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Nonperturbative approach to system-reservoir dynamics in the strong-coupling regime and non-Markovian dynamics

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We present a method to derive an exact master equation for a bosonic system coupled to a set of other bosonic systems, which plays the role of the reservoir, under the strong-coupling regime, i.e., without resorting to either the rotating-wave or secular approximations. Working with phase-space distribution functions, we verify that the dynamics have two different behaviors. Considering that the initial state is a concentrated wave packet in phase space, we see that the center of this wave packet follows classical mechanics while its shape gets distorted. Moreover, we show that this distortion is caused by the counter-rotating terms as well as thermal fluctuations. Finally, we discuss conditions for non-Markovian dynamics.

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I. INTRODUCTION

The subject of open quantum systems has undergone substantial growth in the last three decades, starting with contributions to the field of fundamental quantum physics with the aim of understanding the process of decoherence. Based on the von Neumann approach to the reduction of the state vector [1], these contributions were mainly driven by the pioneering work of Zurek [2], Caldeira and Leggett [3], and Joos and Zeh [4]. The repercussions of their work, together with the advent of the field of quantum information theory, led to renewed interest in open quantum systems, with the focus now shifting from fundamental issues to practical applications in circuits to implement quantum logical operations.

The master-equation approach has long been used to derive system-reservoir dynamics, to account for energy exchange under a weak-coupling regime [5]. Its effectiveness comes from the fact that the energy exchange of most quantum mechanical systems, especially within quantum and atomic optics, can be handled by the single-pole Wigner-Weisskopf approximation [6], where a perturbative expansion is performed in the system-reservoir coupling. Following developments by Caldeira and Leggett [3], more sophisticated methods to deal with the system-reservoir strong-coupling regime have been advanced, such as the Hu-Paz-Zhang [7] master equation with time-dependent coefficients, which allows for non-Markovian dynamics. Halliwell and Yu [8] have published an alternative derivation of the Hu-Paz-Zhang equation, in which the dynamics is represented by the Wigner function, and an exact solution of this equation was given by Ford and O'Connell [9].

Recently, the non-Markovian dynamics of open quantum systems has been studied with renewed interest, especially in connection with quantum information theory, as in Refs. [10,11]. However, in these studies, as well as in most of the derivations of master equations with time-dependent coefficients, the authors assume either the rotating-wave approximation (RWA) or the secular approximation (SA) for the system-reservoir coupling [12]. Since non-Markovian

behavior is sensitive to the counter-rotating terms in the interaction Hamiltonian, important features of the dynamics are missing under the RWA in the strong-coupling regime. It is worth mentioning that a study of the effect of the RWA and the SA on the non-Markovian behavior in the spin-boson model at zero temperature has already been advanced [12], without, however, deriving a master equation.

Our goal in this work is to derive and investigate the consequences of a master equation within the strong-coupling regime, which prevents us from resorting to either the RWA or the SA in the system-reservoir coupling. Moreover, instead of the path-integral approach [13], we use the formalism of quasiprobability distributions, thus enabling us to cast the problem as the solution of a linear system of equations. Our results follow from the general treatment of a bosonic dissipative network that we have previously presented in Ref. [14], where the network dynamics were investigated, and further used for quantum information purposes [15]. However, differently from our previous developments, we first consider the general model for a network of bosonic nondissipative oscillators and, subsequently, we focus on some of these oscillators (or just one of them) as our system of interest, and treat all the others as a (structured) reservoir. The exact dynamics of the network allows us to obtain an exact dynamics of the system-reservoir interaction. Moreover, we present a simple inequality to distinguish between Markovian and non-Markovian dynamics.

Finally, this development enables us to generalize an earlier result by Glauber [16]. When using the RWA and a zero-temperature reservoir, it was shown that the quasiprobability functions maintain their shape while they are displaced in phase space; in particular, coherent states remain coherent states. We find that for a general Gaussian state, the center of its phase-space distribution follows classical dynamics (as in Ref. [16]), but its shape is changed. Furthermore, this change can be derived from the evolution of the vacuum state, which is no longer stationary, because of the counter-rotating terms. The change in shape is affected by both quantum and thermal fluctuations, and these contributions can be distinguished, at least in theory. Our developments can be straightforwardly translated to the derivation of an exact master equation for fermionic systems, using the reasoning in Ref. [17].

