Exact dynamics of the spin-boson model at the Toulouse limit

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Starting from the stochastic Liouville equation, we obtain an integral functional equation for describing the finite-temperature dynamics of the asymmetric spin-boson model. Like the zero-temperature case, this equation displays a hierarchical structure characterizing the multiple-timescale nature of quantum dissipative dynamics. We are thereby able to establish a perturbation series and illustrate the contributions with the conventional concepts of blips and sojourns. We clarify the speciality of the Toulouse limit by presenting the analytical properties of intrablip and blip-sojourn interactions. This speciality leads to a closed-form equation for the blip, from which the exact result of the dissipative dynamics can be obtained. We also demonstrate the exact solution by summing the perturbative series. Moreover, we calculate the exact equilibrium distribution at the Toulouse limit and compare it with the Boltzmann distribution valid for weak dissipation.

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I. INTRODUCTION

The spin-boson model, which describes a spin under the influence of a coupling heat bath, has been a paradigm to understand the fundamental aspects of quantum dissipation [1]. It can be used to understand a qubit perturbed by its environment [2] and tunneling in solvents [3]. Moreover, it can be mapped from the anisotropic Kondo model [4,5] and the ferromagnetic Ising model with long-range forces [6,7]. The spin-boson model thus has fruitful applications in physics and chemistry and plays an important role in understanding quantum phase transitions [8–10], quantum computing [11], quantum coherence [12], quantum optics [13], chemical reactions [14–16], thermodynamics [17,18], and heat conduction [19].

The spin-boson model is described by the Caldeira-Leggett model [20,21] consisting of the system $\hat{H}_{\rm s}$, the bath $\hat{H}_{\rm b}$ and the system-bath interaction $\hat{H}_{\rm sb}$, namely,

$$\hat{H}_{\rm sbm} = \hat{H}_{\rm s} + \hat{H}_{\rm b} + \hat{H}_{\rm sb}. \quad (1)$$

The Hamiltonian of the system is generally expressed in terms of the Pauli matrices $\sigma_{x/y/z}$, $\hat{H}_{\rm s} = -\hbar\Delta\sigma_x/2 - \hbar\epsilon\sigma_z/2$, where $\hbar$ denotes the reduced Planck constant. Note that in principle a reorganization term should be included to counteract the bath-induced system shift. But for a two-state system, the reorganization term is a constant, and its influence on the system evolution is merely a global phase and hence is omitted here. The system Hamiltonian is a reasonable two-state approximation to a double-well system with a high barrier. In this approximation ϵ represents the asymmetricity of the double well [21], which is also called the bias. A symmetric double well will be approximated with $\epsilon = 0$, and Eq. (1) describes a symmetric spin-boson model. Otherwise, when $\epsilon \neq 0$, it characterizes an asymmetric one. For the symmetric case, the ground and first excited states are $|0\rangle = (1, -1)^T/\sqrt{2}$ and $|1\rangle = (1, 1)^T/\sqrt{2}$, respectively, with $\hbar\Delta$ being their energy difference. Their linear superpositions $|L\rangle = (|0\rangle + |1\rangle)/\sqrt{2} = (1, 0)^T$ and $|R\rangle = (|0\rangle - |1\rangle)/\sqrt{2} = (0, 1)^T$ correspond to the localized states of the symmetric double-well system and thus are called the left and right states. The dynamics of the localized states is usually used to visualize quantum coherence. Therefore, the spin-boson model also represents generic dissipative tunneling of particles in double-well potentials.

For the Caldeira-Leggett model the bath comprises infinite independent harmonic oscillators $\hat{H}_{\rm b} = \sum_j (\hat{p}_j^2/2m_j + m_j\omega_j^2\hat{x}_j^2/2)$ which linearly couple to the system $\hat{H}_{\rm sb} = \hat{f}_{\rm s}\hat{g}_{\rm b}$, with $\hat{f}_{\rm s} = \sqrt{\hbar}\sigma_z/2$ and $\hat{g}_{\rm b} = \sum_j c_j\hat{x}_j$. For such a linear coupling scheme, it is shown that the effect of the bath on the evolution of the system is fully characterized by its spectral density function [20]

$$J(\omega) = \frac{\pi}{2}\sum_j \frac{c_j^2}{m_j\omega_j}\delta(\omega - \omega_j). \quad (2)$$

Usually, the bath is assumed to form a continuum, and $J(\omega)$ is thus a continuous function. In the present work, we treat the bath as $J(\omega) = 2\pi K\omega e^{-\omega/\omega_c}$, where K is the dimensionless Kondo parameter characterizing the dissipation strength and ω_c is the high-frequency cutoff. Here, we focus on the dynamical features at the scaling limit $\omega_c \to \infty$. Such a bath is Ohmic as $J(\omega) \propto \omega$ in the low-frequency regime.

Despite the apparent simplicity, the spin-boson model exhibits rich physics [7]. At zero temperature the dissipative dynamics is coherent and exhibits quantum coherence at weak dissipation ($K < \frac{1}{2}$). When K is increased to $\frac{1}{2}$, the Toulouse

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limit, it manifests a coherent-incoherent crossover with an exponential decay. The Toulouse limit is related to the infinite-U Anderson model [22] and has been extensively studied in physics. It has been shown that the dynamics can be solved by the real-time path-integral technique [23–25], mapping to a solvable free-fermion resonant-level model [7,21] and a solvable equivalent noninteracting nonequilibrium problem [26]. When the dissipation strength K further increases, the dynamics becomes incoherent until K reaches a critical value, $K = 1$. Then, the system will be localized in the initial state, manifesting a transition from a delocalized state to a local one, which is a typical signature of the quantum phase transition.

We still do not know how to exactly solve the spin-boson model in the whole physical parameter space because of the involvement of multiple timescales, although it assumes analytical solutions for specific cases such as the Toulouse limit. As such, this model offers both a great challenge and a versatile test bed for methodological developments. There have been several theoretical techniques proposed to attack the spin-boson model and generic quantum dissipative systems as well. For instance, to understand the thermodynamics it is useful to transfer a number of rigorous, thermodynamical results of the inverse-square Ising chain to the spin-boson model by exploiting their equivalence [27–29]. Especially, Anderson used the mapping to show that this model assumes quantum phase transition [6]. For real-time dynamics, the Feynman-Vernon influence functional serves as powerful theoretical machinery [30] and has stimulated a bunch of analytical and numerical methods, such as the noninteraction-blip approximation (NIBA) [31,32], the quantum Monte Carlo method [33], the quasiadiabatic propagator path-integral approach [34], the stochastic Liouville equation (SLE) [35,36], and the functional-integral approach [17,37]. Among these methods, SLE [35,36], first established upon factoring the influence functional [35] and later reformulated with the stochastic decoupling of the dissipative interaction [36], has become a fruitful framework. As a theoretical formulation, it has been shown to be equivalent to the non-Markovian quantum state diffusion and used to derive quantum master equations [38]. More importantly, SLE provides a simulation protocol and a working formula for developing highly efficient numerical procedures. The SLE-based methods, including the hierarchical approach [39–42], hybrid stochastic-hierarchical equations [43,44], and variance reduction schemes [45–47], have already witnessed successful applications to solve quantum dissipative dynamics. Especially, the hierarchical approach and hybrid stochastic-hierarchical equations have now become the benchmark methods for solving the dynamics of the spin-boson model [48,49]. Unfortunately, despite the impressive progress, the zero-temperature dynamics of the spin-boson model at strong dissipation ($K > \frac{1}{2}$) still remains elusive, and results obtained from the hybrid stochastic-hierarchical equations [48] differ from those of the extended hierarchical approach [49] and are challenged by simulations of the multilayer multiconfiguration time-dependent Hartree method [50].

Very recently, with the stochastic Liouville equation and using the auxiliary functional averaging technique, we derived an integral functional equation for the population dynamics [51]. This equation displays a hierarchical structure of motion in the sense that the later dynamics relies on the spontaneous fields induced by the earlier one and allows us to develop a nonperturbative treatment. Indeed, NIBA is feasibly acquired by merely neglecting the earlier spontaneous fields. Moreover, the exact solution at the Toulouse limit is readily obtained for the symmetric spin-boson model. An approximation for dealing with strong dissipation $K > \frac{1}{2}$ is also proposed, which results in an exponential-decay dynamics and in which the scaled time does not change in the range of $\frac{1}{2} \leqslant K < 1$. Of course, it correctly predicts that the decay rate vanishes at the quantum critical point $K = 1$.

In this work we focus on the finite-temperature dissipative dynamics. In particular we aim at exactly solving the Toulouse dynamics of the asymmetric spin-boson model. The asymmetricity makes the numerical simulations and the analytic solution even harder [52,53]. Interestingly, for the symmetric case $\epsilon = 0$, NIBA gives an exponential decay at the Toulouse limit [1,23,25] and yields an overall good approximation for $K < \frac{1}{2}$. However, it is no longer a valid approximation in the presence of a finite bias [21]. This notorious failure even brought about doubt on the NIBA result for the coherent-incoherent transition. Egger *et al.* investigated this transition beyond NIBA and revealed that for the symmetric model at $K \to \frac{1}{2}$ only blips of effectively vanishing length contribute, which causes vanishing interblip interaction and makes NIBA exact [53].

