

Master equation incorporating the system-environment correlations present in the joint equilibrium state

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We present a general master equation, correct to second order in the system-environment coupling strength, that takes into account the initial system-environment correlations. We assume that the system and its environment are in a joint thermal equilibrium state, and thereafter, a unitary operation is performed to prepare the desired initial system state, with the system Hamiltonian possibly changing thereafter as well. We show that the effect of the initial correlations shows up in the second-order master equation as an additional term, similar in form to the usual second-order term describing relaxation and decoherence in quantum systems. We apply this master equation to a generalization of the paradigmatic spin-boson model, namely, a collection of two-level systems interacting with a common environment of harmonic oscillators, as well as a collection of two-level systems interacting with a common spin environment. We demonstrate that, in general, the initial system-environment correlations need to be accounted for in order to accurately obtain the system dynamics.

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I. INTRODUCTION

The study of quantum systems interacting with their environment, namely, open quantum systems, has gained immense importance lately. This is due to both practical reasons and the relevance of open quantum systems to the foundations of quantum mechanics [1]. In particular, precise quantum coherent control and state preparation necessary for quantum computation and information are possible only by taking into account the interaction of a quantum system with its environment, while the process of decoherence sheds light on the so-called measurement problem. Among the variety of tools and techniques developed to tackle the dynamics of open quantum systems, the most popular approach is the quantum-master-equation approach, in which a differential equation for the time evolution of the system state is obtained and solved. The total system-environment Hamiltonian is written down, and then with this total Hamiltonian and the initial system-environment state, the time evolution of the total system-environment state is examined. Since we are typically interested in only the system dynamics, the environment is traced out to obtain the master equation. Unfortunately, performing this process to obtain the master equation for most realistic system-environment models involves making a series of approximations. For example, the system-environment coupling strength is assumed to be weak so that the joint time-evolution operator can be found perturbatively [1,2]. The environment is assumed to have a short “memory time” (the Markovian approximation), means that the environment loses information about the system very quickly [3,4]. Finally, the initial system-environment state is assumed to be a simple product state, with the system and the environment independent of one another [3].

With increasingly sophisticated quantum technologies, each of the assumptions typically made in the derivation of master equations has come under renewed reexamination. Master equations that allow one to deal with stronger system-environment coupling strengths have been formulated (see, for example, Ref. [5]). Measures of non-Markovianity have also been put forward [4]. Most pertinent for us, the role of the initial system-environment correlations—the ones present in the total system-environment state at the initial time—has been investigated widely [3,6–37]. Such studies have generally been performed using exactly solvable models such as the pure dephasing model of a two-level system interacting with a collection of harmonic oscillators [24,26]. Some efforts have, nevertheless, been made to consider master equations beyond exactly solvable regimes that include the effect of the initial correlations. For example, in Ref. [27], the system and its environment were allowed to come to thermal equilibrium, and thereafter a projective measurement was performed on the system to prepare the desired initial system state. It was shown that the effect of the initial correlations appears as an additional term in the second-order master equation, similar in form to the first term in the master equation that describes the free system evolution. This approach was later generalized to higher-order system-environment coupling strengths [33]. Along similar lines, in this paper, we consider the quantum system and its environment to reach a joint equilibrium state. A unitary operator is then performed on the system to prepare (approximately) a desired initial system state, and a time-local master equation, correct to second-order in the system-environment coupling strength, that describes the ensuing dynamics of the system is derived. In fact, the system Hamiltonian before the application of the unitary operator can be different from the system Hamiltonian after the unitary operator—the former plays a role in the initial-state preparation, while the latter plays a role in the dynamics thereafter. We show that the effect of the initial correlations is again

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contained in an additional term in the master equation, but now the form of this additional term is similar to that of the second term in the usual master equation that describes the relaxation and decoherence of open quantum systems. We then apply our master equation to a collection of two-level systems interacting with a common environment of harmonic oscillators. We work out the additional term in the master equation and perform numerical simulations to show that the effect of the initial correlations increases as the number of two-level systems increases. Along similar lines, we also apply our master equation to analyze the effect of initial correlations for a collection of two-level systems interacting with a spin environment.

This paper is organized as follows. In Sec. II, we derive our general time-local second-order master equation. Section III discusses the application of this master equation to the large spin-boson model, while Sec. IV applies the master equation to a collection of two-level systems interacting with a spin environment. We then conclude in Sec. V. The Appendixes consist of some technical details regarding the initial-system-state preparation, the usual relaxation term in the master equation, the exactly solvable pure dephasing limit of the large spin-boson model, the generalization of the master equation to a time-dependent system Hamiltonian, and the derivation of environment correlation functions.

II. THE FORMALISM

We start by briefly discussing the problem we wish to solve. We are given a quantum system which is interacting with its environment and has reached a joint equilibrium state. At the initial time, a unitary operation is performed on the system alone. The system Hamiltonian itself may also be changed—after all, the system Hamiltonian parameters initially may be chosen in order to prepare an approximately pure system state, and the unitary operation thereafter applied prepares a desired approximately pure initial system state. The system Hamiltonian parameters can then be changed to generate the desired nontrivial system quantum dynamics. Our problem is to derive the master equation, correct to second order in the system-environment coupling strength, that describes these system dynamics. We write the system-environment Hamiltonian as

$$H_{\text{tot}} = \begin{cases} H_{S0} + H_B + \alpha V & t \leq 0, \\ H_S + H_B + \alpha V & t > 0. \end{cases} \quad (1)$$

Here H_S is the system Hamiltonian corresponding to coherent evolution of the system only after the initial time $t = 0$ at which the system state is prepared. H_{S0} is similar to H_S in the sense that both operators live in the same Hilbert space, but they may have different parameters. H_B is the Hamiltonian of the environment, and V corresponds to the system-environment coupling. α is simply a dimensionless parameter introduced to keep track of the perturbation order; at the end of the calculation, we will set $\alpha = 1$. Let us now briefly discuss the initial-state preparation.

A. Initial-state preparation

We let our system come to a joint equilibrium state with the environment. What we mean by this is that the equilibrium

state of the system is not simply proportional to $e^{-\beta H_{S0}}$; there are corrections due to the finite system-environment coupling strength [38]. We instead consider the system and the environment together in the thermal equilibrium state proportional to $e^{-\beta H_{\text{tot}}}$ with $H_{\text{tot}} = H_{S0} + H_B + \alpha V$; the system state can be obtained by simply tracing out the environment. A unitary operator Ω is then applied to the system. The initial system-environment state is consequently

$$\rho_{\text{tot}}(0) = \frac{\Omega e^{-\beta H_{\text{tot}}} \Omega^\dagger}{Z_{\text{tot}}}, \quad (2)$$

where $Z_{\text{tot}} = \text{Tr}_{S,B}[e^{-\beta H_{\text{tot}}}]$ is the partition function and $\text{Tr}_{S,B}$ denotes the trace over the system and the environment. Now, assuming the system-environment coupling strength is weak, we can perform a perturbative expansion of this initial system-environment state to second order in the system-environment coupling strength. Writing the system-environment interaction as $V = F \otimes B$, where F and B are operators living in the system and the environment Hilbert space, respectively (the extension to the more general case $V = \sum_a F_a \otimes B_a$ is straightforward), we find that the initial system state is (see Appendix A for details)

$$\rho(0) = \frac{e^{-\beta H_{S0}^R}}{Z_{S0} Z'} \left[\mathbb{1} + \int_0^\beta \int_0^\lambda F^R(\lambda) F^R(\lambda') \times \langle B(\lambda) B(\lambda') \rangle_B d\lambda' d\lambda \right], \quad (3)$$

where $H_{S0}^R = \Omega H_{S0} \Omega^\dagger$, $F^R(\lambda) = \Omega F(\lambda) \Omega^\dagger$, $F(\lambda) = e^{\lambda H_{S0}} F e^{-\lambda H_{S0}}$, $Z_{S0} = \text{Tr}_S[e^{-\beta H_{S0}}]$, $B(\lambda) = e^{\lambda H_B} B e^{-\lambda H_B}$, $\langle \dots \rangle_B = \text{Tr}_B[e^{-\beta H_B}(\dots)]/Z_B$, $Z_B = \text{Tr}_B[e^{-\beta H_B}]$, and

$$Z' = 1 + \int_0^\beta \int_0^\lambda \langle F(\lambda) F(\lambda') \rangle_S \langle B(\lambda) B(\lambda') \rangle_B d\lambda' d\lambda, \quad (4)$$

with $\langle \dots \rangle_S = \text{Tr}_S[e^{-\beta H_{S0}}(\dots)]/Z_{S0}$. With the initial system state correct to second order in the system-environment coupling strength available, we now turn our attention to deriving the second-order master equation.