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II. UNITARY DYNAMICS OF THE UNIVERSE

The universe considered here consists of a set of M+N harmonic oscillators, which are linearly coupled to each other in an arbitrary network. We consider M of them to be part of our system of interest, and the remaining N to be part of a reservoir. However, at this stage, we are concerned with the full dynamics of the universe, and there is actually no difference between system and reservoir modes. The oscillators are described by mass m_k and natural, isolated frequencies ϖ_k ; the coupling between modes k and k, which occurs via their position coordinates, has strength k, (which, without loss of generality, is symmetric in its indices). Before we write the Hamiltonian that describes such a universe, we note that it must be positive definite, in order to be bounded from below and have a well-defined ground state. Then, the Hamiltonian which is compatible with this model is

$$H = \frac{1}{2} \sum_{k=1}^{M+N} \left(\frac{1}{m_k} \hat{p}_k^2 + m_k \varpi_k^2 \hat{q}_k^2 \right) + \frac{1}{4} \sum_{kj=1}^{M+N} \lambda_{kj} (\hat{q}_k - \hat{q}_j)^2,$$
(1)

where the coefficients λ_{kj} form a real, symmetric matrix. We do not assume any particular form for them, so as to generate an arbitrary network, as depicted in Fig. 1. The coupling term induces a change in the natural frequency of each mode, which is now represented by

$$\omega_k = \sqrt{\varpi_k^2 + \frac{1}{m_k} \sum_{j=1}^N \lambda_{kj}}.$$
 (2)

Using this renormalized frequency, we can define annihilation operators a_k and rewrite the Hamiltonian as

$$H = \sum_{k=1}^{M+N} \omega_k a_k^{\dagger} a_k + \frac{1}{2} \sum_{kj=1}^{M+N} g_{kj} (a_k + a_k^{\dagger}) (a_j + a_j^{\dagger}), \quad (3)$$

with the coupling in this picture given by

$$g_{kj} = \frac{\lambda_{kj}}{2\sqrt{m_k m_j \omega_k \omega_j}}. (4)$$

From here on, we will focus on ω_k and g_{kj} , with the latter forming a real, symmetric matrix.

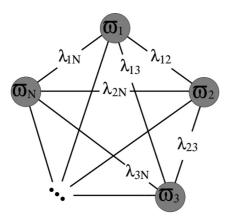


FIG. 1. Network of coupled quantum harmonic oscillators in a general topology.

Characteristic function

The dynamics given by the Hamiltonian of Eq. (3) is best understood in terms of the characteristic function of a state, which is just the expected value of the multimode displacement operator in the symmetric ordering,

$$\chi(\{\beta_k\}) = \left\langle \prod_{k=1}^{M+N} \exp(\beta_k a_k^{\dagger} - \beta_k^* a_k) \right\rangle, \tag{5}$$

where $\{\beta_k\}$ represents all coordinates β_k with k = 1, ..., N, as well as their complex conjugates.

The characteristic function carries the complete information about the state, and in particular information about moments of all orders; this is one of the reasons it is a better approach than using the Heisenberg equations of motion directly. The von Neumann equation in Hilbert space is mapped to a differential equation in dual phase space (where the characteristic function is defined).

$$\frac{\partial \chi}{\partial t} = i \sum_{k=1}^{M+N} \left[\omega_k \beta_k - \sum_{j=1}^N g_{kj} (\beta_j + \beta_j^*) \right] \frac{\partial \chi}{\partial \beta_k} + \text{H.c.} \quad (6)$$

Being linear and of first order, this equation admits a simple ansatz,

$$\chi(\{\beta_k\},t) = \chi(\{\beta_k(t)\},0),\tag{7}$$

which implies that the characteristic function maintains its shape, but the underlying (dual) phase space undergoes a linear transformation, given by

$$\beta_k(t) = \sum_{j=1}^{M+N} [U_{j,k}(t)\beta_j - V_{j,k}(t)\beta_j^*].$$
 (8)

This transformation is defined by the solution to a system of differential equations,

$$\frac{dU_{kj}}{dt} = i\omega_j U_{kj} - i \sum_{n=1}^{M+N} (U_{kn} - V_{kn}) g_{nj},$$
 (9a)

$$\frac{dV_{kj}}{dt} = -i\omega_j V_{kj} - i \sum_{n=1}^{M+N} (U_{kn} - V_{kn}) g_{nj}.$$
 (9b)

The Heisenberg equations of motion for the first moments have a similar structure. However, since they refer only to first moments, they do not represent a complete solution of the problem, which can be obtained from the characteristic function with the same computational effort [18].

III. REDUCED DYNAMICS OF THE SYSTEM

From this point on, we shall be interested only in the behavior of a subset of M oscillators (the ones labeled 1 to M), which form our system of interest, while the oscillators labeled M+1 to M+N play the role of a (structured) reservoir. The complete solution to the dynamics is given by Eq. (7); in order to eliminate the reservoir degrees of freedom, all we need to do is set $\beta_k = 0$ if k > M (i.e., evaluate the characteristic function at the origin of the phase space of the modes we want to eliminate from the description). Before continuing, we observe that although not strictly necessary in our method, for the sake of simplicity we assume the usual sudden-coupling

hypothesis, i.e., that the states of system and reservoir are initially uncorrelated (i.e., it is a product state),

$$\chi_{SR}(\{\beta_k\}, 0) = \chi_S(\{\beta_k\}_{k \le M}, 0) \chi_R(\{\beta_m\}_{m > M}).$$
 (10)

Tracing out the reservoir degrees of freedom, following the procedure above, leads to

$$\chi_{S}(\{\beta_{k}\},t) = \chi_{S}(\{\beta_{k}(t)\},0)\chi_{\text{in}}(\{\beta_{k}\},t), \tag{11}$$

where the indices run only through the degrees of freedom of the system (i.e., k runs from 1 to M). Therefore, we must use Eq. (8) with $\beta_k = 0$ for k > M, and it follows that we only need U_{kj} and V_{kj} for $k \le M$. Equations 9(a) and 9(b), although written as a matrix equation, are actually a set of N independent vector equations and we conclude that only a few of these need to be solved. In fact, if our system of interest were a single oscillator, we would reduce the problem of finding its exact dynamics to a single vector equation of dimension 2N.