In an elaborate work [23] Sassetti and Weiss addressed the exact solution at the Toulouse limit with the path-integral method. Their derivation involves beautiful, profound physical considerations and sophisticated techniques, which motivates us to develop more accessible methods. We find that the integral functional equation developed in Ref. [51] is a suitable one. Indeed, by analyzing the particularity of the Toulouse limit we can either solve the resultant equations of motion or carry out the summation of the perturbation expansion to obtain the exact solution.

The rest of this paper is organized as follows. In Sec. II we outline the key ideas of the stochastic decoupling method and show how to derive the bath-induced field when the bath starts from a state that is equilibrated according to the initial configuration of the two-state system. In Sec. III we give a brief account of the integral functional equation method for solving the dissipative dynamics. In Sec. IV we show that the solution of the single-blip dynamics is available. With this solution the exact Toulouse dynamics is feasibly reached. We also demonstrate that the exact dynamics can be worked out by iterating the integral functional equation and calculating the resultant series. In Sec. V we compare the exact solution and the Boltzmann distribution that is suitable for weak dissipation. We summarize our findings and discuss their implications in Sec. VI.

II. STOCHASTIC DECOUPLING OF THE SPIN-BOSON MODEL

For a given initial state, the dynamics of the spin-boson model is fully characterized by its density operator $\rho(t)$, which evolves according to the quantum Liouville–von Neumann equation, $i\hbar\partial\rho(t)/\partial t = [\hat{H}_{\mathrm{sbm}}, \rho(t)]$. The initial state is generally assumed to be a factorized one, $\rho(0) = \rho_s(0)\rho_b(0)$. In this work we suppose that the system evolves from the left state, that is, $\rho_s(0) = |L\rangle\langle L|$. We will focus on the dynamics $\tilde{z}(t) = \mathrm{Tr}[\rho(t)\sigma_z]$, that is, the population difference between the left and right states. Without the system-bath interaction, the two-state system is a textbook example manifesting quantum coherence with a periodic change in the population in the initial state, resulting in $\tilde{z}(t) = (\epsilon^2 + \Delta^2 \cos\sqrt{\epsilon^2+\Delta^2}t)/(\epsilon^2+\Delta^2)$ [54]. The coupling to a heat bath affects this coherent motion. We compare the quantum coherence between the spin-boson model and a damped harmonic oscillator. As we know, the periodic oscillation of a harmonic oscillator is hampered by friction. When fiction gets stronger, the harmonic oscillator returns to its equilibrium point more slowly and exhibits an underdamped-overdamped transition. The dynamics is frozen only when the dissipation is infinitely strong. For the two-state system, which is a genuine quantum system, its dynamical feature is dramatically changed by quantum dissipation. Like the frictional classical oscillation exhibiting an underdamped-overdamped transition, the dissipative two-state system also shows a coherent-incoherent crossover as the dissipation strength increases. However, there is a drastic difference between the damped harmonic oscillator and the spin-boson model: When the dissipation strength goes beyond a critical value, a dissipative two-state system at zero temperature will be localized in the initial state forever. This is the pivotal feature of the quantum phase transition and has no classical counterpart.

We now consider the initial state of the bath. Usually, the bath is assumed to start from a thermal equilibrium state, i.e., $\rho_b(0) = \exp(-\beta\hat{H}_b)/\mathrm{Tr}[\exp(-\beta\hat{H}_b)]$, where $\beta = 1/k_BT$, with k_B being the Boltzmann constant and T being the temperature. Such an initial bath state might be relevant in chemical reactions and spectroscopic measurements where the bath represents the solvent [55–57]. This choice simplifies theoretical derivation and ensuing computation and is thus widely adopted in the literature. The thermal equilibrium according to the bare bath Hamiltonian is by no means the only choice of the initial condition, and there are studies on different initial preparations [58–62]. A nonfactorized initial state may have different consequences. For instance, Hakim and Ambegaokar investigated a dissipative free particle and revealed that the factorized and nonfactorized initial states lead to different transient dynamics [63]. Qin and coworkers studied the spin-boson model and found that different initial states yield the same long-time dynamics [64]. These results confirm that the two sets of initial states should give the same evolution in the timescale $\gg 1/\omega_c$. Generally speaking, the bath will quickly return to equilibrium regardless of the initial condition, but the difficulty in theoretical treatment differs for different initial conditions. We here set the bath initially equilibrated according to the system. The equilibration can be realized by applying a strong bias $-\hbar\epsilon_0\theta(-t)$, with $\epsilon_0 \gg \Delta$, from an infinite past to trap the spin in the left state. The strong bias is disabled at time $t = 0$, and later, the dynamics is dictated by the Hamiltonian (1). Such a preparation results in a shifted initial bath

$$\rho_b(0) = e^{-\beta(\hat{H}_b + \bar{f}_s\hat{g}_b)}/\mathrm{Tr}\{e^{-\beta(\hat{H}_b+\bar{f}_s\hat{g}_b)}\}, \quad (3)$$

where $\bar{f} = \mathrm{Tr}[\hat{f}_s\rho_s(0)]$.

With the initial state and the equation of motion, we are ready to tackle the dynamics of the spin-boson model. Direct propagation through the quantum Liouville–von Neumann equation, however, has to deal with the coupled infinite degrees of freedom and is impossible. To avoid this difficulty, we adopt a stochastic unraveling scheme [36] to decouple the evolution into a set of equations,

$$i\hbar\frac{\partial\rho_s}{\partial t} = [\hat{H}_s, \rho_s] + \frac{\chi\sqrt{\hbar}}{2}[\hat{f}_s, \rho_s]\mu(t) + \frac{\chi\sqrt{\hbar}}{2}\{\hat{f}_s, \rho_s\}\nu(t), \quad (4a)$$

$$i\hbar\frac{\partial\rho_b}{\partial t} = [\hat{H}_b, \rho_b] + i\frac{\sqrt{\hbar}}{2\chi}[\hat{g}_b, \rho_b]\nu^*(t) + i\frac{\sqrt{\hbar}}{2\chi}\{\hat{g}_b, \rho_b\}\mu^*(t), \quad (4b)$$

where $\mu(t)$ and $\nu(t)$ are two uncorrelated complex white noises satisfying the correlations $\mathcal{M}\langle\mu(t_1)\mu(t_2)\rangle = \mathcal{M}\langle\nu(t_1)\nu(t_2)\rangle = 0$ and $\mathcal{M}\langle\mu^*(t_1)\mu(t_2)\rangle = \mathcal{M}\langle\nu^*(t_1)\nu(t_2)\rangle = 2\delta(t_1 - t_2)$, with $\delta(t)$ being the Dirac delta function. The parameter χ is a free scaling factor with the dimension $[T^{-\frac{1}{2}}]$ to ensure all terms in Eq. (4) have the same dimension. Note that the parameter χ could be important if Eq. (4a) is used to describe the real or virtual stochastic physical processes. When we aim at the exact dissipative dynamics, however, the factors χ and χ^{-1} in Eq. (4a) will be canceled out by their inverse arising from Eq. (4b), and thus, χ becomes irrelevant. Therefore, we simply set $\chi = 1$ in the following.

The exact dynamics of the whole system is produced by the stochastic average, $\rho(t) = \mathcal{M}\langle\rho_s(t)\rho_b(t)\rangle$. Consequently, the reduced dynamics of the system is given by $\tilde{\rho}_s(t) = \mathcal{M}\langle\rho_s(t)\mathrm{Tr}[\rho_b(t)]\rangle$. That is to say, the dissipative dynamics can be acquired directly if the trace of the bath $\mathrm{Tr}[\rho_b(t)]$ instead of the density matrix $\rho_b(t)$ itself is known. Actually, we can feasibly evaluate the trace $\mathrm{Tr}[\rho_b(t)]$ with the operator method [65], obtaining $\mathrm{Tr}[\rho_b(t)] = \exp\{\int_0^t dt_1\mu^*(t_1)[\bar{g}(t_1) - 2\bar{f}F(t_1)]/\sqrt{\hbar}\}$, where $\bar{g}(t)$ is the bath-induced field,

$$\bar{g}(t) = \sqrt{\hbar}\int_0^t dt_1[\alpha_r(t-t_1)\mu^*(t_1) + i\alpha_i(t-t_1)\nu^*(t_1)], \quad (5)$$

and $F(t) = \int_0^\infty d\omega J(\omega)\cos(\omega t)/\omega$, with α_r and α_i respectively being the real and imaginary parts of the bath correlation function $\alpha(t) = \mathrm{Tr}[\exp(i\hat{H}_bt/\hbar)\hat{g}_b\exp(-i\hat{H}_bt/\hbar)\hat{g}_b\exp(-\beta\hat{H}_b)]/\mathrm{Tr}[\exp(-\beta\hat{H}_b)]$. This correlation function can be expressed in terms of the spectral density function

$$\alpha(t) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\hbar\beta\omega}{2}\right)\cos(\omega t) - i\sin(\omega t)\right]. \quad (6)$$