B. Derivation of the master equation

We derive a master equation that describes the time evolution of the system for $t > 0$. The system-environment Hamiltonian is

$$H_{\text{tot}} = H_S + H_B + \alpha V \equiv H_0 + \alpha V.$$

Note that the system Hamiltonian H_S can be different from the previous system Hamiltonian H_{S0} . In fact, H_S can even be a time-dependent Hamiltonian without changing the subsequent derivation. Using perturbation theory, the unitary time evolution with such a Hamiltonian can be written as

$$U(t) \approx U_0(t) \left[1 - \alpha \int_0^t U_0^\dagger(s) V U_0(s) ds \right], \quad (5)$$

where $U_0(t) \equiv U_S(t) \otimes U_B(t)$ is the “free” unitary time-evolution operator corresponding to H_0 , that is, the uncoupled system and its environment. The matrix elements of the system density matrix can be written as $\rho_{mn}(t) = \text{Tr}_S[|n\rangle\langle m| \rho(t)]$, where $|m\rangle$ and $|n\rangle$ are some basis states of the

system. Since $\rho(t) = \text{Tr}_B \rho_{\text{tot}}(t)$, we can alternatively write

$$\rho_{mn}(t) = \text{Tr}_{S,B} [X_{nm}^H(t) \rho_{\text{tot}}(0)],$$

where $X_{nm}^H(t) = U^\dagger(t) (|n\rangle\langle m| \otimes \mathbb{1}_B) U(t)$. The master equation can then be written in the general form

$$\frac{d}{dt} \rho_{mn}(t) = \text{Tr}_{S,B} \left[\rho_{\text{tot}}(0) \frac{d}{dt} X_{nm}^H(t) \right]. \quad (6)$$

To make further progress, we note that $X_{nm}^H(t)$ is a Heisenberg picture operator. Using the Heisenberg equation of motion and Eq. (5), it can be shown that, correct to second order in the system-environment coupling strength,

$$\begin{aligned} \frac{d}{dt} X_{nm}^H(t) &= i[H_0^H(t), X_{nm}^H(t)] + i\alpha[\tilde{V}(t), \tilde{X}_{nm}(t)] \\ &+ \alpha^2 \int_0^t ds [[\tilde{V}(t), \tilde{X}_{nm}(t)], \tilde{V}(s)], \end{aligned} \quad (7)$$

where the tildes denote time evolution under the free unitary operator $U_0(t)$ and the superscript H denotes time evolution with the full time-evolution operator. Using Eq. (7) and given the initial system-environment state $\rho_{\text{tot}}(0)$ in Eq. (2), we can derive the master equation that describes the time evolution of the quantum system by simplifying Eq. (6). The result due to the first term in Eq. (7) is very straightforward. We simply have that

$$\begin{aligned} &\text{Tr}_{S,B} \{ \rho_{\text{tot}}(0) i[H_0^H(t), X_{nm}^H(t)] \} \\ &= i \text{Tr}_{S,B} \{ \rho_{\text{tot}}(t) [H_S + H_B, (|n\rangle\langle m| \otimes \mathbb{1}_B)] \} \\ &= i \text{Tr}_S \{ \rho(t) [H_S, |n\rangle\langle m|] \} \\ &= i \langle m | [\rho(t), H_S] | n \rangle. \end{aligned} \quad (8)$$

This term simply tells us about the free system evolution corresponding to the system Hamiltonian H_S . To calculate the next term in our master equation, that is,

$$i\alpha \text{Tr}_{S,B} \{ \rho_{\text{tot}}(0) [V(t), X_{nm}(t)] \},$$

we perform a perturbative expansion of the initial system-environment state. It is useful to write $\rho_{\text{tot}}(0) = \rho_{\text{tot}}^{(0)} + \rho_{\text{tot}}^{(1)}$, where [see Eq. (A2) in Appendix A]

$$\rho_{\text{tot}}^{(0)}(0) = \frac{\Omega e^{-\beta(H_{S_0} + H_B)} \Omega^\dagger}{Z_{\text{tot}}} = \rho_{S_0}^R \otimes \rho_B, \quad (9)$$

$$\rho_{\text{tot}}^{(1)}(0) = \frac{-\alpha \Omega e^{-\beta(H_{S_0} + H_B)} Q_{SB}(\beta) \Omega^\dagger}{Z_{\text{tot}}}. \quad (10)$$

Here $\rho_{S_0}^R = e^{-\beta H_{S_0}} / Z_{S_0}$, $\rho_B = e^{-\beta H_B} / Z_B$, the partition function $Z_{\text{tot}} = Z_{S_0} Z_B$, and $Q_{SB}(\beta) = \int_0^\beta d\lambda F(\lambda) \otimes B(\lambda)$, with $F(\lambda) = e^{\lambda H_{S_0}} F e^{-\lambda H_{S_0}}$ and $B(\lambda) = e^{\lambda H_B} B e^{-\lambda H_B}$. We do not need the higher-order terms since there is already a factor of α in $i\alpha[V(t), X_{nm}(t)]$. Now, the contribution of $\rho_{\text{tot}}^{(0)}$ is

$$\begin{aligned} &i\alpha \text{Tr}_{S,B} \{ \rho_{\text{tot}}^{(0)}(0) [U_0^\dagger(t) V U_0(t), U_0^\dagger(t) X_{nm} U_0(t)] \} \\ &= i\alpha \text{Tr}_{S,B} \{ \rho_{S_0}^R \otimes \rho_B U_0^\dagger(t) [F \otimes B, |n\rangle\langle m| \otimes \mathbb{1}_B] U_0(t) \} \\ &= i\alpha \text{Tr}_S \{ \rho_{S_0}^R U_S^\dagger(t) [F, Y_{nm}] U_S(t) \} \times \langle B(it) \rangle_B. \end{aligned}$$

Since $\langle B(it) \rangle_B$ is usually zero for most system-environment models, this contribution turns out to be zero. The most interesting contribution is due to $\rho_{\text{tot}}^{(1)}(0)$. Using this along with the second term in Eq. (7), we get

$$\begin{aligned} &i\alpha \text{Tr}_{S,B} \{ \rho_{\text{tot}}^{(1)}(0) [U_0^\dagger(t) V U_0(t), U_0^\dagger(t) X_{nm} U_0(t)] \} \\ &= \frac{-i\alpha^2}{Z_{S_0}} \int_0^\beta \text{Tr}_{S,B} \{ \rho_B \Omega e^{-\beta H_{S_0}} F(\lambda) \Omega^\dagger \otimes B(\lambda) U_S^\dagger(t) [F, |n\rangle\langle m|] U_S(t) U_B^\dagger(t) B U_B(t) \} d\lambda \\ &= \frac{-i\alpha^2}{Z_{S_0}} \int_0^\beta \text{Tr}_S \{ \Omega e^{-\beta H_{S_0}} F(\lambda) \Omega^\dagger U_S^\dagger(t) [F, |n\rangle\langle m|] U_S(t) \} \text{Tr}_B \{ \rho_B B(\lambda) B(it) \} d\lambda \\ &= \frac{-i\alpha^2}{Z_{S_0}} \int_0^\beta \langle m | [U_S(t) \Omega e^{-\beta H_{S_0}} F(\lambda) \Omega^\dagger U_S^\dagger(t), F] | n \rangle B_{\text{corr}}(\lambda, t) d\lambda, \end{aligned} \quad (11)$$

where $B_{\text{corr}}(\lambda, t) = \text{Tr}_B \{ \rho_B B(\lambda) B(it) \}$. This is the additional term in the master equation that takes into account the effect of the initial correlations, correct to second order in the system-environment coupling strength. In basis-independent form, we can write this term as

$$-i[\tilde{\rho}(t) J_{\text{corr}}^R(\beta, t), F], \quad (12)$$

where we have defined $\tilde{\rho}(t) = U_S(t) \rho_{S_0}^R U_S^\dagger(t)$ and

$$J_{\text{corr}}^R(\beta, t) = \int_0^\beta \overleftarrow{F}^R(\lambda, t) B_{\text{corr}}(\lambda, t) d\lambda, \quad (13)$$

$$\overleftarrow{F}^R(\lambda, t) = U_S(t) \Omega e^{\lambda H_{S_0}} F e^{-\lambda H_{S_0}} \Omega^\dagger U_S^\dagger(t). \quad (14)$$

We would like to replace $\tilde{\rho}(t)$ by $\rho(t)$ so that the only density matrix in the master equation is $\rho(t)$, and this seems to be

feasible since the corrections would be of order higher than second order in the system-environment coupling strength. However, it can be checked that $-i[\rho(t) J_{\text{corr}}^R(\beta, t), F]$ is not guaranteed to be Hermitian. To proceed, we first write

$$-i[\tilde{\rho}(t) J_{\text{corr}}^R(\beta, t), F] = -\frac{i}{2} \{ [\tilde{\rho}(t) J_{\text{corr}}^R(\beta, t), F] - \text{H.c.} \}, \quad (15)$$

where H.c. denotes the Hermitian conjugate. This is permitted because $-i[\tilde{\rho}(t) J_{\text{corr}}^R(\beta, t), F]$ is Hermitian, so $[\tilde{\rho}(t) J_{\text{corr}}^R(\beta, t), F]$ is anti-Hermitian. We now replace $\tilde{\rho}(t)$ by $\rho(t)$. This step is also allowed since the corrections are of order higher than the second-order master equation that we are considering. Consequently, the term in the master equation that takes into account the initial correlations

is $-\frac{i}{2}\{[\rho(t)J_{\text{corr}}^R(\beta, t), F] - \text{H.c.}\}$, and this is manifestly Hermitian.