The two terms of Eq. (11) are called the homogeneous (because it depends on the initial state of the system) and inhomogeneous (because it is independent of it, depending only on the initial state of the reservoir) terms. The homogeneous part of the solution is just the linear transformation of phase space induced only by the elements U_{kj} and V_{kj} for which both $k, j \leq M$. These elements can be arranged in two general complex $M \times M$ matrices, resulting in $4M^2$ real parameters.

At this point, we make an additional assumption that the initial state of the reservoir is Gaussian [19], i.e., its characteristic function has the Gaussian form. Moreover, the reservoir is unbiased (i.e., $\langle a_m \rangle = 0$ for m > M). These are reasonable hypotheses, since the Gaussian states include the thermal states of quadratic Hamiltonians. The inhomogeneous characteristic function is then also a Gaussian function:

$$\chi_{\text{in}}(\{\beta_k\},t) = \exp\left[-\frac{1}{2}\sum_{kj=1}^{M} A_{kj}(t)\beta_k\beta_j^*\right]$$

$$\times \exp\left[\sum_{kj=1}^{M} B_{kj}(t)\beta_k\beta_j + \text{c.c.}\right]. \tag{12}$$

The time-dependent functions A_{kj} and B_{kj} may be divided into two terms, in the form $A_{kj} = A_{kj}^{(0)} + A_{kj}^{(\text{th})}$ (and similarly for B), the first of which is the solution for a zero-temperature reservoir,

$$A_{kj}^{(0)} = \frac{1}{2} \sum_{m=M+1}^{M+N} (U_{km} U_{jm}^* + V_{km} V_{jm}^*),$$
 (13a)

$$B_{kj}^{(0)} = \frac{1}{2} \sum_{m=M+1}^{M+N} (U_{km} V_{jm} + V_{km} U_{jm}),$$
 (13b)

while the second incorporates the effects of the reservoir initial state, which is completely characterized by the second-order moments $\langle a_m^{\dagger} a_n \rangle_0$ and $\langle a_m a_n \rangle_0$,

$$A_{kj}^{(\text{th})} = \sum_{m=M+1}^{M+N} \langle a_m^{\dagger} a_n \rangle_0 (U_{km} U_{jn}^* + V_{kn} V_{jm}^*) + \sum_{m=M+1}^{M+N} (\langle a_m a_n \rangle_0 V_{km} U_{jn}^* + \text{c.c.}), \qquad (14a)$$

$$B_{kj}^{(\text{th})} = \sum_{m=M+1}^{M+N} \langle a_m^{\dagger} a_n \rangle_0 (U_{kn} V_{jm} + V_{km} U_{jn}^*) + \sum_{m=M+1}^{M+N} (\langle a_m a_n \rangle_0 V_{km} V_{jn} + \text{c.c.}).$$
 (14b)

Both A and B form complex $M \times M$ matrices; however, A must be Hermitian, while B is not. This represents an additional $3M^2$ real parameters, giving a total of $7M^2$ that completely specifies a given Gaussian evolution map (so called because if the initial state of the system is Gaussian, it will remain Gaussian).

The functions $A_{kj}^{(0)}$ and $B_{kj}^{(0)}$ represent the solution for a zero-temperature reservoir; therefore, they represent the quantum, or zero-point, fluctuations. The functions $A_{kj}^{(th)}$ and $B_{kj}^{(th)}$ represent the thermal fluctuations (when the reservoir is assumed to be in a thermal state), and other effects that may arise due to, e.g., squeezing in the reservoir modes.

Although we have assumed that the initial state of the reservoir is Gaussian, we have not made a similar assumption for the system. In Eq. (11), the function $\chi_S(\{\alpha\},0)$ can represent an arbitrary initial state [with the characteristic function given by Eq. (5)]. The hypotheses made here ensure that the map is Gaussian, but the initial state of the system need not be.

IV. SINGLE-MODE DYNAMICS

The result of Sec. III may be written in a simpler fashion for the case of a single oscillator taken as the system of interest:

$$\chi(\beta,t) = \chi(U\beta - V\beta^*,0)$$

$$\times \exp\left(-A|\beta|^2 + \frac{1}{2}B\beta^2 + \frac{1}{2}B^*\beta^{*2}\right), \quad (15)$$

where the indices 1,1 are dropped. The single-mode Gaussian map is completely characterized by seven real parameters (since A is real, and U, V, and B are complex).

