutions of the shifted equation (41) and the nonlinear equation (43) (long dashed and dotted line, respectively) for $\beta=0.01$ (high temperatures), with an average of $\kappa=1000$ trajectories. The result of the master equation is displayed with a solid line.

number of trajectories, the linear equation, in contrast, presents a solution which during the evolution becomes more and more fluctuating and far away from the master equation curve. These results, shown in Figs. 4 and 5 for $\kappa=100$ and $\kappa=10\,000$ trajectories, respectively, suggest that the shift becomes essential for the true evolution at high temperature, improving significantly the results in comparison with those of the linear (nonshifted) equation.

A further question shall be addressed next: Does a normalization of the wave function during the evolution still improve the statistics? To answer we compare in Fig. 6 the results of the shifted equation (41) and the nonlinear (also shifted) equation (43), which evolves normalized states. Using an ensemble of $\kappa=1000$ trajectories it appears that they both give the same degree of accuracy. To be more specific, for this number of trajectories it seems that the solutions of both equations still present some fluctuations around the result of the master equation, but these have the same amplitude in both cases. As a consequence, we can conclude that, at least for the spin-boson model, no further improvement of the statistics is achieved when averaging over the normalized solutions of Eq. (43). We conclude that in practice, it is irrelevant whether one normalizes after each time step. As long as one uses the shifted noise and keeps track of the norm in order to evaluate expectation values with the correct normalization factor, both the linear shifted equation (41) and the full nonlinear equation (43) give results of equal quality.

It is now important to study whether the shifted equation (41) still presents a better sampling than the linear equation (16) for low temperatures ($\beta=10$). As shown by Gaspard and Nagaoka,[8] the linear equation already gives averages that are in good agreement with the master equation. Figures 7 and 8 show that indeed, there is no appreciable improvement of the shifted equation with respect to the linear one in any of the two statistical ensembles of trajectories used (10 000 and

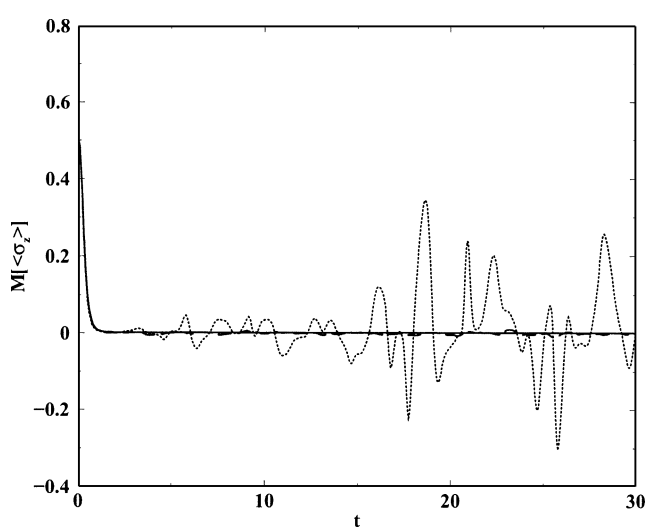

FIG. 5. Same as Fig. 4 but with $\kappa=10\,000$ trajectories.

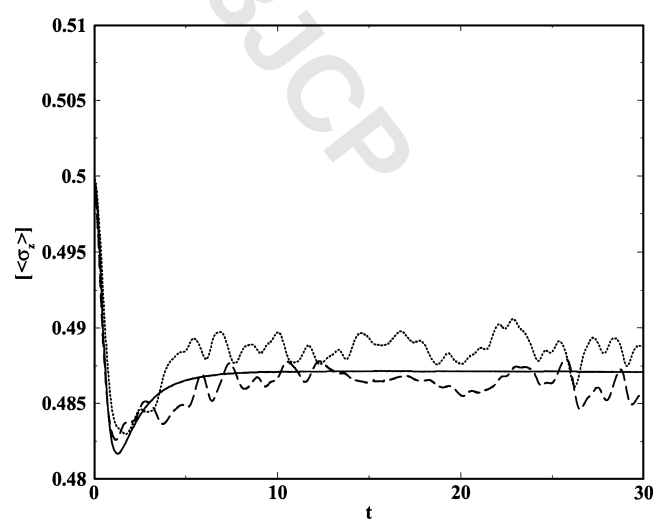

FIG. 7. Solutions of the linear equation (long dashed line) and the shifted equation (dotted line) for $\beta=10$, averaged for 10 000 trajectories. The results are compared to the one obtained from the master equation (thick line).