We next simplify the contribution of the third term in Eq. (7). It is clear that now only $\rho_{\text{tot}}^{(0)}(0)$ contributes. Manipulations similar to those performed above lead to (see Appendix B for details)

$$\alpha^2 \int_0^t \langle m | \{ [\bar{F}(t, s) \tilde{\rho}(t), F] C_{ts} + \text{H.c.} \} | n \rangle ds,$$

where the environment correlation function is $C_{ts} = \langle B(it)B(is) \rangle_B$, $\bar{F}(t, s) = U_S(t, s)F U_S^\dagger(t, s)$. We can further replace $\tilde{\rho}(t)$ by $\rho(t)$ to get

$$\alpha^2 \int_0^t \langle m | \{ [\bar{F}(t, s) \rho(t), F] C_{ts} + \text{H.c.} \} | n \rangle ds.$$

Once again, this is permitted since the corrections lead to terms of higher order in the master equation (compared to the second-order master equation that we are considering). We now put all the terms together to arrive at the general basis-independent form of the master equation, given by

$$\begin{aligned} \frac{d}{dt} \rho(t) = & i[\rho(t), H_S] - \frac{i}{2} \{ [\rho(t)J_{\text{corr}}^R(\beta, t), F] - \text{H.c.} \} \\ & + \int_0^t \{ [\bar{F}(t, s) \rho(t), F] C_{ts} + \text{H.c.} \} ds. \end{aligned} \quad (16)$$

Let us note that we have assumed implicitly that the timescale on which the unitary operator Ω is implemented and the time taken to change the system Hamiltonian from H_{S0} to H_S are much smaller than the other timescales such as the environment correlation time, the relaxation time, and the free system evolution timescale. We also emphasize that the same master equation applies if the system Hamiltonian is time dependent with the caveat that finding the free system time-evolution operator $U_S(t)$ will then be, in general, highly nontrivial. In fact, we use such a time-dependent Hamiltonian in Appendix D to examine more carefully what happens when the system Hamiltonian parameters are not changed instantaneously.

III. APPLICATION TO THE LARGE SPIN-BOSON MODEL

We now apply our derived master equation to a variant of the paradigmatic spin-boson model [1] with N two-level systems interacting with a common environment of harmonic oscillators [26,27,39]. Recall that the total system-environment Hamiltonian is given by $H_{\text{tot}} = H_{S0} + H_B + V$ for $t < 0$, while $H_{\text{tot}} = H_S + H_B + V$ for $t \geq 0$. For the large

spin-boson model, we consider

$$H_{S0} = \varepsilon_0 J_z + \Delta_0 J_x, \quad (17)$$

$$H_S = \varepsilon J_z + \Delta J_x, \quad (18)$$

$$H_B = \sum_k \omega_k b_k^\dagger b_k, \quad (19)$$

$$V = J_z \sum_k (g_k^* b_k + g_k b_k^\dagger), \quad (20)$$

where J_x, J_y, J_z are the collective spin operators with $J^2 = J_x^2 + J_y^2 + J_z^2$, ε is the energy bias, Δ is the tunneling amplitude, H_B is the bath of harmonic oscillators (we are ignoring the zero-point energy), and V describes the interaction between the common harmonic oscillator bath and the spin system. We have set $\hbar = 1$ throughout, and the values of other parameters are in dimensionless units. Note that the system operator $F = J_z$, and the bath operator $B = \sum_k (g_k^* b_k + g_k b_k^\dagger)$. One imagines that the large-spin system has been interacting with the environment for a long time with a relatively large value of ε_0 and a small value of Δ_0 . In such a situation with $\beta\varepsilon_0 \gg 1$, realized, for example, by applying a suitably large static magnetic field, the state of the system will approximately correspond to the state with all spins down in the z direction. At time $t = 0$, we then apply a unitary operator to prepare the desired initial state. For example, if the desired initial state is one with all spins in the x direction, then the unitary operator that should be applied is $\Omega = e^{i\pi J_y/2}$. In other words, a $\frac{\pi}{2}$ pulse is used to prepare the initial system state, with the assumption that this pulse takes a very short time to apply. In particular, we assume that the duration of the pulse is smaller than the inverse of the effective Rabi frequency $\tilde{\Delta} = \sqrt{\varepsilon^2 + \Delta^2}$ as well as the inverse of the environment cut-off frequency. With the initial state approximately prepared, we can then change the parameters of the system Hamiltonian to whatever values we desire to generate any required system evolution; in our example, this entails changing the energy bias from ε_0 to ε so that the effect of the tunneling term ΔJ_x becomes more evident. Again, we assume that this change takes place over a very short time interval; this approximation is further critically examined in Appendix D. Let us, then, look at how the initial system-environment correlations appear in the system evolution using our general master equation.

Our first objective is to calculate the operator J_{corr}^R . To do so, we first find [see Eq. (14)]

$$\begin{aligned} \overleftarrow{F}^R(\lambda, t) = & U_S(t) [\Omega (e^{\lambda H_{S0}} F e^{-\lambda H_{S0}}) \Omega^\dagger] U_S^\dagger(t) \\ = & J_x [a_x d_x + a_y c_x - a_z b_x] + J_y [a_x d_y + a_y c_y - a_z b_y] \\ & + J_z [a_x d_z + a_y c_z - a_z b_z], \end{aligned}$$

with

$$\begin{aligned} a_x = & \frac{\varepsilon_0 \Delta_0}{\Delta^2} \{1 - \cosh(\lambda \Delta')\}, & a_y = & \frac{-i \Delta_0}{\Delta'} \sinh(\lambda \Delta'), & a_z = & \frac{\varepsilon_0^2 + \Delta_0^2 \cosh(\lambda \Delta')}{\Delta^2}, & b_x = & \frac{\Delta^2 + \varepsilon^2 \cos(\tilde{\Delta} t)}{\tilde{\Delta}^2}, \\ b_y = & \frac{\varepsilon}{\tilde{\Delta}} \sin(\tilde{\Delta} t), & b_z = & \frac{\varepsilon \Delta}{\tilde{\Delta}^2} \{1 - \cos(\tilde{\Delta} t)\}, & c_x = & -\frac{\varepsilon}{\tilde{\Delta}} \sin(\tilde{\Delta} t), & c_y = & \cos(\tilde{\Delta} t), & c_z = & \frac{\Delta}{\tilde{\Delta}} \sin(\tilde{\Delta} t), \\ d_x = & \frac{\varepsilon \Delta}{\tilde{\Delta}^2} \{1 - \cos(\tilde{\Delta} t)\}, & d_y = & -\frac{\Delta}{\tilde{\Delta}} \sin(\tilde{\Delta} t), & d_z = & 1 + \frac{\Delta^2}{\tilde{\Delta}^2} \{\cos(\tilde{\Delta} t) - 1\}. \end{aligned}$$

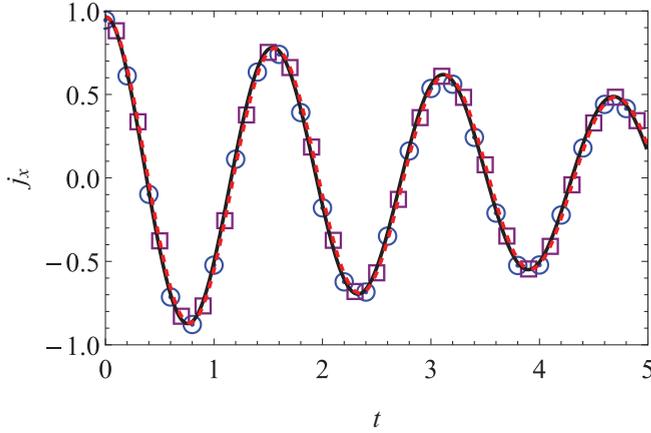


FIG. 1. Behavior of $j_x = 2\langle J_x \rangle / N$ versus t for $N = 1$ using the exact solution with (blue circled dots) and without (purple squares) initial correlations and using the master equation with (solid black line) and without (dashed red line) initial correlations. We have used dimensionless units with $\hbar = 1$ for all the figures. Here we have set $\varepsilon = \varepsilon_0 = 4$, $G = 0.05$, $\beta = 1$, and $\omega_c = 5$.

Here $\Delta^2 = \varepsilon_0^2 + \Delta_0^2$, and $\tilde{\Delta}^2 = \varepsilon^2 + \Delta^2$. In short,

$$\overleftarrow{F}^R(\lambda, t) = \alpha_1(\lambda, t)J_x + \alpha_2(\lambda, t)J_y + \alpha_3(\lambda, t)J_z, \quad (21)$$

where

$$\alpha_1(\lambda, t) = a_x d_x + a_y c_x - a_z b_x,$$

$$\alpha_2(\lambda, t) = a_x d_y + a_y c_y - a_z b_y,$$

$$\alpha_3(\lambda, t) = a_x d_z + a_y c_z - a_z b_z.$$

It then follows that [see Eq. (13)]

$$J_{\text{corr}}^R(\beta, t) = P(\beta, t)J_x + Q(\beta, t)J_y + R(\beta, t)J_z, \quad (22)$$

with

$$P(\beta, t) = \int_0^\beta \alpha_1(\lambda, t) B_{\text{corr}}(\lambda, t) d\lambda,$$

$$Q(\beta, t) = \int_0^\beta \alpha_2(\lambda, t) B_{\text{corr}}(\lambda, t) d\lambda,$$

$$R(\beta, t) = \int_0^\beta \alpha_3(\lambda, t) B_{\text{corr}}(\lambda, t) d\lambda.$$

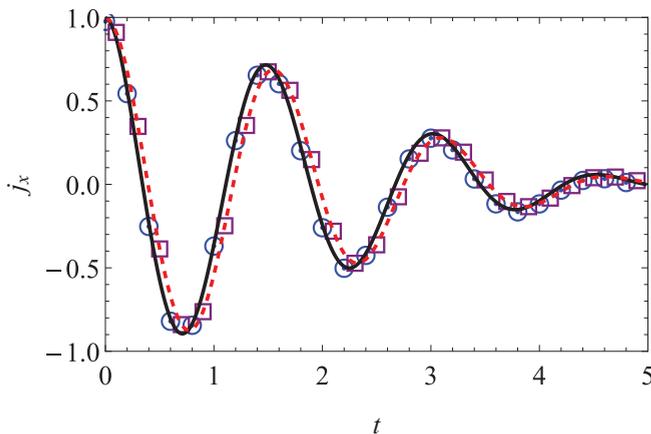


FIG. 2. Same as Fig. 1, except $N = 4$.