When a single mode is considered as the system of interest, we can perform a diagonalization of the reservoir part of the Hamiltonian, and consider the interaction of the system with each of the reservoir normal modes, as depicted in Fig. 2 (normal modes of the reservoir do not interact with each other, but interact with the system). Without loss of generality, we assume that the central oscillator has mass M and the reservoir modes have masses μ , leading to the renormalized frequencies and couplings.

$$\omega_1 = \sqrt{\varpi_1^2 + \frac{1}{M} \sum_{j=2}^{N+1} \lambda_{1j}},$$
 (16a)

$$\omega_j = \sqrt{\varpi_j^2 + \frac{1}{\mu} \lambda_{1j}} \quad (2 \leqslant j \leqslant N+1), \tag{16b}$$

$$g_j = \frac{1}{2\sqrt{\mu M}} \frac{\lambda_{1j}}{\sqrt{\omega_1 \omega_j}} \quad (2 \leqslant j \leqslant N+1). \quad (16c)$$

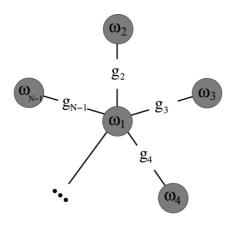


FIG. 2. The system of interest (represented by a single harmonic oscillator of the original network) interacting with the normal modes of the diagonalized reservoir (represented by the remaining oscillators of the network).

Dropping the first index, Eqs. (9a) and (9b) become

$$\frac{dU_1}{dt} = i\omega_1 U_1 - i \sum_{j=2}^{N} g_j (U_j - V_j),$$
 (17a)

$$\frac{dV_1}{dt} = -i\omega_1 V_1 - i \sum_{j=2}^{N} g_j (U_j - V_j),$$
 (17b)

$$\frac{dU_j}{dt} = i\omega_j U_j - ig_j (U_1 - V_1) \quad (j \neq 1), \tag{17c}$$

$$\frac{dV_j}{dt} = -i\omega_j V_j - ig_j (U_1 - V_1) \quad (j \neq 1). \tag{17d}$$

The bottom two equations can be solved by considering U_1 and V_1 as external parameters. Then, by substituting them into the top two equations, we get a pair of coupled integrodifferential equations,

$$\frac{dU_1}{dt} = i\omega_1 U_1 + i \int_0^t d\tau h(t - \tau) [U_1(\tau) - V_1(\tau)], \quad (18a)$$

$$\frac{dV_1}{dt} = -i\omega_1 V_1 + i \int_0^t d\tau h(t - \tau) [U_1(\tau) - V_1(\tau)], \quad (18b)$$

which depends on the reservoir topology only through the function

$$h(t) = \sum_{j=2}^{N+1} g_j^2 \sin(\omega_j t) = \frac{1}{4\mu M \omega_1} \sum_{j=2}^{N+1} \frac{\lambda_j^2}{\omega_j} \sin(\omega_j t), \quad (19)$$

which in turn is related to the Fourier transform of the reservoir spectral density

$$J(\omega) = \sum_{j=2}^{N+1} g_j^2 \delta(\omega - \omega_j) = \frac{1}{4\mu M \omega_1} \sum_{j=2}^{N+1} \frac{\lambda_j^2}{\omega_j} \delta(\omega - \omega_j).$$
(20)

This is the homogeneous part of the solution. To obtain the inhomogeneous one, we need to use the solution found previously for U_k and V_k in terms of the now-known U_1 and V_1 , and then use Eqs. (13) and (14).

The zero-temperature part [Eqs. (13)] of the inhomogeneous solution is

$$A^{(0)} = \int_0^t dt_1 \int_0^t dt_2 [U_1(t_1) - V_1(t_1)] [U_1(t_2) - V_1(t_2)]^*$$

$$\times \text{Re} \int_0^\infty d\omega J(\omega) e^{-i\omega(t_1 - t_2)}, \qquad (21a)$$

$$B^{(0)} = \int_0^t dt_1 \int_0^t dt_2 [U_1(t_1) - V_1(t_1)] [U_1(t_2) - V_1(t_2)]$$

$$\times \int_0^\infty d\omega J(\omega) e^{-i\omega(t_1 - t_2)}. \qquad (21b)$$

The spectral density contains all of the necessary information to describe the dynamics at zero temperature.

Limit of a large reservoir

So far, we have dealt exclusively with a finite number of modes, but at this point, a commentary is in order with respect to the limit $N \to \infty$, which represents the definition of a reservoir as having an infinite number of modes (or infinite heat capacity). This limit cannot be taken too naively, since we see that in Eq. (16a), if we take λ_{1j} and M fixed, the central oscillator's natural frequency grows without bound with N. In order to ensure physical results, one possible solution is to take $M \propto N$, in a way that the sum in Eq. (16a) becomes a proper integral. Essentially, the central oscillator must be much more massive than the reservoir modes. This is the case with Brownian motion, where the observed particle, though mesoscopic, is still much larger than the bath of fluid molecules it interacts with. It is also the case in quantum optics, where the mode inside a cavity has a much smaller mode volume (i.e., it is concentrated in a small region) than the vacuum modes outside the cavity.