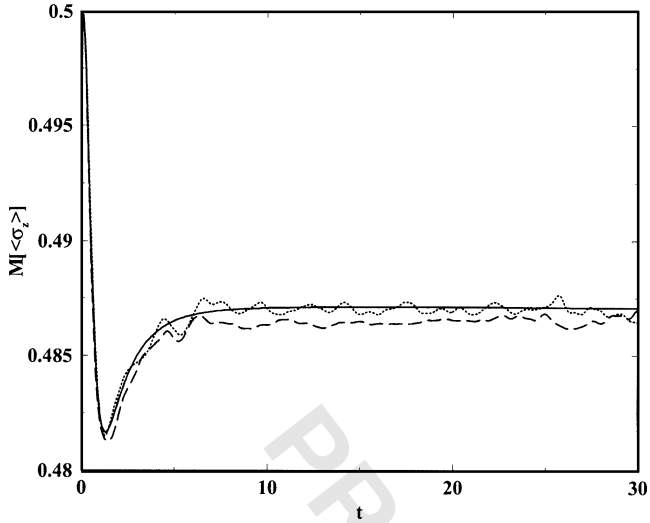

FIG. 8. Same as Fig. 7 but now with 150 000 trajectories.

150 000 trajectories, respectively). These results, added to the fact that the shifted equation is numerically slower, make the linear equation a more sensible choice in the low temperature regime.

D. A study of the noise and the shifted noise

When comparing the shift term $[g\int_0^t d\tau\alpha(t-\tau)^*\langle\sigma_x^\dagger\rangle_\tau]$ and the original noise z_t that appear in expression (40) for both temperature regimes, we find the reason for the previous observations. We present in Fig. 9 the time evolution of the real and imaginary parts of both quantities. For low temperatures $\beta=10$, the shift remains close to zero during the whole evolution, and therefore its significance relative to the noise z_t is small. However, the situation changes for high temperatures, ($\beta=0.01$), in which the real part of the shift reaches an amplitude of fluctuations equal to that of the noise, producing a shifted noise very distant from the non-shifted one.

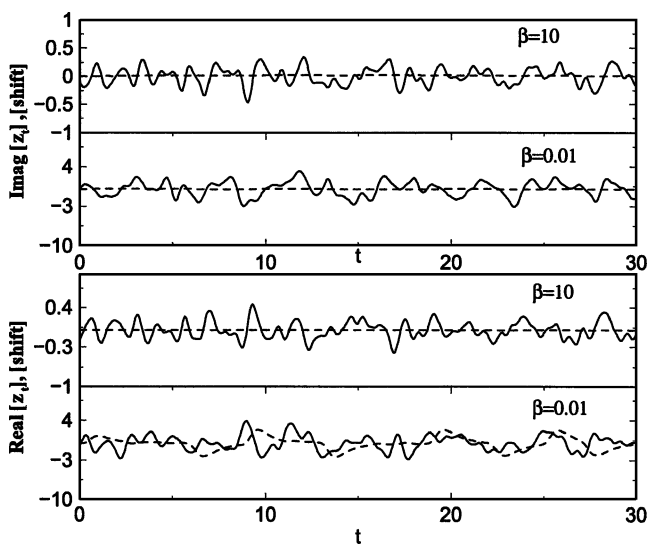

FIG. 9. Real and imaginary part of the noise (solid lines) and the shift term (dashed lines) as a function of time for both temperature regimes.