In calculating the stochastic average of $\rho_s(t)\mathrm{Tr}[\rho_b(t)]$, it is more convenient to work out a variant of ρ_s, a new stochastic density matrix $\hat{\rho}_s$, whose average directly produces the exact reduced density matrix, $\tilde{\rho}_s(t) = \mathcal{M}\langle\hat{\rho}_s(t)\rangle$. To this end, we absorb the trace of the bath $\mathrm{Tr}[\rho_b(t)]$ into the stochastic measure via the Girsanov transformation, which is essentially a shift of the noise, $\mu(t) \to \mu(t) + 2\bar{g}(t)/\sqrt{\hbar}$ [36,66]. Accordingly, the stochastic reduced density matrix ρ_s is modified to $\hat{\rho}_s$, which satisfies the equation of motion

$$i\hbar\frac{\partial\hat{\rho}_s}{\partial t} = [\hat{H}_s + \bar{g}(t)\hat{f}_s, \hat{\rho}_s] + \frac{\sqrt{\hbar}}{2}[\hat{f}_s, \hat{\rho}_s]\mu(t) + \frac{\sqrt{\hbar}}{2}\{\hat{f}_s, \hat{\rho}_s\}\nu(t). \tag{7}$$

Equation (7) is the stochastic Liouville equation derived from a microscopic model. Kubo originally suggested the stochastic Liouville approach as a phenomenological one [67,68], which can be viewed as the high-temperature limit of Eq. (7). The ordinary stochastic differential equation in Eq. (7) is straightforward to implement in numerics. Its performance for strong dissipation, however, degrades due to the drastic increase in the numerical errors at large times [45,46]. Regardless, Eq. (7) may serve as a starting point to derive new efficient algorithms. We now apply it to the spin-boson model. Because the three Pauli matrices and the identity matrix construct a complete basis for two dimensions, the stochastic density matrix can be expressed as $\hat{\rho}_s(t) = [I(t) + x(t)\sigma_x + y(t)\sigma_y + z(t)\sigma_z]/2$. Substituting it into Eq. (7) yields stochastic equations of motion for the coefficients

$$\frac{dI(t)}{dt} = -i\xi_2(t)z(t), \tag{8a}$$

$$\frac{dx(t)}{dt} = [\epsilon + F(t) - \xi_1(t)]y(t), \tag{8b}$$

$$\frac{dy(t)}{dt} = \Delta z(t) - [\epsilon + F(t) - \xi_1(t)]x(t), \tag{8c}$$

$$\frac{dz(t)}{dt} = -\Delta y(t) - i\xi_2(t)I(t). \tag{8d}$$

The initial condition $\hat{\rho}_s(0)$ then accordingly converts to $I(0) = 1$, $x(0) = 0$, $y(0) = 0$, and $z(0) = 1$. Here, for convenience, we have regrouped the white noises and the bath-induced stochastic field as $\xi_1(t) = \bar{g}(t)/\sqrt{\hbar} + \mu(t)/2$ and $\xi_2(t) = \nu(t)/2$. The two noises ξ_1 and ξ_2 are of zero mean and assume the covariances $\mathcal{M}\langle\xi_1(t)\xi_1(t')\rangle = \alpha_r(t-t')$, $\mathcal{M}\langle\xi_2(t)\xi_2(t')\rangle = 0$, and $\mathcal{M}\langle\xi_1(t)\xi_2(t')\rangle = i\theta(t-t')\alpha_i(t-t')$, where $\theta(t)$ is the Heaviside step function, which is unity for $t > 0$ and zero otherwise.

III. FUNCTIONAL EQUATION OF POPULATION DYNAMICS

Our task is to work out the exact dynamics $\tilde{z}(t) = \mathcal{M}\langle z(t)\rangle$. To this end, we derive the stochastic integral equation for $z(t)$ and establish equations for its stochastic average.

We first show how to achieve deterministic functional equations dictating the dynamics. We solve the linear differential equations (8b) and (8c) by treating $z(t)$ as an inhomogeneous term and obtain the solution

$$x(t) = -\Delta\int_0^t dt_1 \sin[\phi_1(t,t_1) - F(t,t_1) - \epsilon(t-t_1)]z(t_1), \tag{9a}$$

$$y(t) = \Delta\int_0^t dt_1 \cos[\phi_1(t,t_1) - F(t,t_1) - \epsilon(t-t_1)]z(t_1), \tag{9b}$$

where, for simplicity, we denote $F(t_1,t_2) = F(t_1) - F(t_2)$ and $\phi_a(t_1,t_2) = \int_{t_2}^{t_1} d\tau\,\xi_a(\tau)$ for $a = 1, 2$. Substituting the solution (9b) into Eqs. (8a) and (8d), we find

$$z(t) = e^{-i\phi_2(t,0)} - \Delta^2\int_0^t dt_1\int_0^{t_1} dt_2 \cos\phi_2(t,t_1) \times \cos[\phi_1(t_1,t_2) - F(t_1,t_2) - \epsilon(t_1-t_2)]z(t_2). \tag{10}$$

In taking the average it becomes convenient to convert the exponential inhomogeneous term in the linear integral equation (10) to unity. To this purpose, we recast $z(t)$ as $z(t) = e^{-i\phi_2(t,0)}\breve{z}(t)$, where $\breve{z}(t)$ satisfies the following equation:

$$\breve{z}(t) = 1 - \Delta^2\int_0^t dt_1\int_0^{t_1} dt_2 \cos\phi_2(t,t_1)e^{i\phi_2(t,t_2)} \times \cos[\phi_1(t_1,t_2) - F(t_1,t_2) - \epsilon(t_1-t_2)]\breve{z}(t_2). \tag{11}$$

We now work out a variant of $\breve{z}(t)$, denoted as $\bar{z}(t)$, whose stochastic average directly produces the dynamics, i.e., $\tilde{z}(t) = \mathcal{M}\langle\bar{z}(t)\rangle$. For this purpose, we invoke the Girsanov transformation $\xi_1(t) \to \xi_1(t) + F(t) - \Lambda t$, with $\Lambda = F(0) = \int_0^\infty d\omega\,J(\omega)/\pi\omega$, to absorb the factor $e^{-i\phi_2(t,0)}$ in $z(t) = e^{-i\phi_2(t,0)}\breve{z}(t)$ into the stochastic measure [51,69]. Then $\bar{z}(t)$ is acquired via the Girsanov transformation of $\breve{z}(t)$ and obeys the equation of motion,

$$\bar{z}(t) = 1 - \Delta^2\int_0^t dt_1\int_0^{t_1} dt_2 \cos\phi_2(t,t_1)e^{i\phi_2(t,t_2)} \times \cos[\phi_1(t_1,t_2) - (\Lambda+\epsilon)(t_1-t_2)]\bar{z}(t_2). \tag{12}$$

Note that the noises $\phi_2(t,t_1)$ and $\phi_2(t_1,t_2)$ do not correlate with $\bar{z}(t_2)$ and thus can be handled independently in averaging. By contrast, the correlation between $\phi_1(t_1,t_2)$ and $\bar{z}(t_2)$ persists and causes the difficulty. Therefore, we try to disentangle this correlation by decomposing the noise $\phi_1(t_1,t_2)$ into two uncorrelated parts, $\phi_1(t_1,t_2) = \phi_1^{(a)}(t_1,t_2) + \phi_1^{(b)}(t_1,t_2)$, so that only $\phi_1^{(b)}(t_1,t_2)$ correlates with $\bar{z}(t_2)$. Such a decomposition can be conveniently realized via the white noise representation of the noise ξ_1, resulting in

$$\phi_1^{(a)}(t_1,t_2) = \int_{t_2}^{t_1} dt_3\left\{\int_{t_2}^{t_3} dt_4[\alpha_r(t_3-t_4)\mu^*(t_4) + i\alpha_i(t_3-t_4)\nu^*(t_4)] + \frac{\mu(t_3)}{2}\right\}, \tag{13a}$$

$$\phi_1^{(b)}(t_1,t_2) = \int_0^{t_2} dt_3\big[B'_{t_1,t_2}(t_3)\mu^*(t_3) + iB''_{t_1,t_2}(t_3)\nu^*(t_3)\big], \tag{13b}$$

where B' and B'' are integrals of the real and imaginary parts of the bath correlation function, respectively,

$$B'_{t_1,t_2}(t_3) = \int_{t_2}^{t_1} dt_4\alpha_r(t_4-t_3), \tag{14a}$$

$$B''_{t_1,t_2}(t_3) = \int_{t_2}^{t_1} dt_4\alpha_i(t_4-t_3). \tag{14b}$$

To go further, we exploit the auxiliary functional technique in calculating stochastic averages [70]. The key point is to view $\bar{z}(t)$ as a functional of the noises ξ_1 and ξ_2. Then we may shift ξ_1 and ξ_2 with arbitrary deterministic functions B_1 and B_2, respectively. As a consequence, the equation of motion of

$\bar{z}(t)$, Eq. (12), is transformed as

$$\bar{z}([\xi_1+B_1,\xi_2+B_2],t) = 1-\frac{\Delta^2}{4}\int_0^t dt_1\int_0^{t_1} dt_2\big[1+e^{2i\phi_2(t,t_1)+2i\int_{t_1}^t d\tau B_2(\tau)}\big]e^{i\phi_2(t_1,t_2)+i\int_{t_2}^{t_1} d\tau B_2(\tau)}\big\{e^{i\phi_1^{(a)}(t_1,t_2)+i\phi_1^{(b)}(t_1,t_2)+i\int_{t_2}^{t_1}d\tau[B_1(\tau-\Lambda-\epsilon]} + e^{-i\phi_1^{(a)}(t_1,t_2)-i\phi_1^{(b)}(t_1,t_2)-i\int_{t_2}^{t_1} d\tau[B_1(\tau)-\Lambda-\epsilon]}\big\}\bar{z}([\xi_1+B_1,\xi_2+B_2],t_2). \quad (15)$$

We now take the average with respect to the noises ξ_1 and ξ_2. To do so, we have to deal with mutual correlations among processes $e^{2i\phi_2(t,t_1)}$, $e^{i\phi_2(t_1,t_2)\pm i\phi_1^{(a)}(t_1,t_2)}$, $e^{\phi_1^{(b)}(t_1,t_2)}$, and $\bar{z}(t_2)$. The averaging can be simplified by noticing the following facts.