It is true that even though λ_{1j} can be arbitrary, the effective couplings g_j will become small when N gets large (in fact, $g_j \propto N^{-1/2}$). This is to be expected, for instance, from Fermi's golden rule, which states that the transition rate is proportional to the density of states and the square of the transition matrix elements. As the density of states increases (proportional to N), the matrix elements must decrease (proportional to $N^{-1/2}$) so that the transition rates stay finite.

In fact, we have seen that through Eqs. (18) and (21), the reservoir spectral density $J(\omega)$ governs the dynamics at zero temperature. We can then consider the limit $N \to \infty$ in Eq. (20), by proposing $M = N\mu_1$, and getting

$$J_{\infty}(\omega) = \lim_{N \to \infty} \frac{1}{4\mu N \mu_1 \omega_1} \sum_{j=2}^{N+1} \frac{\lambda_j^2}{\omega_j} \delta(\omega - \omega_j) \equiv \frac{\lambda^2(\omega)}{4\mu \mu_1 \omega \omega_1},$$
(22)

which has a smoother behavior than the sum of δ peaks in Eq. (20).

Finally, it must be remarked that the system-reservoir coupling g_j can be taken arbitrarily large when considering an equally arbitrarily large, but still finite, reservoir.

V. MASTER EQUATION

The complete solution for single-mode dynamics is Eq. (15), with time-dependent functions U, V, A, and B. It was derived by assuming an explicit microscopic model for the reservoir as a set of other modes, which are coupled to the mode of interest, but over which the experimenter has little control (except for macroscopic parameters such as temperature). In this section, our goal is to find a dynamical equation (in fact, a master equation) whose solution is precisely Eq. (15), but which does not need to involve any other degrees of freedom, besides those of the system.

We start by differentiating Eq. (15) with respect to time, and then mapping it from phase space back to Hilbert space:

$$\frac{d\rho}{dt} = -i[H_S(t), \rho(t)] + \mathcal{D}_t(\rho(t)), \tag{23}$$

where we have a time-dependent effective Hamiltonian,

$$H_S(t) = \omega(t)a^{\dagger}a + \xi(t)a^{\dagger 2} + \xi^*(t)a^2,$$
 (24)

and a time-dependent dissipation superoperator,

$$\mathcal{D}_{t}(\rho) = \frac{\gamma_{1}(t) + \gamma_{2}(t)}{2} ([a\rho, a^{\dagger}] + [a, \rho a^{\dagger}]) + \frac{\gamma_{2}(t)}{2} ([a^{\dagger}\rho, a] + [a^{\dagger}, \rho a]) - \frac{1}{2} \{\eta(t)([a^{\dagger}\rho, a^{\dagger}] + [a^{\dagger}, \rho a^{\dagger}]) + \text{H.c.}\}.$$
 (25)

This master equation depends on seven real time-dependent parameters, which in turn depend on the seven real parameters that define the solution given by Eq. (15): the three real parameters

$$\omega(t) = \frac{1}{|U|^2 - |V|^2} \operatorname{Im} \left(U^* \frac{dU}{dt} - V^* \frac{dV}{dt} \right), \quad (26a)$$

$$\gamma_1(t) = \frac{-2}{|U|^2 - |V|^2} \operatorname{Re} \left(U^* \frac{dU}{dt} - V^* \frac{dV}{dt} \right)$$

$$= -\frac{d}{dt} \ln(|U|^2 - |V|^2), \quad (26b)$$

$$\gamma_2(t) = \frac{dA}{dt} + \gamma_1 \left(A - \frac{1}{2} \right) + 2\operatorname{Im}(\xi^* B), \tag{26c}$$

and the two complex parameters

$$\xi(t) = \frac{-i}{|U|^2 - |V|^2} \left(U \frac{dV}{dt} - V \frac{dU}{dt} \right), \tag{26d}$$

$$\eta(t) = \frac{dB}{dt} + (\gamma_1 + 2i\omega)B + 2i\xi A. \tag{26e}$$

The time-dependent functions $\omega(t)$, $\gamma_1(t)$, and $\xi(t)$ are independent of the initial state of the reservoir, while $\gamma_2(t)$ and $\eta(t)$ depend on it.

The dissipator, given by Eq. (25), is not explicitly in Lindblad-like form, but can be put into it as follows:

$$\mathcal{D}_{t}(\rho) = \sum_{n=1}^{2} \frac{\lambda_{n}(t)}{2} \{ [L_{n}(t)\rho, L_{n}^{\dagger}(t)] + [L_{n}(t), \rho L_{n}^{\dagger}(t)] \}, \tag{27}$$

by defining the Lindblad operators

$$L_1(t) = \cos\left[\frac{\theta(t)}{2}\right] a - \sin\left[\frac{\theta(t)}{2}\right] \frac{\eta(t)}{|\eta(t)|} a^{\dagger}, \quad (28a)$$

$$L_2(t) = \cos \left[\frac{\theta(t)}{2} \right] a^{\dagger} + \sin \left[\frac{\theta(t)}{2} \right] \frac{\eta^*(t)}{|\eta(t)|} a, \quad (28b)$$