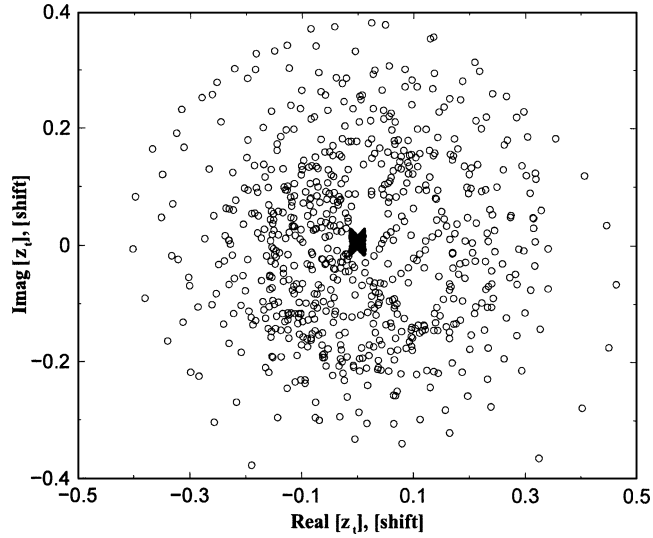

FIG. 10. Real and imaginary part of the noise (circles) and shift term (crosses) for low temperature $\beta=10$.

These results can be seen more clearly in Figs. 10 and 11, which show the real and imaginary parts of the shift term and the noise for low and high temperatures, respectively. We observe that at low temperatures the region in which the shift is distributed (a black point located around the center of the coordinate system in Fig. 10) is small in comparison to the region of values of z_t. The situation at high temperatures is different, as we can see in Fig. 11. Here, the values of the shift term spreads horizontally across the real axis with magnitudes equal to those of the noise.

The latter results explain why at high temperatures it is essential to use the shifted noise equation (41), taking into account dynamically the dynamics of the probability distribution. For lower temperatures this shift is much less important, and the original linear equation can still be used satisfactorily.

E. Noise and shift for other temperatures

Let us study the time averaged magnitude of the shift term in comparison to that of the noise for other temperature

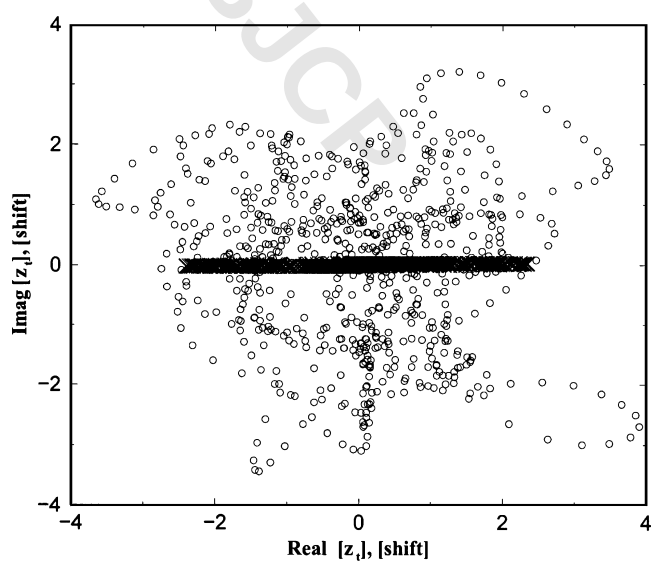

FIG. 11. Same as Fig. 10 but now for high temperature $\beta=0.01$.