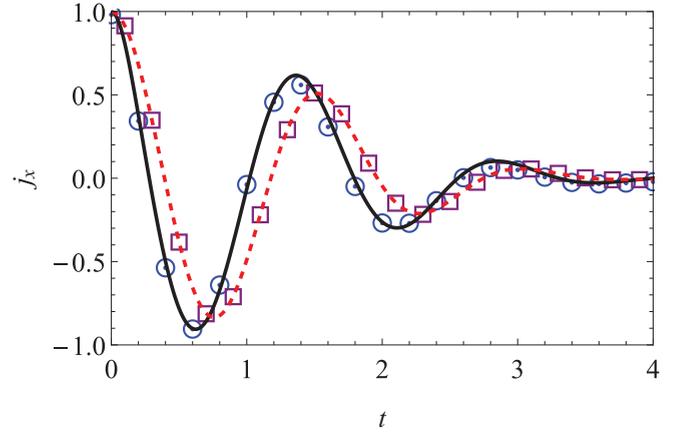


FIG. 3. Same as Fig. 1, except $N = 10$.

We now calculate the bath correlation term $B_{\text{corr}}(\lambda, t)$. First,

$$B(\lambda) = \sum_k (g_k^* e^{-\lambda \omega_k} b_k + g_k e^{\lambda \omega_k} b_k^\dagger). \quad (23)$$

Since $B_{\text{corr}}(\lambda, t) = \text{Tr}[\rho_B B(\lambda) B(it)]$, we find (see Appendix E for details)

$$B_{\text{corr}}(\lambda, t) = \sum_k |g_k|^2 \{ e^{-\omega_k(\lambda - it)} + 2n_k \cosh(\lambda \omega_k - i\omega_k t) \}, \quad (24)$$

with n_k given by Bose-Einstein statistics as

$$n_k = \frac{1}{2} \left\{ \coth\left(\frac{\beta \omega_k}{2}\right) - 1 \right\}. \quad (25)$$

To perform the sum over the environment modes, we use the spectral density $J(\omega)$ via $\sum_k |g_k|^2 (\dots) \rightarrow \int_0^\infty d\omega J(\omega) (\dots)$. We generally use an Ohmic spectral density of the form $J(\omega) = G\omega e^{-\omega/\omega_c}$. The integrals are performed numerically to find $J_{\text{corr}}(\beta, t)$, and the results are incorporated in the numerical simulations of the master equation. We first look at the pure dephasing case ($\Delta = \Delta_0 = 0$)

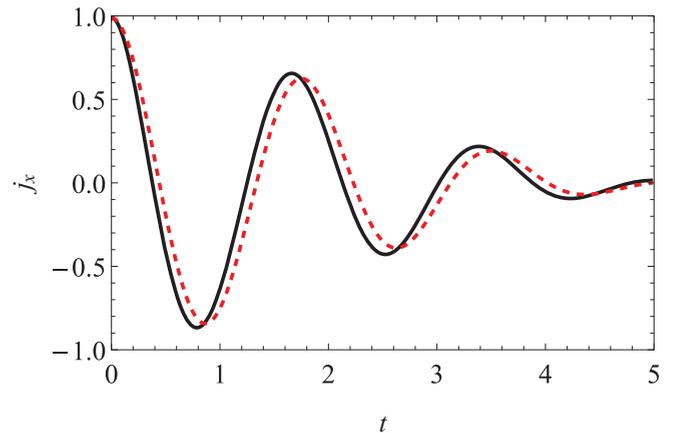
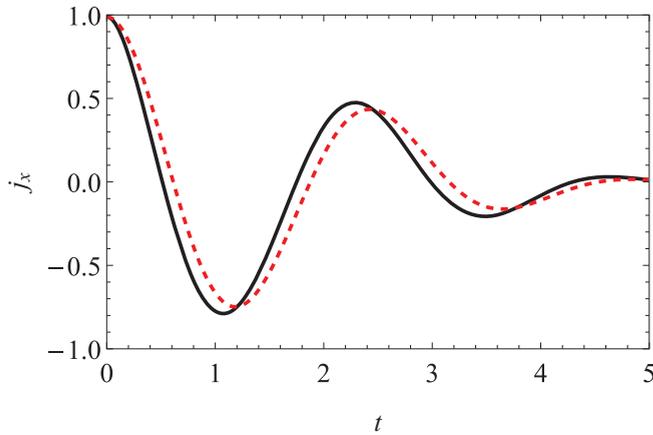
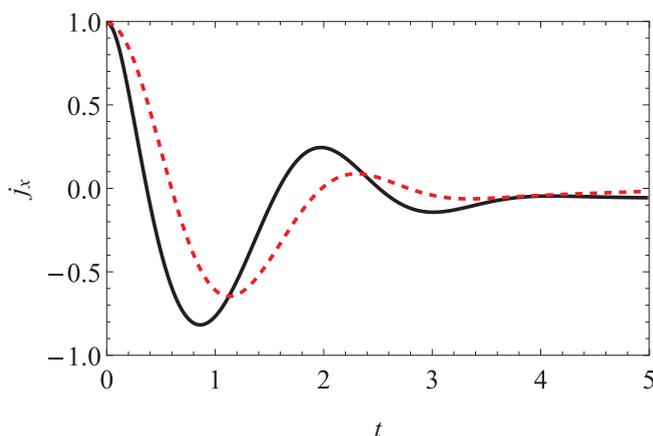
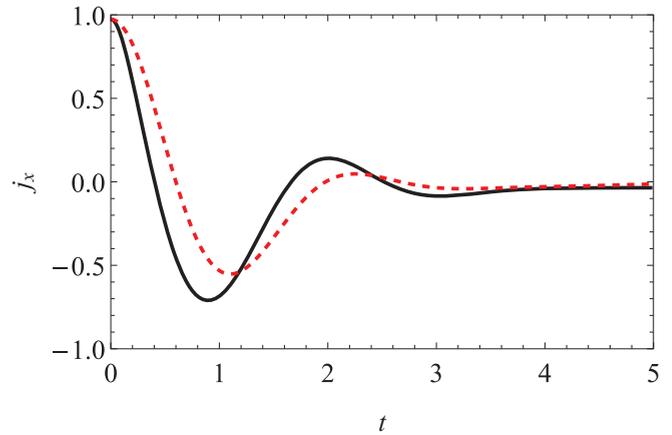


FIG. 4. Behavior of j_x versus t for $N = 2$ with (black solid line) and without (dashed red line) taking into account initial correlations. Here we have used $\varepsilon_0 = 4$, $\varepsilon = 2.5$, and $\Delta = \Delta_0 = 0.5$, while the rest of the parameters are the same as in Fig. 1.

FIG. 5. Same as Fig. 4, except $N = 4$.

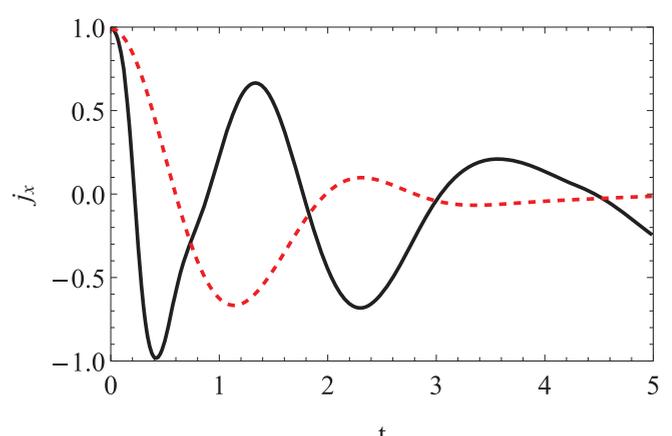
since this case can be solved exactly and serves as a useful benchmark (details of the exact solution are given in Appendix C). We illustrate our results in Fig. 1 for $N = 1$ by plotting $j_x = 2\langle J_x \rangle / N$. Two points should be noted. First, the role played by initial correlations is very small in this case. Second, our master equation reproduces the exact results very well. Since we expect that the role of the initial correlations increases with increasing N , we next look at $N = 4$ and $N = 10$. Results are shown in Figs. 2 and 3. It is clear that as N increases, the initial correlations play a larger and larger role. This is a manifestation of the fact that the environment harmonic oscillators can be understood to be displaced as a result of the system-environment interaction [see the displaced harmonic oscillator modes after Eq. (C7)], and as N increases, the environment harmonic oscillator modes are displaced more. Moreover, the extra term in our master equation is able to take into account the effect of the initial correlations very well.