and Lindblad rates

$$\lambda_1(t) = \frac{\gamma_1(t)}{2} + \frac{\gamma_1(t)}{|\gamma_1(t)|} \sqrt{\frac{\gamma_1^2(t)}{4} + |\eta(t)|^2} + \gamma_2(t), \quad (29a)$$

$$\lambda_2(t) = \frac{\gamma_1(t)}{2} - \frac{\gamma_1(t)}{|\gamma_1(t)|} \sqrt{\frac{\gamma_1^2(t)}{4} + |\eta(t)|^2} + \gamma_2(t), \quad (29b)$$

with the auxiliary definition

$$\theta(t) = \arctan\left[\frac{2|\eta(t)|}{\gamma_1(t)}\right] \left[-\frac{\pi}{2} \leqslant \theta(t) \leqslant \frac{\pi}{2}\right].$$
 (30)

The standard master equation derived with the Born-Markov approximation has the same form as Eqs. (23)–(25), but with constant-in-time parameters. In it, each term has a physical meaning:

- (i) The first term in Eq. (24), with $\omega(t) = \omega_1 + \Delta \omega(t)$, accounts for the free dynamics of the system, modified by a frequency shift due to its interaction with the reservoir.
- (ii) The second term in Eq. (24) is a squeezing term, arising from an asymmetry between position and momentum variables in the coupling Hamiltonian. However, in the weak-coupling regime, this term is small (being exactly zero in the RWA), leading to a negligible squeezing effect.
- (iii) $\gamma_1(t)$ is a decay rate, which drives the center of the system wave packet towards its equilibrium at the origin of phase space.
- (iv) $\gamma_2(t)$ is a diffusion coefficient, related to injection of extra noise into the system due to nonzero reservoir temperature and counter-rotating terms, which only spreads the wave packet without affecting the trajectory of its center.
- (v) $\eta(t)$ is a coefficient of anomalous diffusion, which injects different levels of noise in position and momentum. From Eqs. (28a) and (28b), we see that when $\eta \neq 0$, the Lindblad operators are not given by a and a^{\dagger} , but by linear combinations of the two, giving rise to anomalous diffusion. The master equation derived in this section is exact in the sense that its solution is guaranteed to agree with the reduced state of a unitary dynamics of the universe. It relies on two hypotheses: that the initial state of the universe is a product state and that the initial state of the reservoir is Gaussian. All features of the system-reservoir energy and information exchange are codified in the specific ways that the coefficients [Eqs. (26)] vary in time.

Markovian and non-Markovian behavior

An interesting discussion in the current literature (see Ref. [20] and references therein) concerns non-Markovian behavior. The Born-Markov approximation always leads to a Lindblad equation with a dissipator written in the form of Eq. (27), with rates $\lambda_n(t)$ which are positive but may vary in time (in which case it can be called a *time-dependent*

Markovian process). If, at any given time, one of these rates assumes a negative value, then it is said to be a *non-Markovian process*, according to the divisibility criterion of Rivas-Huelga-Plenio [20,21]. The model we have developed allows us to compute these rates exactly from the solution, obtained through the system-reservoir interaction Hamiltonian. We can thus describe the system as *Markovian* if the following conditions hold for all times *t*:

$$\gamma_1(t) + 2\gamma_2(t) \geqslant 0, \tag{31a}$$

$$\gamma_1(t)\gamma_2(t) + \gamma_2^2(t) - |\eta(t)|^2 \ge 0,$$
 (31b)

where the functions are defined in Eqs. (26b), (26c), and (26e). These conditions will be satisfied in the limit of vanishingly small system-reservoir coupling, a scenario in which the Born-Markov approximation holds well, when the coupling strength is quantified by the spectral density, given by Eq. (20), or its continuous limit, given by Eq. (22). However, the so-called strong-coupling regime is not a precondition for non-Markovianity, which is mainly determined by the shape of the spectral density $J(\omega)$. In general, Markovianity is associated with a broadband spectrum, such that its typical width is much larger than its typical height [since $J(\omega)$ has the dimension of frequency, we can compare its height and width], while non-Markovian behavior is associated with a narrow spectral width (again, as compared with the typical coupling strength).

The master equation defines a family of dynamical maps $\mathcal{E}_{t,0}$, where the state ρ_t depends on the initial state ρ_0 through a linear superoperator as $\rho_t = \mathcal{E}_{t,0}(\rho_0)$. At the initial instant t = 0, we have made the assumption of a product state between the system and reservoir, and thus the initial system state ρ_0 can be arbitrary. Since ρ_0 and ρ_t are by definition always physically acceptable states, the map $\mathcal{E}_{t,0}$ is necessarily completely positive.

A given family of dynamical maps can be considered divisible if it can be written as $\mathcal{E}_{t,0}(\rho_0) = \mathcal{E}_{t,s}(\mathcal{E}_{s,0}(\rho_0))$, and the map $\mathcal{E}_{t,s}$ is completely positive for every s such that 0 < s < t. This last assumption does not follow from the fact that $\mathcal{E}_{t,0}$ and $\mathcal{E}_{s,0}$ indeed are completely positive. In fact, $\mathcal{E}_{t,s}$ is not completely positive when one of the rates $\lambda_n(t_1)$ is negative on the whole interval $s \leq t_1 \leq t$, which may be infinitesimal.