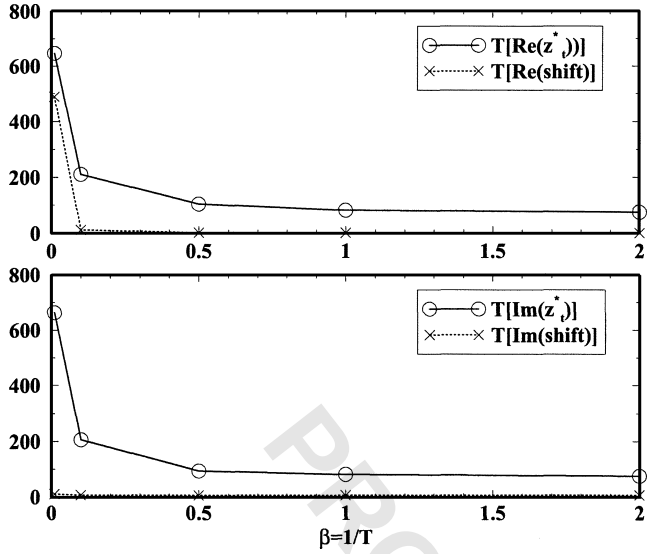

FIG. 12. Real and imaginary part of the time average (denoted as $T[*]$) of the absolute value of the noise (solid line with circles) and shift term (dotted line with crosses) for different inverse temperatures β. Only for very high temperatures the time average of the shift is relevant in comparison to the nonshifted noise.

values. Here we define the time averaged magnitude of a stochastic quantity $f(t)$ simply as $T[f]=1/T\int_0^T d\tau|f(\tau)|$. The relation between these values will again give us an idea of the necessity of using a nonlinear equation instead of the linear one. For intermediate temperatures (for values of β between 0.01 and 10) we see in Fig. 12 that only for very high temperatures (values of β close to zero), the magnitude of the real part of the shift is comparable to that of the noise, and therefore a nonlinear equation is needed. However, for β greater than 0.1, even the real part of the shift term saturates to magnitudes very close to zero in comparison to the magnitude of the noise, which saturates to values of ≈ 100 (in inverse time units).

V. CONCLUSIONS

Two different stochastic linear equations which describe the dynamics of a quantum open system, the convolutionless equation (13) (Refs. 17 and 19) and the convoluted equation (23),[16] have been compared and shown to be equivalent up to second order in the perturbation parameter. We have verified their equivalence numerically for a spin-boson system with a Hermitian coupling operator σ_x. The linear equation (13), when considering the effects of the interaction with the quantum open system in the probability distribution of the bath, gives rise to a second type of stochastic equation which is nonlinear with the wave function $|\psi_t\rangle$, but which still evolves non-normalized states [in the case of Eq. (41)] or normalized states, in the case of Eq. (43).[16,25] For the spin-boson model, the linear and the two nonlinear equations have been studied for high and low temperatures, showing how the temperature is a very important parameter to decide whether it is necessary to use a nonlinear equation. Indeed, in the high temperature regime, the shifted noise $\tilde{z}_t$ appearing in the two nonlinear equations becomes very different from the original noise z_t of the linear equation. The physical reason underlying this behavior is the dynamics of the environmental distribution (Husimi) function $Q_t(z,z^*)$ that may evolve considerably throughout the phase space of the bath. In such a case, nonlinear equations lead to a much more efficient sampling than linear ones. At low temperatures, however, we show that the noise probability distribution does not evolve significantly and the shifted noise remains approximately equal to the nonshifted noise which drives the linear equation. As a consequence, the improvement in the sampling provided by nonlinear equations is not very appreciable, and the best choice in this case is the simpler linear equation. It is also interesting to point out that the nonlinear equation that evolves normalized states (43) does not present a further improvement in the sampling (at least in the spin-boson model) in comparison with the nonlinear equation (41) which still evolves non-normalized states, with the need, however, to keep track of the norm. While mathematically, both equations should give identical results anyway, we here see that even in practical applications, there is no difference in the quality or efficiency of the results obtained from these two nonlinear equations.

ACKNOWLEDGMENTS

The authors thank G. Nicolis and José M. Gómez Llorente for their encouragement and support, and M. Esposito and A. Ruíz for fruitful discussions at Brussels and La Laguna. Support was provided by Gobierno de Canarias (Grant No. PI2002/009), Ministerio de Ciencia y Tecnología (Grant No. BFM2001-3349), and the EU (CERION II). I.d.V. was financially supported by a Ministerio de Ciencia y Tecnología doctoral fellowship (Grant No. AP2001-2226). P.G. thanks the "Communauté française de Belgique-Actions de Recherche Concertées," the F.N.R.S. (Belgium), the F.R.N.C., and U.L.B for financial support.

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