(1) The stochastic processes $\phi_2(t,t_1)$ and $i\phi_2(t_1,t_2)\pm i\phi_1^{(a)}(t_1,t_2)$ do not correlate with other processes, and the averages $\mathcal{M}\langle e^{2i\phi_2(t,t_1)}\rangle$ and $\mathcal{M}\langle e^{i\phi_2(t_1,t_2)\pm i\phi_1^{(a)}(t_1,t_2)}\rangle$ can be carried out independently. The corresponding results are $\mathcal{M}\langle e^{2i\phi_2(t,t_1)}\rangle = 1$ and $\mathcal{M}\langle e^{i\phi_2(t_1,t_2)+i\lambda\phi_1^{(a)}(t_1,t_2)}\rangle = Q(t_1-t_2;\lambda)e^{i\lambda\Lambda(t_1-t_2)}$, where

$$Q(t;\lambda) = e^{-B(t)-i\lambda A(t)-i\lambda\Lambda t}, \quad (16)$$

with $A(t)=\int_0^t dt_1\int_0^{t_1} dt_2\alpha_i(t_1-t_2)$ and $B(t)=\int_0^t dt_1\int_0^{t_1} dt_2\alpha_r(t_1-t_2)$.

(2) The correlation between $\bar{z}(t_2)$ and $\phi_1^{(b)}(t_1,t_2)$ can be solved with the help of the Girsanov transform, $\mathcal{M}\langle e^{\pm i\phi_1^{(b)}(t_1,t_2)}\bar{z}([\xi_1+B_1,\xi_2+B_2],t_2)\rangle = \tilde{z}([B_1\pm iB'_{t_1,t_2}, B_2\mp B''_{t_1,t_2}],t_2)$. Accordingly, upon the stochastic averaging, Eq. (15) becomes

$$\tilde{z}([B_1,B_2],t) = 1-\frac{\Delta^2}{4}\int_0^t dt_1\int_0^{t_1} dt_2\big[1+e^{2i\int_{t_1}^t d\tau B_2(\tau)}\big] \times\sum_{\lambda=\pm1} Q(t_1-t_2;\lambda)e^{i\lambda\int_{t_2}^{t_1} d\tau[B_1(\tau)+\lambda B_2(\tau)-\epsilon]} \times\tilde{z}\big(\big[B_1+i\lambda B'_{t_1,t_2}, B_2-\lambda B''_{t_1,t_2}\big],t_2\big). \quad (17)$$

A remark on the averaging procedure is in order. If it directly applies to Eq. (10), we then end up with the following integral functional equation:

$$\underline{z}([B_1,B_2],t) = e^{-i\int_0^t d\tau B_2(\tau)} - \frac{\Delta^2}{2}\int_0^t dt_1\int_0^{t_1} dt_2\sum_{\lambda=\pm1} \times\cos\left[\int_{t_1}^t d\tau B_2(\tau)\right]Q(t_1-t_2;\lambda) \times e^{i\lambda\int_{t_2}^{t_1} d\tau[B_1(\tau)-\epsilon]} \times\underline{z}\big(\big[B_1+i\lambda B'_{t_1,t_2}, B_2-\lambda B''_{t_1,t_2}\big],t_2\big). \quad (18)$$

These two equations can be transformed into each other by using $\underline{z}([B_1,B_2],t)=e^{-i\int_0^t d\tau B_2(\tau)}\tilde{z}([B_1,B_2],t)$, which keeps the population dynamics unchanged, i.e., $\underline{z}([0,0],t)=\tilde{z}([0,0],t)$. However, it turns out that Eq. (17) makes approximations such as NIBA easier and is thus the focus in the following.

In Eq. (17) functions $B'_{t_1,t_2}(\tau)$ and $B''_{t_1,t_2}(\tau)$ may be regarded as dissipative fields spontaneously produced during evolution. They will be induced as $\tilde{z}([B_1,B_2],t)$ propagates and in turn exert a feedback on the evolution. To further illustrate this idea, we simply set the auxiliary functions B_1 and B_2 to zero and thereby obtain the wanted quantity $\tilde{z}(t)\equiv\tilde{z}([0,0],t)$, which reads

$$\tilde{z}(t) = 1-\frac{\Delta^2}{2}\int_0^t dt_1\int_0^{t_1} dt_2\sum_{\lambda=\pm1} Q(t_1-t_2;\lambda) \times e^{-i\lambda\epsilon(t_1-t_2)}\tilde{z}_{\lambda,t_1}(t_2), \quad (19)$$

where $\tilde{z}_{\lambda,t_1}(t_2)=\tilde{z}([\lambda iB'_{t_1,t_2}, -\lambda B''_{t_1,t_2}],t_2)$. When $t_1=t_2$, $\tilde{z}_{\pm1,t_1}(t_2)=\tilde{z}(t_1)$ by definition. In addition, we have $\tilde{z}_{-1,t_1}(t_2)=[\tilde{z}_{1,t_1}(t_2)]^*$, which ensures a real $\tilde{z}(t)$. Equation (19) presents the exact dissipative dynamics. Unfortunately, it is not in closed form because the relation between $\tilde{z}([\pm iB'_{t_1,t_2}, \mp B''_{t_1,t_2}],t_2)$ and $\tilde{z}(t)$ is unknown. To solve these equations, therefore, we have to know $\tilde{z}_{1,t_1}(t_2)$, which can be deduced from Eq. (17) [71]:

$$\tilde{z}_{1,t_1}(t_2) = 1-\frac{\Delta^2}{2}\int_0^{t_2} dt_3\int_0^{t_3} dt_4 P(t_1,t_2,t_3) \times\big\{Q(t_3-t_4;+1)S(t_1,t_2,t_3,t_4;+1)e^{-i\epsilon(t_3-t_4)} \times\tilde{z}\big(\big[iB'_{t_1,t_2}+iB'_{t_3,t_4}, -B''_{t_1,t_2}-B''_{t_3,t_4}\big],t_4\big) + Q(t_3-t_4;-1)[S(t_1,t_2,t_3,t_4;-1)]^{-1}e^{i\epsilon(t_3-t_4)} \times\tilde{z}\big(\big[iB'_{t_1,t_2}-iB'_{t_3,t_4}, -B''_{t_1,t_2}+B''_{t_3,t_4}\big],t_4\big)\big\}, \quad (20)$$

where

$$P(t_1,t_2,t_3) = \tfrac{1}{2}+\tfrac{1}{2}e^{-\frac{2i}{\hbar}\int_{t_3}^{t_2} dt_4 B''_{t_1,t_2}(t_4)} \quad (21)$$

and

$$S(t_1,t_2,t_3,t_4;\lambda) = \frac{Q(t_1-t_4;\lambda)}{Q(t_1-t_3;\lambda)}\frac{Q(t_2-t_3;\lambda)}{Q(t_2-t_4;\lambda)}. \quad (22)$$

Equation (20) is not in closed form either, and more dissipative fields B'_{t_3,t_4} and B''_{t_3,t_4} are included. The above procedure shows that evolution continuously induces dissipative fields and the motion of $\tilde{z}(t)$ involves $\tilde{z}([i\lambda_1 B'_{t_1,t_2}, -\lambda_1 B''_{t_1,t_2}],t_2)$, whose propagation in turn generates dissipative fields in more periods and depends on $\tilde{z}([i\lambda_1 B'_{t_1,t_2}+i\lambda_2 B'_{t_3,t_4}, -\lambda_1 B''_{t_1,t_2}-\lambda_2 B''_{t_3,t_4}],t_4)$. For convenience we introduce the notation $Z_n=\tilde{z}([i\lambda_1 B'_{t_1,t_2}+\cdots+i\lambda_n B'_{t_{2n-1},t_{2n}}, -\lambda_1 B''_{t_1,t_2}-\cdots-\lambda_n B''_{t_{2n-1},t_{2n}}],t_{2n})$ by omitting the arguments. Iterating Eq. (17) repeatedly, we discover that the equation for Z_n is determined by an integral over Z_{n+1} that involves more complex, more time-advanced dissipative fields. This procedure essentially establishes a hierarchical description for the dissipative dynamics.