Having shown that our master equation is able to reproduce results for the pure dephasing model, we are now in a position to go beyond the pure dephasing model and see the effects of the initial correlations. In Fig. 4, we have shown the dynamics of j_x with a nonzero value of the tunneling amplitude for $N = 2$. It is clear that the initial correlations do have a small influence on the dynamics. This effect becomes more pronounced as we increase N (see Figs. 5 and 6), which

FIG. 6. Same as Fig. 4, except $N = 10$.FIG. 7. Behavior of j_x versus t for $N = 10$ with (black solid line) and without (dashed red line) taking into account initial correlations. Here we have used the same parameters as in Fig. 6, except that $\beta = 0.5$.

signifies that the environment harmonic oscillators are more influenced by the system as N increases. We have also looked at how the role played by the initial correlations changes as the temperature changes. To this end, we compare Fig. 6, where the inverse temperature is $\beta = 1$, with Fig. 7, where $\beta = 0.5$, and Fig. 8, where $\beta = 1.5$. At higher temperatures, the effect of the initial correlations decreases, while at lower temperatures, the effect of the initial correlations increases. Mathematically, this can be seen in Eq. (22), where $P(\beta, t)$, $Q(\beta, t)$, and $R(\beta, t)$ become negligible as the temperature increases. This illustrates that our master equation produces sensible results since we do expect the role of the initial correlations to decrease as the temperature increases.

Let us now demonstrate that the effect of the initial correlations is not manifested in the dynamics of j_x alone. We show in Fig. 9 the dynamics of $j_x^{(2)} \equiv 4\langle J_x^2 \rangle / N^2$, which is not merely the sum of single-particle operators. Such an observable is relevant in the study of spin squeezing and entanglement. It is clear from Fig. 9 that the effect of the initial correlations may also need to be accounted for when studying the dynamics of quantities beyond single-particle observables. Finally, in order to illustrate that we can deal equally well with other kinds

FIG. 8. Same as Figs. 6 and 7, except $\beta = 1.5$.

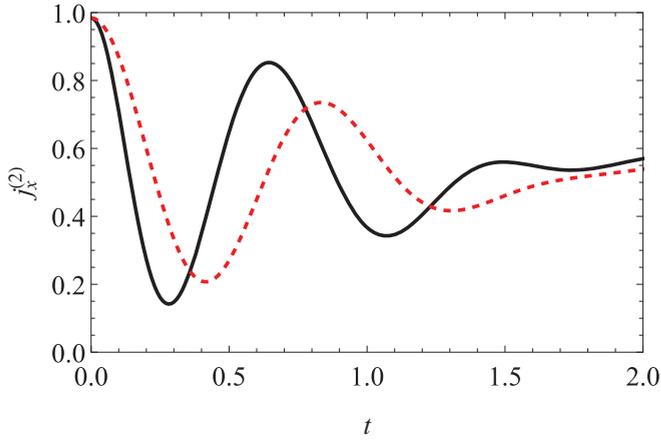


FIG. 9. Behavior of $j_x^{(2)}$ versus t for $N = 10$ with (black solid line) and without (dashed red line) taking into account initial correlations. The rest of the parameters are the same as those in Fig. 4.

of environment, we also demonstrate the effect of the initial correlations with a sub-Ohmic environment, that is, $J(\omega) = G\omega^s\omega_c^{1-s}e^{-\omega/\omega_c}$, with $s < 1$. Since sub-Ohmic environments have longer correlation times, we expect that the effect of the initial correlations will be greater as well. This is, indeed, the case, as can be seen by comparing Figs. 10 and 11 with Figs. 5 and 6, where an Ohmic environment is used.

IV. APPLICATION TO THE SPIN-SPIN ENVIRONMENT MODEL

We now consider a collection of N identical two-level systems interacting with an environment consisting of two-level systems [40–44]. We have

$$H_{S0} = \varepsilon_0 J_z + \Delta_0 J_x, \quad H_S = \varepsilon J_z + \Delta J_x,$$

$$H_B = \sum_k \frac{\omega_k}{2} \sigma_x^{(k)}, \quad V = J_z \otimes \sum_k g_k \sigma_z^{(k)},$$

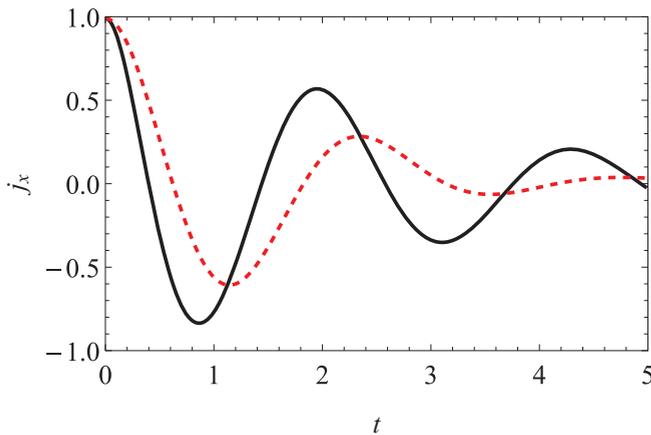


FIG. 10. Behavior of j_x versus t for $N = 4$ with (black solid line) and without (dashed red line) taking into account initial correlations. Here we have used a sub-Ohmic environment with $s = 0.5$. We also have $\varepsilon_0 = 4$, $\varepsilon = 2.5$, and $\Delta = \Delta_0 = 0.5$, while the rest of the parameters are the same as in Fig. 1.

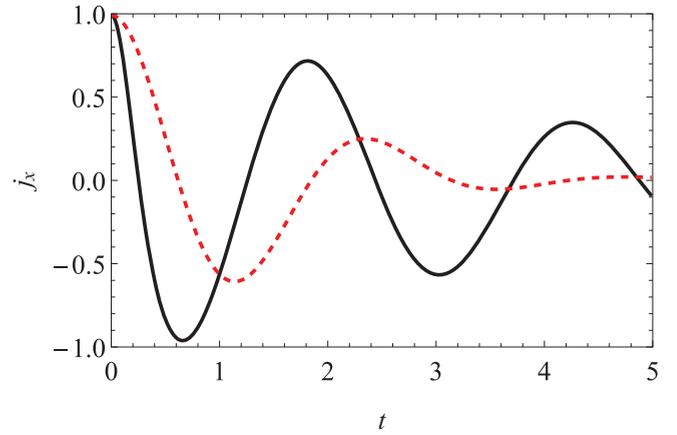


FIG. 11. Same as Fig. 10, except $N = 10$.

where $\sigma_z^{(k)}$ and $\sigma_x^{(k)}$ are the Pauli z -spin and x -spin operators of the k th environment spin, respectively, ω_k denotes the tunneling matrix element for the k th environment spin, and g_k quantifies the coupling strength. The different environment leads to a different correlation function C_{ts} as well as a different factor $J_{\text{corr}}^R(\beta, t)$ that takes into account the effect of the initial system-environment correlations. The calculation of the environment correlation function is sketched out in Appendix F. A similar calculation leads to

$$B_{\text{corr}}(\lambda, t) = \sum_k g_k^2 \left\{ \tanh\left(\frac{\beta\omega_k}{2}\right) e^{-\omega_k(\lambda-it)} + 2n_k \sinh(\lambda\omega_k - i\omega_k t) \right\}, \quad (26)$$

where n_k is given by Eq. (25). Since the factors $\alpha_1(\lambda, t)$, $\alpha_2(\lambda, t)$, and $\alpha_3(\lambda, t)$ are the same as before, this allows us to easily work out the role of the initial correlations [see Eq. (22)]. As before, to perform the sum over the environment modes, we use $\sum_k g_k^2(\dots) \rightarrow \int_0^\infty d\omega J(\omega)(\dots)$. Results are shown in Figs. 12 and 13. Once again, the role of the initial correlations is relatively small for a smaller value of

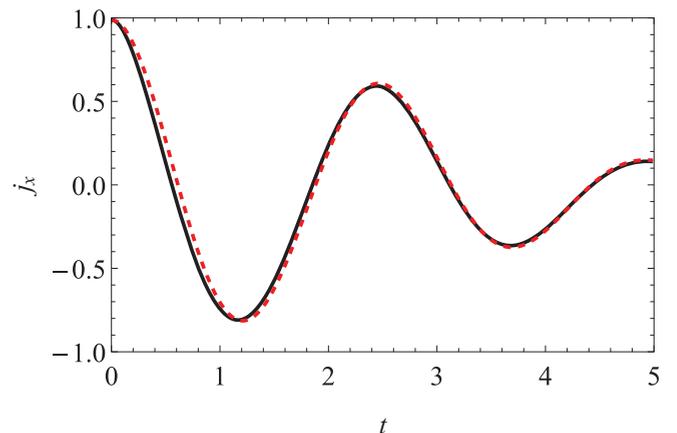
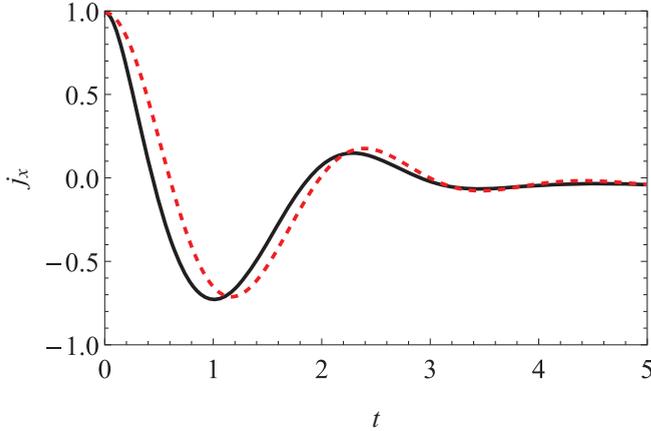


FIG. 12. Behavior of j_x versus t for $N = 4$ with (black solid line) and without (dashed red line) taking into account initial correlations. Here we have $\varepsilon_0 = 4$, $\varepsilon = 2.5$, $\Delta = \Delta_0 = 0.5$, $G = 0.05$, $\beta = 1$, and $\omega_c = 5$.