At time s > 0, correlations between the system and reservoir have built up, and they have possibly become entangled. Thus, the reduced system state ρ_s , which acts as an initial state for the map $\mathcal{E}_{t,s}$, cannot be arbitrary. In particular, it cannot be pure because a pure reduced state means that it is not correlated with any other part of the universe. Therefore, the map $\mathcal{E}_{t,s}$ may fail to be completely positive, but it will not lead to nonphysical states because it can act only on a restricted subset of all possible system states.

VI. ROTATING-WAVE APPROXIMATION

In many physical systems described by the Hamiltonian of Eq. (3), the typical coupling intensity $|g_{kj}|$ is many orders of magnitude smaller than the frequencies ω_k , characterizing the *weak-coupling regime*. It is then a good approximation to drop the counter-rotating terms $(a_k a_j$ and $a_k^{\dagger} a_j^{\dagger})$, a procedure which is known as the *rotating-wave approximation (RWA)*.

Equations (9a) and (9b) are greatly simplified, with $V_{kj} = 0$ and U_{kj} obeying

$$\frac{dU_{kj}}{dt} = i\omega_j U_{kj} - i\sum_{n=1}^N U_{kn} g_{nj}.$$
 (32)

For single-mode dynamics, Eqs. (18a) and (21a) are simplified to

$$\frac{dU_1^{(\text{RWA})}}{dt} = i\omega_1 U_1^{(\text{RWA})} - \int_0^t dt_1 \int_0^\infty d\omega J(\omega)$$
$$\times e^{-i\omega(t-t_1)} U_1^{(\text{RWA})}(t_1), \tag{33}$$

$$A^{(0)} = \int_0^t dt_1 \int_0^t dt_2 U_1^{\text{RWA}}(t_1) U_1^{\text{RWA}*}(t_2)$$

$$\times \text{Re} \int_0^\infty d\omega J(\omega) e^{-i\omega(t_1 - t_2)}.$$
(34)

The condition $V_{kj}=0$ (for all kj) implies both $\xi(t)=0$ (no squeezing term in the effective system Hamiltonian) and $B^{(0)}=0$ and, unless the reservoir initial state has some degree of squeezing [i.e., $\langle a_m a_n \rangle_0 \neq 0$ for some m,n], then also $B^{(\text{th})}=0$. Together, this implies that $\eta(t)=0$. The condition $\xi(t)=\eta(t)=0$ is required to maintain the symmetry between position and momentum variables, since the exchange $(\hat{q},\hat{p}) \leftrightarrow (\hat{p},-\hat{q})$ leaves the RWA Hamiltonian unchanged, while it changes the one in Eq. (1). Therefore, in RWA, the squeezing term in Eq. (24) and the last term in Eq. (25) both vanish at all times, leading to the usual three terms (frequency shift, dissipation, and diffusion) in the expression. The Markovianity condition is then simplified to

$$\gamma_1(t) + 2\gamma_2(t) \geqslant 0, \tag{35a}$$

$$\gamma_2(t) \geqslant 0. \tag{35b}$$

VII. NATURAL BASIS FOR SYSTEM EVOLUTION

It is a well-known result [16] that a coherent state remains coherent when in contact with a reservoir at absolute zero, if one assumes RWA. This makes coherent states a natural basis to analyze the system dynamics, ultimately motivating Glauber and Sudarshan to define the normal-order quasiprobability *P* function,

$$\rho(t) = \int d^{2M}\{\alpha\} P(\{\alpha\}, t) |\{\alpha\}\rangle \langle \{\alpha\}|. \tag{36}$$

We have returned to the general case, where the system is composed of M modes. The coherent state follows a dynamics in phase space that can be written $|\{\alpha\}\rangle \rightarrow |\{\alpha(t)\}\rangle$, where $\{\alpha(t)\}$ is given by [compare with Eq. (8)]

$$\alpha_k(t) = \sum_{j=1}^{M} (U_{kj}\alpha_j + V_{kj}\alpha_j^*) \quad (1 \leqslant k \leqslant M).$$
 (37)

Combining these two equations, we have the familiar result

$$\rho(t) = \int d^{2M}\{\alpha\} P(\{\alpha\}, 0) |\{\alpha(t)\}\rangle \langle \{\alpha(t)\}|.$$
 (38)

The fact that coherent states remain coherent is intimately connected with the fact that the vacuum is a stationary state of

this nonunitary evolution. However, for nonzero temperature, or when one includes the counter-rotating terms, this is no longer true: coherent states do not maintain their coherence and we must resort to another basis, formed by Gaussian states. In the same way that the coherent states are generated by displacing the vacuum, the time-dependent Gaussian basis states are generated by displacing a squeezed thermal state,

$$\rho_B(\{\alpha\},t) = D(\{\alpha\})\rho_o(t)D^{\dagger}(\{\alpha\}),\tag{39}$$

where $\rho_o(t)$ is obtained by allowing an initial vacuum state $|0\rangle\langle 0|$ to evolve to $\rho_o(t)$ in accordance with the solution presented in Eq. (15),

$$\rho_o(t) = \int d^{2M}\{\alpha\} P_o(\{\alpha\}, t) |\{\alpha\}\rangle \langle \{\alpha\}|. \tag{40}$$