The hierarchical structure may be explained in terms of blips and sojourns [21]. To clarify this connection we iterate Eq. (17) to express $\tilde{z}(t)$ as an infinite series of Δ^2,

$$\tilde{z}(t) = 1 + \sum_{n=1}\left(\frac{-\Delta^2}{2}\right)^n \int_0^t \mathcal{D}_n\{t\} \sum_{\lambda_1,\dots,\lambda_n=\pm1} \prod_{j=1}^n Q(t_{2j-1}-t_{2j};\lambda_j)e^{-i\lambda_j\epsilon(t_{2j-1}-t_{2j})}\frac{1}{2}\left[1+\prod_{k=j+1}^n W(t_{2j-1},t_{2j},t_{2k-2},t_{2k-1};\lambda_j)\right] \times \prod_{k=j+1}^n [S(t_{2j-1},t_{2j},t_{2k-1},t_{2k};\lambda_k)]^{\lambda_j\lambda_k}, \tag{23}$$

where $\int_0^t \mathcal{D}_n\{t\} = \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{2n-1}} dt_{2n}$ and $W(t_1,t_2,t_3,t_4;\lambda) = \exp\{-2i\lambda[A(t_2-t_3)+A(t_1-t_4)-A(t_2-t_4)-A(t_1-t_3)]\}$. Here, a blip corresponds to the period $t_{2n} < t < t_{2n-1}$ spanned by dissipative fields $B'_{t_{2n-1},t_{2n}}$ and $B''_{t_{2n-1},t_{2n}}$, whereas a sojourn is the period $t_{2n+1} < t < t_{2n}$ between two successive blips. Correspondingly, the function Z_n describes the n-blip dynamics containing the effect of all the blip-blip and blip-sojourn interactions.

Note that Eq. (23) can also be obtained by iterating Eq. (12) and then taking the stochastic average. Within the framework of stochastic processes, interactions among blips and sojourns becomes clearer: They are nothing but consequences of their stochastic correlations. The nth-order term in the series actually is the n-blip contribution and compromises all possible interactions between n blips and n sojourns. For instance, the W function in Eq. (23) arises from the factor $\exp\{-2\lambda_j\mathcal{M}\langle\phi_1(t_{2j-1},t_{2j})\phi_2(t_{2k-2},t_{2k-1})\rangle\}$ defining the correlation between a blip noise $\phi_1(t_{2j-1},t_{2j})$ and a sojourn noise $\phi_2(t_{2k-2},t_{2k-1})$ and hence stands for the blip-sojourn correlation or interaction. The Q function is rooted in the autocorrelation of the blip noise $\lambda_j\phi_1(t_{2j-1},t_{2j}) + \phi_2(t_{2j-1},t_{2j})$, i.e., $\mathcal{M}\langle\exp\{i[\lambda_j\phi_1(t_{2j-1},t_{2j})+\phi_2(t_{2j_1},t_{2j})]\}\rangle$ and corresponds to the intrablip correlation. Meanwhile, the S function originates from the correlation between two different blip noises, i.e., $\exp\{-\mathcal{M}\langle[\lambda_j\phi_1(t_{2j-1},t_{2j})+\phi_2(t_{2j-1},t_{2j})][\lambda_k\phi_1(t_{2k-1},t_{2k})+\phi_2(t_{2k-1},t_{2k})]\rangle\}$ and stands for the interblip interaction. In addition, $\lambda_j = \pm1$ can be viewed as the phase factor for the jth blip. When two blips $t_{2j} < t < t_{2j-1}$ and $t_{2k} < t < t_{2k-1}$ assume the same phase factors, their interblip interaction is given by $S(t_{2j-1},t_{2j},t_{2k-1},t_{2k};\lambda_k)$ itself. Otherwise, the interaction is described by its inverse, $[S(t_{2j-1},t_{2j},t_{2k-1},t_{2k};\lambda_k)]^{-1}$.

Upon clarifying the blip-and-sojourn concept, the connection to NIBA may be revealed straightforwardly. As illustrated by Dekker [32] and Aslangul *et al.* [72], NIBA can be obtained by using the Born approximation after a polaron transformation. In the path-integral formulation NIBA neglects the contribution of the sojourns and adopts vanishing sojourn-blip and interblip interactions [1]. In our case NIBA neglects the evolution-induced fields B_1 and B_2 in Eq. (19), yielding the differential equation

$$\frac{d\tilde{z}(t)}{dt} = -\frac{\Delta^2}{2}\int_0^t d\tau \sum_{\lambda=\pm1} Q(t-\tau;\lambda)e^{-i\lambda\epsilon(t-\tau)}\tilde{z}(\tau), \tag{24}$$

which is the NIBA equation obtained with the path-integral method.

We now use these results to solve the dynamics at the Toulouse limit.

IV. TOULOUSE LIMIT: EXACT SOLUTION

Let us first look at the correlation function $\alpha(t)$ that determines the bath-induced noise. At temperature T it reads

$$\alpha(t) = \frac{2K\omega_c^2(\omega_c^2t^2 - 2i\omega_c t - 1)}{(1+\omega_c^2t^2)^2} + \frac{4K}{\hbar^2\beta^2}\mathrm{Re}\psi'\left(\frac{1+i\omega_c t}{\hbar\beta\omega_c}\right),$$

where ψ is the digamma function. Functions $A(t)$ and $B(t)$, the double integrals of $\alpha(t)$, become $A(t) = 2K\arctan\omega_c t - 2K\omega_c t$ and $B(t) = -K\ln(1+\omega_c^2t^2) + 2\ln\Gamma(1/\hbar\beta\omega_c) - \ln\{\Gamma[(1+i\omega_c t)/\hbar\beta\omega_c]\,\Gamma[(1-i\omega_c t)/\hbar\beta\omega_c]\}$, where Γ denotes the gamma function. By noticing the identities $\Gamma(a+bi)\Gamma(a-bi) = \Gamma^2(a)/\prod_{k=0}^\infty[1+b^2/(a+k)^2]$ and $\prod_{k=1}^\infty(1+b^2/k^2)^{-1} = b\pi/\sinh b\pi$ for real quantities a and b [73], at the scaling limit $\omega_c\to\infty$ we readily find the asymptotic form $B(t) = K\ln(1+\omega_c^2t^2) - 2K\ln(\kappa t/2) + 2K\ln\sinh(\kappa t/2)$, where $\kappa = 2\pi/\hbar\beta$ is the Matsubara frequency.

At the Toulouse limit $K=\frac{1}{2}$ functions $Q(t;\lambda)$ and $P(t_1,t_2,t_3)$ acquire the following results:

$$Q(t;\lambda) = \frac{1}{1+i\lambda\omega_c t}\frac{\kappa t}{2\sinh\frac{1}{2}\kappa t}, \tag{25a}$$

$$P(t_1,t_2,t_3) = \frac{1}{2} + \frac{1}{2}\exp(2i\{\arctan[\omega_c(t_1-t_2)] - \arctan[\omega_c(t_1-t_3)] + \arctan[\omega_c(t_2-t_3)]\}). \tag{25b}$$

The function $Q(t;\lambda)$, acting as a kernel of the integral over positive time, assumes the asymptotic behavior

$$Q(t;\lambda) = \frac{\pi}{2\omega_c}\delta(t) - \frac{\lambda\kappa i}{2\omega_c}\mathrm{P}\frac{1}{\sinh\frac{1}{2}\kappa t}, \tag{26}$$

where P denotes the Cauchy principal value. The P function at the scaling limit turns out to be real because its imaginary part is of $O(1/\omega_c)$ and negligible compared to the real part. Its asymptotic form reads $P(t_1,t_2,t_3) = [1+\omega_c^2(t_1-t_2)^2]^{-1} + [1+\omega_c^2(t_1-t_3)^2]^{-1} + [1+\omega_c^2(t_2-t_3)^2]^{-1}$. Because $P(t_1,t_2,t_3)$ is defined with the constraint $t_1 \geqslant t_2 \geqslant t_3$ except $t_1 = t_3$, the P function can be replaced with Dirac δ functions when serving as an integral kernel,

$$P(t_1,t_2,t_3) = \frac{\pi}{2\omega_c}[\delta(t_1-t_2)+\delta(t_2-t_3)]. \tag{27}$$

The zero-temperature dynamics of a symmetric spin-boson model can feasibly be solved by taking advantage of the asymptotic property of the kernel $Q(t;\lambda)$ [51]. Indeed, when $\epsilon = 0$ and $\kappa\to 0$, we substitute Eq. (26) into Eq. (19)

and obtain

$$\tilde{z}(t) = 1 - \Delta_r \int_0^t dt_1 \tilde{z}(t_1) + i\frac{\Delta_r}{\pi}\mathrm{P}\int_0^t dt_1 \int_0^{t_1} dt_2 \frac{1}{t_1 - t_2} \times \{\tilde{z}_{1,t_1}(t_2) - [\tilde{z}_{1,t_1}(t_2)]^*\}, \tag{28}$$

where $\Delta_r = \pi\Delta^2/2\omega_c$. The third term can be neglected because $\tilde{z}_{1,t_1}(t_2)$ becomes real at the scaling limit for $t_1 - t_2 > 1/\omega_c$. Consequently, Eq. (28) yields the exact solution $\tilde{z}(t) = e^{-\Delta_r t}$.