FIG. 13. Same as Fig. 12, except $N = 10$.

N . However, as N increases, it is clear that we need to take into account the role of the initial correlations to obtain an accurate picture of the system dynamics even in the case of a spin environment.

V. CONCLUSION

To conclude, we have shown that if we start from the joint thermal equilibrium state of a quantum system and its environment and then apply a unitary operation to the system to prepare the system quantum state, the initial correlations that exist in the joint thermal equilibrium state influence the subsequent dynamics of the system. We have derived a time-local master equation, correct to second order in the system-environment coupling strength, that takes into account the effect of these correlations, showing therefore that one need not necessarily be in the strong system-environment coupling regime to observe the effects of the initial correlations. The structure of this master equation is very interesting, as the form of the term that takes into account the initial correlations is the same as the relaxation and dephasing term. In this sense, one can say that the initial correlations affect the decoherence and dephasing rates, a fact which was already pointed out in studies of the role of initial correlations in pure dephasing models [24]. Finally, we actually applied our master equation to the large spin-boson model as well as to a collection of two-level systems interacting with a spin environment to quantitatively investigate the role of the initial correlations. We found that when the number of spins is small, then the initial correlations do not play a significant role. However, for a larger number of spins, the initial correlations must be accounted for in order to explain the dynamics accurately.

ACKNOWLEDGMENTS

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APPENDIX A: THE INITIAL STATE

As explained in the main text, we consider the total system-environment Hamiltonian to be $H = H_{S0} + H_B + V$.

Assuming the system-environment coupling strength is weak, we can use the Kubo identity to expand the joint state given by Eq. (2). The Kubo identity tells us that for any two arbitrary operators X and Y ,

$$e^{\beta(X+Y)} = e^{\beta X} \left[\mathbb{1} + \int_0^\beta e^{-\lambda X} Y e^{\lambda(X+Y)} d\lambda \right]. \quad (\text{A1})$$

By setting $X = -(H_{S0} + H_B)$ and $Y = -\alpha V$ and using the Kubo identity twice, we find that to second order in the system-environment coupling strength

$$\begin{aligned} e^{-\beta(H_{S0}+H_B+\alpha V)} &= e^{-\beta(H_{S0}+H_B)} - \alpha e^{-\beta(H_{S0}+H_B)} \int_0^\beta e^{\lambda(H_{S0}+H_B)} V e^{-\lambda(H_{S0}+H_B)} d\lambda \\ &\quad + \alpha^2 e^{-\beta(H_{S0}+H_B)} \int_0^\beta d\lambda e^{\lambda(H_{S0}+H_B)} V \\ &\quad \times e^{-\lambda(H_{S0}+H_B)} \int_0^\lambda e^{\lambda'(H_{S0}+H_B)} V e^{-\lambda'(H_{S0}+H_B)} d\lambda'. \end{aligned} \quad (\text{A2})$$

We now write the system environment coupling V as $F \otimes B$, where F and B are operators living in the system and environment Hilbert space, respectively. The extension to the more general case where $V = \sum_\alpha F_\alpha \otimes B_\alpha$ is straightforward. Equation (A2) can then be simplified as

$$\begin{aligned} e^{-\beta(H_{S0}+H_B+\alpha V)} &= e^{-\beta(H_{S0}+H_B)} - \alpha e^{-\beta(H_{S0}+H_B)} \\ &\quad \times \int_0^\beta F(\lambda) \otimes B(\lambda) d\lambda + \alpha^2 e^{-\beta(H_{S0}+H_B)} \\ &\quad \times \int_0^\beta d\lambda F(\lambda) \otimes B(\lambda) \int_0^\lambda F(\lambda') \otimes B(\lambda') d\lambda', \end{aligned} \quad (\text{A3})$$

where $F(\lambda) = e^{\lambda H_{S0}} F e^{-\lambda H_{S0}}$ and $B(\lambda) = e^{\lambda H_B} B e^{-\lambda H_B}$. We now use this in Eq. (2) in the main text and thereafter take the trace over the environment to find the initial system state correct to second order in the system-environment coupling strength. This is important because our aim is to derive a master equation correct to second order in the system-environment strength. For consistency, the initial system state used to solve this master equation should also be accurate to second order in the system-environment coupling strength. For ease of notation, we write the initial system state as

$$\rho(0) = \rho^{(0)}(0) + \rho^{(1)}(0) + \rho^{(2)}(0), \quad (\text{A4})$$

where

$$\rho^{(0)}(0) = \frac{\text{Tr}_B[\Omega(e^{-\beta(H_{S0}+H_B)})\Omega^\dagger]}{Z_{\text{tot}}}, \quad (\text{A5})$$

$$\rho^{(1)}(0) = \frac{\text{Tr}_B\{-\alpha\Omega[e^{-\beta(H_{S0}+H_B)}\int_0^\beta F(\lambda)\otimes B(\lambda)d\lambda]\Omega^\dagger\}}{Z_{\text{tot}}}, \quad (\text{A6})$$

$$\begin{aligned} \rho^{(2)}(0) &= \frac{1}{Z_{\text{tot}}} \times \text{Tr}_B\left\{\alpha^2\Omega\left[e^{-\beta(H_{S0}+H_B)}\int_0^\beta d\lambda F(\lambda)\otimes B(\lambda)\right.\right. \\ &\quad \left.\left.\times \int_0^\lambda F(\lambda')\otimes B(\lambda')d\lambda'\right]\Omega^\dagger\right\}. \end{aligned} \quad (\text{A7})$$

Let us simplify these relations one by one. $\rho^{(0)}(0)$ can be simplified as

$$\rho^{(0)}(0) = \frac{e^{-\beta H_{S0}} Z_B}{Z_{\text{tot}}},$$

where $Z_B = \text{Tr}_B[e^{-\beta H_B}]$. As for $\rho^{(1)}(0)$, we can write

$$\rho^{(1)}(0) = \frac{-\alpha Z_B \int_0^\beta \Omega e^{-\beta H_{S0}} F(\lambda) \Omega^\dagger \langle B(\lambda) \rangle_B d\lambda}{Z_{\text{tot}}},$$

where $\langle \dots \rangle_B = \text{Tr}_B[e^{-\beta H_B}(\dots)]/Z_B$. Since $\langle B(\lambda) \rangle_B$ is zero for most system-environment models, we simply get that $\rho^{(1)}(0) = 0$. Carrying on, $\rho^{(2)}(0)$ can be simplified as

$$\rho^{(2)}(0) = \frac{\alpha^2 Z_B \Omega e^{-\beta H_{S0}} \int_0^\beta \int_0^\lambda F(\lambda) F(\lambda') \Omega^\dagger \langle B(\lambda) B(\lambda') \rangle_B d\lambda' d\lambda}{Z_{\text{tot}}}.$$

To proceed further, we evaluate the partition function Z_{tot} . We note that Z_{tot} has to be such that the trace of the system state $\rho(0)$ in Eq. (A4) is 1. It is then clear that

$$Z_{\text{tot}} = Z_B \text{Tr}_S[e^{-\beta H_{S0}}] + \alpha^2 Z_B \text{Tr}_S[\Omega e^{-\beta H_{S0}} \times \int_0^\beta \int_0^\lambda F(\lambda) F(\lambda') \Omega^\dagger \langle B(\lambda) B(\lambda') \rangle_B d\lambda' d\lambda].$$

Putting these results together,

$$\rho(0) = \frac{e^{-\beta H_{S0}}}{Z_{S0} Z'} \left[\mathbb{1} + \int_0^\beta \int_0^\lambda F^R(\lambda) F^R(\lambda') \times \langle B(\lambda) B(\lambda') \rangle_B d\lambda' d\lambda \right], \quad (\text{A8})$$

where $F^R(\lambda) = \Omega F(\lambda) \Omega^\dagger$, $Z_{S0} = \text{Tr}_S[e^{-\beta H_{S0}}]$ and

$$Z' = 1 + \int_0^\beta \int_0^\lambda \langle F(\lambda) F(\lambda') \rangle_S \langle B(\lambda) B(\lambda') \rangle_B d\lambda' d\lambda, \quad (\text{A9})$$

with $\langle \dots \rangle_S = \text{Tr}_S[e^{-\beta H_{S0}}(\dots)]/Z_{S0}$.