Adopting then this natural Gaussian basis, we can write the evolution of any arbitrary initial state as

$$\rho(t) = \int d^{2M}\{\alpha\} P(\{\alpha\}, 0) \rho_B(\{\alpha(t)\}, t). \tag{41}$$

Combining Eqs. (40) and (41), we can rewrite the evolution of an arbitrary initial state (albeit one with a reasonably well-defined P function) as

$$\rho(t) = \int d^{2M}\{\alpha\} \int d^{2M}\{\eta\} P(\{\alpha\}, 0) P_o(\{\eta\}, t)$$

$$\times |\{\eta + \alpha(t)\}\rangle \langle \{\eta + \alpha(t)\}|. \tag{42}$$

There are two different behaviors associated with this evolution, which are codified in different mathematical objects. The first behavior is associated with the first moments of the distribution, or the trajectory of the center of a wave packet in phase space, given by $\{\alpha(t)\}\$ defined in Eq. (37). It is independent of the state of the reservoir, as it is only affected by dissipation effects. It is also exactly equivalent to the solution to classical equations of motion. The situation is different when we analyze the evolution of the shape of the wave packet, which is given by $P_o(\{\eta\},t)$, defined through Eq. (40). It depends both on thermal fluctuations (caused by the initial state of the reservoir being different from the vacuum) and on quantum fluctuations (caused by the presence of counter-rotating terms). The latter is responsible for the entire difference between quantum and classical dynamics governed by quadratic Hamiltonians.

When the RWA and an absolute-zero reservoir are assumed, the wave packet is not distorted, and $P_o(\{\eta\},t)$ reduces to a δ function at the origin, making Eq. (42) identical to Eq. (38). Therefore, Eq. (42) is a generalization of Eq. (38), and we have obtained a generalization of the dynamics described in Ref. [16].

Another way to look at this result is that the displaced phasespace quasiprobability function is convoluted with another function, which accounts for the change in shape,

$$P(\{\alpha\},t) = \int d^{2M}\{\gamma\} P(\{\gamma\},0) P_o(\{\alpha - \gamma(t)\},t). \tag{43}$$

For a single mode, the center path follows $\alpha(t) = U_1\alpha + V_1\alpha^*$, with U_1 and V_1 being given by the solutions to Eqs. (18a) and (18b). The function $P_o(\{\alpha\},t)$ is just the solution when the initial state is the vacuum, i.e., it satisfies the initial condition $P_o(\{\alpha\},0) = \delta^{(2)}(\alpha)$. Under the RWA, this continues to be

true at all times, $P_o^{\text{RWA}}(\{\alpha\},t) = \delta^{(2)}(\alpha)$, and the wave packet wanders around phase space undistorted.

VIII. CONCLUSIONS

We have presented a technique to derive an exact master equation for the system-reservoir dynamics under the strongcoupling regime, where neither the rotating-wave approximation nor the secular approximation apply. To this end, we adopted the strategy of considering a network of bosonic systems coupled to each other, picking out one of them as the system of interest and leaving the rest to play the role of the reservoir. Working with phase-space distribution functions and Gaussian states, we generalize an earlier result by Glauber that a coherent state remains coherent despite dissipation when coupled to a zero-temperature reservoir. We demonstrate that there is a class of Gaussian states which serves as a generalization of the coherent-state basis of the Glauber-Sudarshan P representation. This class of Gaussian states follows from the distortion of the vacuum state which, in the strong-coupling regime, is no longer a stationary state, even for a zero-temperature reservoir.

We have also presented an investigation of the conditions that lead to a non-completely-divisible map, and thus non-Markovian dynamics. So far, conditions for non-Markovianity have been studied for finite Hilbert spaces under the rotating-wave and/or secular approximations. We remark that a master equation similar to the one derived here has been obtained using the path-integral approach [7]. The simplicity of our development, using phase-space distribution functions, offers the significant advantage of enabling us to cast the problem as the solution of a linear system of equations.

We finally address some interesting issues to be further investigated. We first observe that the asymptotic state of a non-Markovian open system may depend on the initial conditions when the initial state of the system plus reservoir is correlated [22]. In fact, although we have assumed for simplicity the usual sudden-coupling hypothesis, we emphasize that our approach is particularly useful for considering the situation where the initial states are not separable. In light of this result, it is worth studying the asymptotic dynamics under the strongcoupling regime, as well as a study of the differences coming when the RWA is used and when the counter-rotating terms are added, for different ranges of couplings [23], both in the short-time and the asymptotic limits. As the main goal of the present work is to present our method to deal with the system-reservoir coupling under the strong-coupling regime, a detailed analysis of the dynamics of the system under distinct initial states and sets of parameters will be addressed in another contribution.

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