Now we consider the asymmetric case at finite temperature. Inserting Eq. (26) into Eq. (19) and regarding $z_{\pm 1,t_1}(t_2)$ as known functions, we readily solve this equation and obtain

$$\tilde{z}(t) = e^{-\Delta_r t} + \frac{\Delta^2}{2\omega_c}\int_0^t dt_1 \mathrm{P}\int_0^{t_1} dt_2 \frac{\kappa e^{-\Delta_r(t-t_1)}}{\sinh\frac{1}{2}\kappa(t_1 - t_2)} \times \mathrm{Im}\left[e^{-i\epsilon(t_1-t_2)}\tilde{z}_{1,t_1}(t_2)\right]. \tag{29}$$

Now we only need to solve $\tilde{z}_{1,t_1}(t_2)$ for $t_1 > t_2$ due to the presence of the Cauchy principle integral. To this end, we substitute the expressions for Q and P into Eq. (20) to get

$$\begin{aligned}\tilde{z}_{1,t_1}(t_2) = 1 - \frac{\pi\Delta^2}{4\omega_c}\int_0^{t_2} dt_3 \{&Q(t_2 - t_3; +1)e^{-i\epsilon(t_2-t_3)} \\ &\times S(t_1, t_2, t_2, t_3; +1)\tilde{z}_{1,t_1}(t_3) \\ &+ Q(t_2 - t_3; -1)[S(t_1, t_2, t_2, t_3; -1)]^{-1}e^{i\epsilon(t_2-t_3)} \\ &\times \tilde{z}([iB'_{t_1,t_2} - iB'_{t_2,t_3}, -B''_{t_1,t_2} + B''_{t_2,t_3}], t_3)\}.\end{aligned} \tag{30}$$

Now a key step is to calculate the products $Q(t_3 - t_4; \lambda)S(t_1, t_2, t_3, t_4; \lambda)$ and $Q(t_3 - t_4; \lambda)[S(t_1, t_2, t_3, t_4; \lambda)]^{-1}$ under the constraint $t_2 = t_3$. Recognizing the definition of the S function given in Eq. (22), we immediately obtain the following results for $t_2 = t_3$:

$$Q(t_3 - t_4; \lambda)S(t_1, t_2, t_3, t_4; \lambda) = \frac{Q(t_1 - t_4; \lambda)}{Q(t_1 - t_2; \lambda)} \tag{31}$$

and

$$\frac{Q(t_3 - t_4; \lambda)}{S(t_1, t_2, t_3, t_4; \lambda)} = \frac{[Q(t_2 - t_4; \lambda)]^2 Q(t_1 - t_2; \lambda)}{Q(t_1 - t_4; \lambda)}. \tag{32}$$

Note that once the constraint $t_2 = t_3$ is imposed, t_1, t_2, and t_4 are mutually different times. Therefore, Eq. (31) is of the order $O(1)$, whereas Eq. (32) is of the order $O(1/\omega_c^2)$. Exploiting these results and based on Eq. (30), we obtain

$$\tilde{z}_{1,t_1}(t_2) = 1 - \frac{\pi\Delta^2}{4\omega_c}\int_0^{t_2} dt_3 e^{-i\epsilon(t_2-t_3)}\tilde{z}_{1,t_1}(t_3)\frac{Q(t_1 - t_3; +1)}{Q(t_1 - t_2; +1)}. \tag{33}$$

Equation (33) is an integral equation and can feasibly be solved with iteration, yielding

$$\tilde{z}_{1,t_1}(t_2) = 1 + \sum_{n=1}^{\infty}\left(-\frac{\Delta_r}{2}\right)^n \int_0^{t_2} dt_3 \cdots \int_0^{t_{n+1}} dt_{n+2} \times \frac{Q(t_1 - t_{n+2}; +1)}{Q(t_1 - t_2; +1)}e^{-i\epsilon(t_2-t_{n+2})}. \tag{34}$$

Here, the multidimensional integral can be simplified to a simple one-dimensional one. With the expression $Q(t;\lambda)$ we have

$$\tilde{z}_{1,t_1}(t_2) = 1 - \frac{\Delta_r}{2}\int_0^{t_2} dt_3 \frac{\sinh\frac{\kappa}{2}(t_1 - t_2)}{\sinh\frac{\kappa}{2}(t_1 - t_3)}e^{-(\frac{\Delta_r}{2} + i\epsilon)(t_2 - t_3)}. \tag{35}$$

Inserting it into Eq. (29) and carrying out the involved multidimensional integral, we find

$$\tilde{z}(t) = e^{-\Delta_r t} + \frac{\kappa}{\pi}\int_0^t dt_1 \frac{\sin\epsilon t_1}{\sinh\frac{\kappa t_1}{2}}e^{-\frac{\Delta_r t_1}{2}}[1 - e^{-\Delta_r(t-t_1)}], \tag{36}$$

which is the exact result first obtained by Sassetti and Weiss [24].

With the above procedure, we can also calculate the quantity $\tilde{x}(t) = \mathcal{M}\langle x(t)\rangle$ characterizing the change in coherence. Starting with Eq. (9a) and following the derivation of Eq. (19), we find that $\tilde{x}(t)$ can be related to $\tilde{z}_{\lambda,t}(t_1)$,

$$\tilde{x}(t) = -\frac{\Delta}{2i}\int_0^t dt_1 \sum_{\lambda=\pm 1}\lambda Q(t - t_1; \lambda)e^{-i\lambda_1\epsilon(t-t_1)}\tilde{z}_{\lambda,t}(t_1). \tag{37}$$

Substituting Eq. (35) into Eq. (37), we get

$$\tilde{x}(t) = \frac{1}{2}\omega_c\kappa\Delta\int_0^t dt_1 \frac{t_1^2\cos\epsilon t_1}{(1 + \omega_c^2 t_1^2)\sinh\frac{1}{2}\kappa t_1}e^{-\frac{\Delta_r}{2}t_1}. \tag{38}$$

In order to understand the interaction between blips and sojourns, we will also solve the dynamics with the perturbative expansion (23). For $k > j + 1$ and at the scaling limit, the function $W(t_{2j-1}, t_{2j}, t_{2k-2}, t_{2k-1}; \lambda) = 1$. Then Eq. (23) simplifies to $\tilde{z}(t) = 1 + \sum_{n=1}^{\infty} z_n(t)$, where $z_n(t)$ is the nth-order contribution

$$\begin{aligned}z_n(t) = \left(\frac{-\Delta^2}{2}\right)^n \int_0^t \mathcal{D}_n\{t\} \sum_{\lambda_1,\ldots,\lambda_n=\pm 1}\prod_{j=1}^{n} &\times e^{-i\lambda_j\epsilon(t_{2j-1}-t_{2j})}Q(t_{2j-1} - t_{2j}; \lambda_j) \\ &\times P(t_{2j-3}, t_{2j-2}, t_{2j-1}) \\ &\times \prod_{k<j}[S(t_{2k-1}, t_{2k}, t_{2j-1}, t_{2j}; \lambda_j)]^{\lambda_j\lambda_k}.\end{aligned} \tag{39}$$

Here, $P(t_{-1}, t_0, t_1) = 1$ is introduced. In calculating the term $z_n(t)$ we have to deal with the Q, P, and S functions simultaneously. We find that the asymptotic form of P should be taken before that of Q, and Eqs. (31) and (32) will be useful in omitting higher-order terms in $1/\omega_c$. These two equations actually reflect the interplay between the intra- and interblip interactions and imply that when a sojourn collapses, its preceding and subsequent blips merge into a longer one only when they have the same phase factors. This is the key observation that helps us complete multiple integrations in the perturbative treatment. To illustrate this point clearly, we first treat the cases with $n = 1$ and $n = 2$. For $n = 1$, the P and S functions are not involved. Substituting Eq. (26) into Eq. (39), we obtain

$$z_1(t) = -\Delta_r t - \frac{\kappa\Delta_r}{\pi}\int_0^t dt_1 \frac{\sin\epsilon t_1}{\sinh\frac{1}{2}\kappa t_1}(t - t_1). \tag{40}$$