APPENDIX B: THE RELAXATION AND DEPHASING TERM IN THE MASTER EQUATION

We look at the contribution of the third term in Eq. (7). We need to consider only $\rho_{\text{tot}}^{(0)}(0)$ since we are restricted to only second-order terms in the master equation. We obtain

$$\begin{aligned} & \alpha^2 \text{Tr}_{S,B} \left\{ \rho_{\text{tot}}^{(0)}(0) \int_0^t [[\tilde{V}(t), \tilde{X}_{nm}(t)], \tilde{V}(s)] ds \right\} \\ &= \alpha^2 \text{Tr}_{S,B} \left\{ \rho_{S0}^R \otimes \rho_B \int_0^t [[\tilde{V}(t), \tilde{X}_{nm}(t)], \tilde{V}(s)] ds \right\} \\ &= \alpha^2 \text{Tr}_{S,B} \left\{ \rho_{S0}^R \otimes \rho_B \left(\int_0^t \tilde{V}(t) \tilde{X}_{nm}(t) \tilde{V}(s) ds \right. \right. \\ &\quad \left. \left. - \int_0^t \tilde{V}(s) \tilde{V}(t) \tilde{X}_{nm}(t) ds - \int_0^t \tilde{X}_{nm}(t) \tilde{V}(t) \tilde{V}(s) ds \right. \right. \\ &\quad \left. \left. + \int_0^t \tilde{V}(s) \tilde{X}_{nm}(t) \tilde{V}(t) ds \right) \right\}. \quad (\text{B1}) \end{aligned}$$

The first term is

$$\begin{aligned} & \alpha^2 \text{Tr}_{S,B} \left\{ \rho_{S0}^R \otimes \rho_B \int_0^t \tilde{V}(t) \tilde{X}_{nm}(t) \tilde{V}(s) ds \right\} \\ &= \alpha^2 \int_0^t \text{Tr}_{S,B} \left\{ \rho_{S0}^R \otimes \rho_B U_0^\dagger(t) V U_0(t) U_0^\dagger(t) X_{nm} U_0(t) \right. \\ &\quad \left. \times U_0^\dagger(s) V U_0(s) \right\} ds \\ &= \alpha^2 \int_0^t \text{Tr}_S \left\{ \rho_{S0}^R U_S^\dagger(t) F Y_{nm} U_S(t, s) F U_S(s) \right\} \\ &\quad \times \text{Tr}_B \left\{ \rho_B B(t) B(s) \right\} ds \\ &= \alpha^2 \int_0^t \langle m | \bar{F}(t, s) \tilde{\rho}(t) F | n \rangle C_{ts} ds. \end{aligned}$$

In similar fashion, we can simplify the other terms. Putting them all back together and shifting to the basis-independent representation, we obtain the third term in Eq. (16).

APPENDIX C: PURE DEPHASING MODEL

For completeness, we now sketch the derivation of the system dynamics for the large spin-boson model. We have N identical two-level systems interacting with a common environment of harmonic oscillators. The dynamics of such a system can be described by the Hamiltonian

$$H_{\text{tot}} = H_S + H_B + V,$$

where $H_S = \varepsilon J_z$, $H_B = \sum_k \omega_k b_k^\dagger b_k$, and $V = J_z \sum_k (g_k^* b_k + g_k b_k^\dagger)$. In the interaction picture, the Hamiltonian becomes

$$\begin{aligned} H_I(t) &= e^{i(H_B + H_S)t} V e^{-i(H_B + H_S)t} \\ &= J_z \sum_k (g_k^* b_k e^{-i\omega_k t} + g_k b_k^\dagger e^{i\omega_k t}). \end{aligned}$$

The corresponding unitary time-evolution operator can be found exactly via the Magnus expansion, leading to

$$U_I(t) = \exp \left\{ J_z \sum_k [\alpha_k(t) b_k^\dagger - \alpha_k^*(t) b_k] - i J_z^2 \Delta(t) \right\},$$

where $\alpha_k(t) = \frac{g_k(1 - e^{-i\omega_k t})}{\omega_k}$ and $\Delta(t) = \sum_k |g_k|^2 \frac{[\sin(\omega_k t) - \omega_k t]}{\omega_k^2}$. The unitary operator for the complete Hamiltonian is $U(t) = e^{-i\varepsilon J_z t} e^{-iH_B t} U_I(t)$. We can use this to work out the reduced density operator of the system in the J_z eigenbasis. Note that

$$[\rho(t)]_{mn} = \text{Tr}_{S,B}[U(t)\rho(0)U^\dagger(t)P_{nm}], \quad (\text{C1})$$

where $P_{nm} \equiv |n\rangle\langle m|$, such that $J_z|n\rangle = n|n\rangle$. We can write Eq. (C1) in the Heisenberg picture, where $P_{nm}(t) = U^\dagger(t)P_{nm}U(t)$ is the Heisenberg picture operator. It follows that

$$[\rho(t)]_{mn} = \text{Tr}_{S,B}[\rho(0)P_{nm}(t)].$$

It is straightforward to find that

$$P_{nm}(t) = e^{-i\varepsilon(m-n)t} e^{-i\Delta(t)(m^2 - n^2)} e^{-R_{nm}(t)} P_{nm},$$

where

$$R_{nm}(t) = (n - m) \sum_k [\alpha_k(t) b_k^\dagger - \alpha_k^*(t) b_k].$$

Hence, it follows that

$$[\rho(t)]_{mn} = e^{-i\epsilon(m-n)t} e^{-i\Delta(t)(m^2-n^2)} \text{Tr}_{S,B}[\rho(0)e^{-R_{nm}(t)}P_{nm}]. \quad (\text{C2})$$

This is a general result because we have not yet defined the joint system-environment initial state $\rho(0)$. Hence, it can be applied to both uncorrelated and correlated initial states. We will derive an expression for $[\rho_S(t)]_{mn}$ for both cases. First, without considering the initial system-environment correlations,

$$\rho_{\text{tot}}(0) = \rho(0) \otimes \rho_B,$$

where $\rho_B = \frac{e^{-\beta H_B}}{Z_B}$, with $Z_B = \text{Tr}_B[e^{-\beta H_B}]$. We then get

$$[\rho(t)]_{mn} = [\rho(0)]_{mn} e^{-i\epsilon(m-n)t} e^{-i\Delta(t)(m^2-n^2)} \text{Tr}_B[\rho_B e^{-R_{nm}(t)}]. \quad (\text{C3})$$

Simplifying the trace over the environment, we obtain

$$[\rho(t)]_{mn} = [\rho(0)]_{mn} e^{-i\epsilon(m-n)t} e^{-i\Delta(t)(m^2-n^2)} e^{-\gamma(t)(m-n)^2}, \quad (\text{C4})$$

with

$$\gamma(t) = \sum_k \frac{|g_k|^2 [1 - \cos(\omega_k t)]}{\omega_k^2} \coth\left(\frac{\beta\omega_k}{2}\right). \quad (\text{C5})$$

Next, we look at the case where the initial system-environment state is of the form

$$\rho(0) = \frac{\Omega e^{-\beta H_{\text{tot}}} \Omega^\dagger}{Z}, \quad (\text{C6})$$

where $Z = \text{Tr}_{S,B}[\Omega e^{-\beta H_{\text{tot}}} \Omega^\dagger]$ and Ω is a unitary operator. We first simplify Z by introducing a completeness relation,

$$\begin{aligned} Z &= \sum_l \text{Tr}_{S,B}[\Omega e^{-\beta H_{\text{tot}}} |l\rangle\langle l| \Omega^\dagger] \\ &= \sum_l e^{-\beta\epsilon l} \langle l| \Omega^\dagger \Omega |l\rangle \text{Tr}_B[e^{-\beta H_B^{(l)}}], \end{aligned}$$

where

$$H_B^{(l)} = H_B + l \sum_k (g_k^* b_k + g_k b_k^\dagger). \quad (\text{C7})$$

Using the displaced harmonic oscillator modes $B_{k,l} = b_k + \frac{l g_k}{\omega_k}$ and $B_{k,l}^\dagger = b_k^\dagger + \frac{l g_k^*}{\omega_k}$, we obtain

$$Z = \sum_l e^{-\beta\epsilon l} \langle l| \Omega^\dagger \Omega |l\rangle e^{\beta l^2 \mathcal{C}} Z_B,$$

where $\mathcal{C} = \sum_k \frac{|g_k|^2}{\omega_k}$. Proceeding further, again using a completeness relation, we note that

$$\begin{aligned} [\rho(t)]_{mn} &= \frac{1}{Z} \sum_l e^{-i\epsilon(m-n)t} e^{-i\Delta(t)(m^2-n^2)} \\ &\quad \times \langle l| \Omega^\dagger P_{nm} \Omega |l\rangle \text{Tr}_B[e^{-\beta H_B^{(l)}} e^{-R_{nm}(t)}], \end{aligned}$$

where $R_{nm}(t)$ is written as

$$R_{nm}(t) = (n-m) \sum_k [\alpha_k(t) b_k^\dagger - \alpha_k^*(t) b_k] + i\Phi_{nm}^{(l)}(t),$$

with

$$\Phi_{nm}^{(l)}(t) = l(n-m)\Phi(t), \quad \Phi(t) = \sum_k \frac{|g_k|^2}{\omega_k^2} \sin(\omega_k t).$$