For $n = 2$, Eqs. (31) and (32) are needed to deal with the product between the Q and S functions. Substituting the asymptotic behavior of the P function and using Eq. (32), we find that for the summation over λ_1 and λ_2, terms with $\delta(t_2 - t_3)$ for $\lambda_1 \neq \lambda_2$ are of high order in $1/\omega_c$ and thus neglectable. Recognizing the fact that $Q(t_1 - t_2; \lambda) = S(t_1, t_2, t_3, t_4; \lambda) = 1$ for $t_1 = t_2$, we may write $z_2(t)$ as

$$\begin{aligned} z_2(t) = &\left(\frac{-\Delta^2}{2}\right)^2 \int_0^t dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \frac{2\pi}{\omega_c} \\ &\times \mathrm{Re}\big[Q(t_3 - t_4; +1)e^{-i\epsilon(t_3 - t_4)}\big] \\ &+ \left(\frac{-\Delta^2}{2}\right)^2 \sum_{\lambda=\pm 1} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_4 \frac{\pi}{2\omega_c} \\ &\times Q(t_1 - t_2; \lambda)e^{-i\lambda\epsilon(t_1 - t_4)} \\ &\times Q(t_2 - t_4; \lambda)S(t_1, t_2, t_2, t_4; \lambda). \end{aligned} \tag{41}$$

Calculating the product between the Q and S functions with Eq. (31) and rearranging the triple integrals, we may rewrite Eq. (41) in a compact form:

$$\begin{aligned} z_2(t) = &(-\Delta_r)^2 \frac{\omega_c}{2\pi} \sum_{k=1}^{2} 2^k \int_0^t dt_1 \int_0^{t_1} dt_2 \int_{t_k}^{t_{k-1}} dt' \\ &\times \mathrm{Re}\big[Q(t' - t_2; +1)e^{-i\epsilon(t' - t_2)}\big]. \end{aligned} \tag{42}$$

For general cases $n > 2$, the product of the P functions has 2^{n-1} terms. By using Eqs. (31) and (32) repeatedly, terms involving $\delta(t_{2j+1} - t_{2j})\delta(t_{2j+1} - t_{2j+2})$, which collapse a sojourn and its successive blip at the same time, turn out to be of higher order in $1/\omega_c$ and can be omitted. Taking these results into account, we find that only n terms $\prod_{l=1}^{m} \delta(t_{2l-1} - t_{2l}) \prod_{l=m+1}^{n-1} \delta(t_{2l} - t_{2l+1})$ for $1 \leqslant m \leqslant n$ contribute out of the 2^{n-1} above-mentioned terms. By noticing $Q(t_1 - t_2; \lambda) = S(t_1, t_2, t_3, t_4; \lambda) = 1$ for $t_1 = t_2$ again, Eq. (39) reduces to

$$\begin{aligned} z_n(t) = &\frac{2\omega_c}{\pi}(-\Delta_r)^n \int_0^t dt_1 \int_0^{t_1} dt_3 \cdots \int_0^{t_{2n-3}} dt_{2n-1} \\ &\times \int_0^{t_{2n-1}} dt_{2n} \sum_{\lambda_1,\ldots,\lambda_n=\pm 1} \sum_{m=1}^{n} \\ &\times \prod_{j=m+1}^{n} Q(t_{2j-1} - t_{2j+1}; \lambda_j)e^{-i\lambda_j\epsilon(t_{2j-1} - t_{2j+1})} \\ &\times \prod_{k=m+1}^{j-1} [S(t_{2k-1}, t_{2k+1}, t_{2j-1}, t_{2j+1}; \lambda_j)]^{\lambda_j\lambda_k}, \end{aligned} \tag{43}$$

where $t_{2n+1} = t_{2n}$ is assumed. The next step is to simplify the summation over $\lambda_1, \ldots, \lambda_n$. Indeed, Eq. (32) reveals that in Eq. (43) the terms with $\lambda_l \neq \lambda_{l+1}$ for $l > m$ are of higher order in $1/\omega_c$, which implies $\lambda_l = \lambda_{m+1}$ for all $l > m$. That is to say, we now need to solve only the product of the P and S functions, and terms involving S^{-1} can be neglected. To deal with this product, a direct calculation using Eq. (22) yields

$$\prod_{j=m}^{n} Q(t_j - t_{j+1}; \lambda) \prod_{k=m}^{j-1} S(t_k, t_{k+1}, t_j, t_{j+1}; \lambda) = Q(t_m - t_{n+1}; \lambda). \tag{44}$$

Substituting Eq. (44) into Eq. (43), we find that the integrand of the multidimensional integral in Eq. (43) depends on only two time variables. Again, such an integral can be simplified to a one-dimensional one. Putting all results together, we finally get

$$\begin{aligned} z_n(t) = &\frac{(-\Delta_r)^n}{n!} \frac{2\omega_c}{\pi} \int_0^t dt_1 \mathrm{Re}\big[Q(t_1; +1)e^{-i\epsilon t_1}\big] \\ &\times \left[\left(t - \frac{t_1}{2}\right)^n - \left(\frac{t_1}{2}\right)^n\right], \end{aligned} \tag{45}$$

which is the analytical result for the nth-order contribution. It is straightforward to verify that Eqs. (40) and (42) are special cases of Eq. (45) with $n = 1$ and $n = 2$, respectively. Summing up all contributions and imposing the scaling limit on $Q(t; \lambda)$, the exact result naturally comes out as it should be.

Equation (35) is the central result of this work. We would like to point out that it is the scaling-limit speciality of the interaction between blips and sojourns that allows us to work out analytical results. This speciality is rigorously reflected in the asymptotic behavior of the P and Q functions in Eq. (39). A qualitative description goes as follows. At the scaling limit, the P function becomes real and local. Meanwhile, the real part of the Q function becomes local, and the imaginary part becomes nonlocal but is treatable. Accordingly, the nonlocal component affects the dynamics by acting on the imaginary part of the single-blip function. In the symmetric case the single-blip function is real, and therefore, only the local part contributes, which coincides with the findings by Egger *et al.* [53]. In the asymmetric case, however, the finite bias introduces a phase to the single-blip function, so that nonlocal interactions also play a role. The presence of the nonlocal component involves the blip-sojourn, intrablip, and interblip correlations. As suggested in Eqs. (31) and (32), the interplay among these interactions may merge successive blips into longer ones and reduces the n-blip contribution to the intrablip interaction with different lengths. It is this consequence of the scaling-limit speciality that leads to the solvability of the Toulouse limit.

A comparison to the derivation using the real-time path integral by Sassetti and Weiss [23,24] is worthwhile. They also started with the exact series of $\tilde{z}(t)$. In their treatment, however, all relevant coefficients were set to the scaling limit, and the time length $O(1/\omega_c)$ was omitted at the very beginning. As a result, they had to deal with the series of $\Delta^2 \cos K\pi$, which is zero for the Toulouse limit $K = \frac{1}{2}$. Instead of $K = \frac{1}{2}$ they used $K = \frac{1}{2} - \delta$, the analysis of interactions of charges and dipoles and a trick of regularization to compensate the omission of time length $O(1/\omega_c)$. They finally took the limit $\delta \to 0$ to obtain the desired result. In contrast, our procedure based on the asymptotic behavior defining the interactions between blips and sojourns is more straightforward and easy to follow.

V. COMPARISON BETWEEN THE EXACT SOLUTION AND THE BOLTZMANN DISTRIBUTION

After sufficiently long time evolution the spin-boson model approaches the thermal equilibrium, and all the dynamical quantities take their static values. At the Toulouse limit the

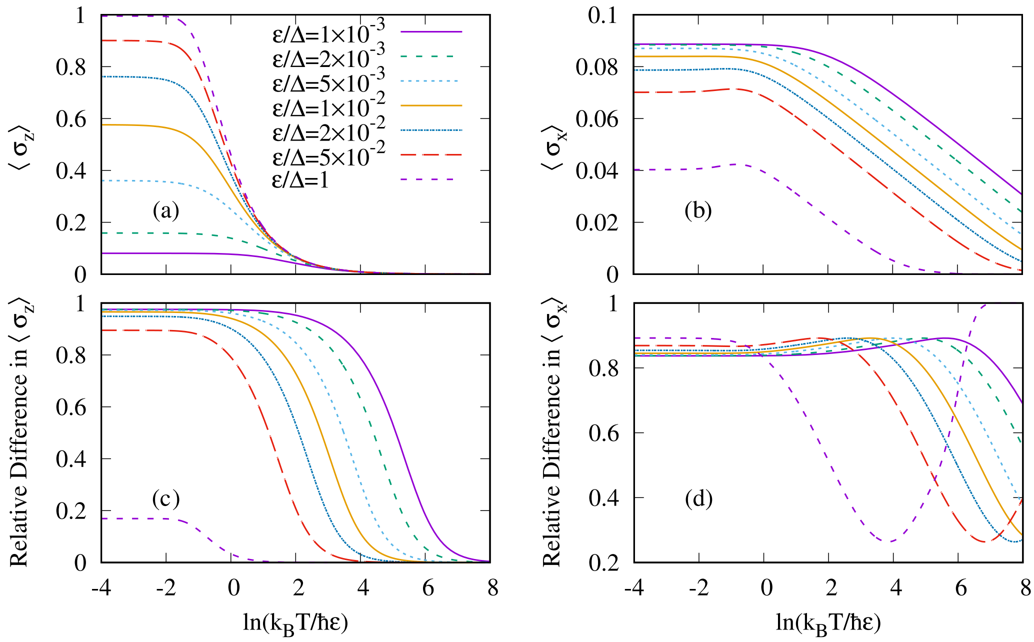

FIG. 1. The exact equilibrium (a) population difference and (b) coherence of the spin-boson model at the Toulouse limit and the relative differences from that given by the Boltzmann distribution. The depicted relative difference is $|\tilde{z}_{\text{eq}}^{(\text{tl})} - \tilde{z}_{\text{eq}}^{(\text{bl})}|/(\tilde{z}_{\text{eq}}^{(\text{tl})} + \tilde{z}_{\text{eq}}^{(\text{bl})})$ for (c) and $|\tilde{x}_{\text{eq}}^{(\text{tl})} - \tilde{x}_{\text{eq}}^{(\text{bl})}|/(\tilde{x}_{\text{eq}}^{(\text{tl})} + \tilde{x}_{\text{eq}}^{(\text{bl})})$ for (d). The high-frequency cutoff is $\omega_c = 100\Delta$.