It can be shown that

$$\text{Tr}_B[e^{-\beta H_B^{(l)}} e^{-R_{nm}(t)}] = e^{-i\Phi_{nm}^{(l)}(t)} e^{\beta l^2 \mathcal{C}} Z_B e^{-\gamma(t)(m-n)^2}.$$

Hence, we obtain

$$\begin{aligned} [\rho(t)]_{mn} &= [\rho(0)]_{mn} e^{-i\epsilon(m-n)t} e^{-i\Delta(t)(m^2-n^2)} \\ &\quad \times e^{-\gamma(t)(m-n)^2} \frac{\sum_l [\langle l| \Omega^\dagger P_{nm} \Omega |l\rangle e^{-i\Phi_{nm}^{(l)}(t)} e^{-\beta\epsilon l} e^{\beta l^2 \mathcal{C}}]}{\sum_l [\langle l| \Omega^\dagger P_{nm} \Omega |l\rangle e^{-\beta\epsilon l} e^{\beta l^2 \mathcal{C}}]}. \end{aligned} \quad (\text{C8})$$

APPENDIX D: MASTER EQUATION WITH A TIME-DEPENDENT SYSTEM HAMILTONIAN

In Sec. III, we applied the master equation [see Eq. (16)] to the large spin-boson model with the system Hamiltonian parameters changed suddenly. In particular, for the numerical results presented, the tunneling amplitude was not changed, that is, $\Delta_0 = \Delta$, while the energy-level splitting was changed from ϵ_0 to ϵ instantaneously at $t = 0$. We examine in this Appendix what happens if we do not change the energy-level spacing instantaneously. In particular, we consider that for $t \geq 0$, the system Hamiltonian is $H_S(t) = \frac{\epsilon(t)}{2} J_z + \Delta J_x$, where $\epsilon(t) = (\epsilon_0 - \epsilon)e^{-t/t_\epsilon} + \epsilon$. t_ϵ is a measure of how quickly we change the energy-level spacing, with a smaller value of t_ϵ indicating a quicker transition from ϵ_0 to ϵ . This time-dependent Hamiltonian can be used in the master equation (16), with the system unitary time-evolution operator calculated numerically via the split-operator method, thereby also entailing numerical evaluation of the operator $J_{\text{corr}}^R(\beta, t)$ as well as the third term in the master equation. Results for different values of t_ϵ are illustrated in Fig. 14. As expected, for small values of t_ϵ , the results

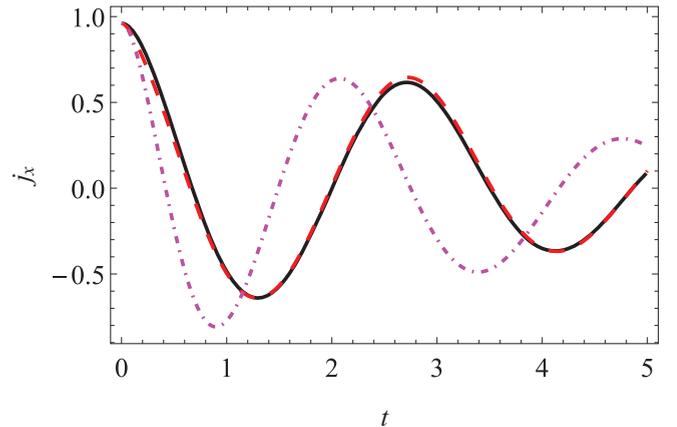


FIG. 14. Behavior of j_x versus t for $N = 2$, taking into account the initial correlations, with the time-dependent system Hamiltonian. The solid black curve is for $t_\epsilon \rightarrow 0$; for the dashed red curve $t_\epsilon = 0.1$, while $t_\epsilon = 1$ for the dot-dashed magenta curve. As usual, we have used dimensionless units with $\hbar = 1$, with the rest of the parameters being $\epsilon_0 = 4$, $\epsilon = 2$, $\Delta = \Delta_0 = 1$, $G = 0.05$, $\beta = 1$, and $\omega_c = 5$.

with the time-dependent Hamiltonian agree very closely with our previous results, in which we assumed that the system Hamiltonian is changed instantaneously. Such agreement is expected when t_ε is smaller than the environment correlation time (which is related to the inverse of the cutoff frequency) as well as the timescale set by the system Hamiltonian (which is on the order of the inverse of $\sqrt{\varepsilon^2 + \Delta^2}$).

APPENDIX E: BATH CORRELATION FUNCTION FOR THE HARMONIC OSCILLATOR ENVIRONMENT

To calculate $B_{\text{corr}}(\lambda, t) = \text{Tr}_B[\rho_B B(\lambda) B(it)] = \langle B(\lambda) B(it) \rangle_B$ for the harmonic oscillator environment, we first note that

$$B(\lambda) = \sum_k (g_k^* e^{-\lambda \omega_k} b_k + g_k e^{\lambda \omega_k} b_k^\dagger).$$

Using this, we find that

$$\begin{aligned} B_{\text{corr}}(\lambda, t) &= \sum_{k, k'} (g_k^* g_{k'} e^{-\lambda \omega_k} e^{i \omega_{k'} t} (\mathbb{1} + b_k^\dagger b_{k'}) \\ &\quad + g_k g_{k'}^* e^{\lambda \omega_k} e^{-i \omega_{k'} t} b_k^\dagger b_{k'})_B \\ &= \sum_k |g_k|^2 \{ e^{-\omega_k(\lambda - it)} + (e^{-\omega_k(\lambda - it)} + e^{\omega_k(\lambda - it)}) n_k \} \\ &= \sum_k |g_k|^2 \{ e^{-\omega_k(\lambda - it)} + 2n_k \cosh(\lambda \omega_k - i \omega_k t) \}, \end{aligned}$$

with n_k given by

$$n_k = \frac{1}{2} \left\{ \coth \left(\frac{\beta \omega_k}{2} \right) - 1 \right\}.$$

APPENDIX F: ENVIRONMENT CORRELATION FUNCTION WITH THE SPIN ENVIRONMENT

Consider the system-environment Hamiltonian given in Sec. IV. We evaluate

$$C(\tau) = \text{Tr}_B \{ \rho_B B(i\tau) B \}.$$

Here $B(i\tau) = e^{iH_B \tau} B e^{-iH_B \tau}$ denotes the collective environment operator $B = \sum_k g_k \sigma_z^{(k)}$ in the interaction picture. The exponential $e^{iH_B \tau}$ factors into single-spin terms, leading to

$$e^{iH_B \tau} \equiv e^{i \sum_k H_B^{(k)} \tau} = \prod_k e^{iH_B^{(k)} \tau}.$$

Therefore, we can write the environment self-correlation function as

$$C(\tau) = \sum_{kj} g_k g_j \text{Tr}_B \{ \rho_B e^{iH_B^{(k)} \tau} \sigma_z^{(k)} e^{-iH_B^{(j)} \tau} \sigma_z^{(j)} \}.$$

Using the fact that the environmental spins do not directly interact with each other and are therefore uncorrelated, this can be simplified to [42]

$$C(\tau) = \sum_k g_k^2 \text{Tr}_B \{ \rho_B \sigma_z^{(k)}(\tau) \sigma_z^{(k)} \},$$

where $\sigma_z^{(k)}(\tau) = e^{iH_B^{(k)} \tau} \sigma_z^{(k)} e^{-iH_B^{(k)} \tau}$ and $H_B^{(k)} = \frac{\omega_k}{2} \sigma_x^{(k)}$. This simplifies to a product of traces over the individual environment spins, that is,

$$C(\tau) = \sum_k g_k^2 \frac{1}{Z_k} \text{Tr}_{B_k} \{ e^{-\beta H_B^{(k)}} \sigma_z^{(k)}(\tau) \sigma_z^{(k)} \}, \quad (\text{F1})$$

where $Z_k = \text{Tr}_{B_k} \{ e^{-\beta H_B^{(k)}} \}$. These traces are most easily evaluated by working in the eigenbasis of $\sigma_x^{(k)}$. We find that

$$\begin{aligned} e^{-\beta H_B^{(k)}} \sigma_z^{(k)}(\tau) \sigma_z^{(k)} &= e^{-\beta \omega_k / 2 + i \omega_k \tau} |+\rangle_k \langle +|_k + e^{\beta \omega_k / 2 - i \omega_k \tau} |-\rangle_k \langle -|_k, \end{aligned}$$

where $|+\rangle_k$ and $|-\rangle_k$ are the eigenstates of $\sigma_x^{(k)}$ and

$$Z_k = \text{Tr}_{B_k} \{ e^{-\beta H_B^{(k)}} \} = e^{\beta \omega_k / 2} + e^{-\beta \omega_k / 2}.$$

Using these, we obtain the environment correlation function

$$C(\tau) = \sum_k g_k^2 \left\{ \cos(\omega_k \tau) - i \tanh \left(\frac{\omega_k}{2k_B T} \right) \sin(\omega_k \tau) \right\}.$$

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