equilibrium value of $\tilde{z}(t)$ and $\tilde{x}(t)$ can feasibly be obtained from Eqs. (36) and (38). To separate the asymptotic values from these exact expressions, we may also analyze how these quantities reach the equilibrium. For the coherence $\tilde{x}(t)$ there is

$$\tilde{x}(t) = \tilde{x}(\infty) - \frac{\omega_c \kappa \Delta}{2} \int_t^\infty dt_1 \frac{t_1^2 \cos \epsilon t_1}{(1 + \omega_c^2 t_1^2) \sinh \frac{\kappa t_1}{2}} e^{-\frac{\Delta_r t_1}{2}}. \tag{46}$$

When $\kappa t_1 \gg 1$, the function $\sinh(\kappa t_1/2)$ may be replaced by $\exp(\kappa t_1/2)$, which leads to $\tilde{x}(t) = \tilde{x}(\infty) - \kappa \Delta \omega_c^{-1}[4\epsilon^2 + (\Delta_r + \kappa)^2]^{-1}[(\Delta_r + \kappa)\cos \epsilon t - 2\epsilon \sin \epsilon t] \exp[-(\Delta_r + \kappa) t/2]$. Therefore, the coherence assumes a damped oscillation with the damping rate $(\Delta_r + \kappa)/2$ and the oscillation frequency ϵ. The same dynamical feature applies to $\tilde{z}(t)$.

We now compare the exact thermal equilibrium and that dictated by the Boltzmann distribution that is valid only for weak dissipation. For the exact Toulouse solution, the equilibrium value $\tilde{x}_{\text{eq}}^{(\text{tl})} = \tilde{x}(\infty)$ is of $O(1/\omega_c)$, which is consistent with the physical intuition that equilibrium means no quantum coherence. The population difference $\tilde{z}_{\text{eq}}^{(\text{tl})} = \tilde{z}(\infty)$ at equilibrium reads [1]

$$\tilde{z}_{\text{eq}}^{(\text{tl})} = \frac{2}{\pi} \text{Im} \psi \left(\frac{1}{2} + \frac{\Delta_r + i2\epsilon}{2\kappa} \right), \tag{47}$$

which is nonvanishing as long as $\epsilon \neq 0$. For the Boltzmann distribution, $\tilde{\rho}_{\text{bl}} = \exp(-\beta \hat{H}_{\text{s}})/\,\text{Tr}[\exp(-\beta \hat{H}_{\text{s}})]$, which gives $\tilde{x}_{\text{eq}}^{(\text{bl})} \equiv \text{Tr}[\tilde{\rho}_{\text{bl}} \sigma_x] = \Delta/\sqrt{\Delta^2 + \epsilon^2} \tanh(\hbar\beta\sqrt{\Delta^2 + \epsilon^2}/2)$ and $\tilde{z}_{\text{eq}}^{(\text{bl})} \equiv \text{Tr}[\tilde{\rho}_{\text{bl}} \sigma_z] = \epsilon/\sqrt{\Delta^2 + \epsilon^2} \tanh(\hbar\beta\sqrt{\Delta^2 + \epsilon^2}/2)$. Hereafter, the superscripts (tl) and (bl), corresponding to the exact Toulouse solution and the Boltzmann distribution, respectively, will be omitted if no confusion arises. We notice that $\tilde{y}_{\text{eq}}$ is zero for either the exact equilibrium or the Boltzmann distribution, which reflects the invariance of $\hat{H}_{\text{sbm}}$ under the symmetry transformation $\sigma_y \to -\sigma_y$.

The exact thermal equilibrium depends on Δ, ϵ, T, and ω_c. Here, we use Δ as the reference quantity and choose a fixed, large cutoff $\omega_c = 100\Delta$. The equilibrium population difference and coherence are plotted against $k_B T/\hbar\epsilon$ in Figs. 1(a) and 1(b), respectively, for $\epsilon/\Delta = 1 \times 10^{-3}$, 2×10^{-3}, 5×10^{-3}, 1×10^{-2}, 2×10^{-2}, 5×10^{-2}, and 1. The curves clearly show that the bias, which differentiates the two local states, enhances the population difference and suppresses the coherence. For a given bias, the population difference and the coherence generally decrease as the temperature increases. In the low-temperature regime we observe a temperature-independent feature both for $\tilde{z}_{\text{eq}}^{(\text{tl})}$ and for $\tilde{x}_{\text{eq}}^{(\text{tl})}$. This happens because at low temperature $T \ll \hbar\sqrt{4\epsilon^2 + \Delta_r^2}/k_B$, the function $\sinh(\pi k_B T t/\hbar)$ can be replaced with $\pi k_B T t/\hbar$. Consequently, the equilibrium expectations given by Eqs. (36) and (38) become temperature independent at low temperature,

$$\tilde{x}_{\text{eq}} = -\frac{\Delta}{2\omega_c} \left(2\gamma + \ln \frac{4\epsilon^2 + \Delta_r^2}{4\omega_c^2} \right), \tag{48a}$$

$$\tilde{z}_{\text{eq}} = \frac{2}{\pi} \arctan \left(\frac{2\epsilon}{\Delta_r} \right), \tag{48b}$$

where γ is the Euler gamma constant. The deviations of the exact results from Eq. (48), scaling as $\epsilon \Delta_r T^2/(4\epsilon^2 + \Delta_r^2)^2$, decrease quadratically with decreasing temperature. The high-temperature behaviors of x_{eq} and z_{eq} are different from the low-temperature ones. It turns out that in the high-temperature regime z_{eq} is a univariate function of $k_B T/\hbar\epsilon$, while x_{eq} is independent of ϵ.

The dependence of the exact Toulouse solution on ϵ/Δ and T differs qualitatively from that of the Boltzmann distribution. Figure 1(c) displays the relative difference

$|\tilde{z}_{\rm eq}^{(\rm tl)} - \tilde{z}_{\rm eq}^{(\rm bl)}|/(\tilde{z}_{\rm eq}^{(\rm tl)} + \tilde{z}_{\rm eq}^{(\rm bl)})$ in predicting $z_{\rm eq}$ between the exact Toulouse solution and the Boltzmann distribution. We observe that in the high-temperature regime the difference gradually declines with temperature because at the limit $T \to \infty$ both the exact Toulouse solution and the Boltzmann distribution yield a zero expectation for $z_{\rm eq}$. But in the low-temperature regime the difference, which becomes independent of temperature, is significant even for a very small bias. The reason is that the Boltzmann distribution at low temperature is dominated by the ground state and gives $z_{\rm eq}^{(\rm bl)} = \epsilon/\sqrt{\Delta^2 + \epsilon^2}$, while the exact Toulouse solution predicts Eq. (48b), a drastically different picture about the bias-dependence. Regarding the coherence, the difference, as illustrated in Fig. 1(d), is big even at high temperature because $\tilde{x}_{\rm eq}/\tilde{z}_{\rm eq} = \Delta/\epsilon$ for the Boltzmann distribution but $\tilde{x}_{\rm eq}/\tilde{z}_{\rm eq} = 0$ for the Toulouse solution at the scaling limit.

VI. SUMMARY AND OUTLOOK

Starting with the stochastic decoupling and the resultant stochastic Liouville equation, we were able to establish an integral functional equation (IFE) describing the finite-temperature dynamics of the asymmetric spin-boson model. We first developed a stochastic integral equation and then resorted to the Girsanov transform and the auxiliary functional approach in taking the average, arriving at a deterministic IFE. It is clear that the desired dissipative dynamics comes out when the auxiliary function is set to zero. The evolution of the dissipative dynamics, however, spontaneously produces extra fields exerting on itself, which may change the dynamics and makes the solution extremely difficult, if not impossible. Further, the induced fields determine a new kind of dynamics that fully defines the original one. The new dynamics is not independent and also induces more new fields and leads to next level dynamics. Therefore, the functional equation provides a picture of a hierarchical structure for dissipative dynamics. The key to solving the IFE lies in the properties of spontaneous fields.

Note that the concepts of blips and sojourns expounded in the framework of the influence functional theory correspond to the duration of evolution without the influence of the spontaneous field and the interval between such evolutions. The interaction between the blips and sojourns is also illustrated as the consequence of their random correlations in the stochastic description. When the spontaneous field or the blip-blip correlation is neglected, the functional equation reproduces the result from the noninteracting blip approximation, which has witnessed widespread applications. As is well known, however, NIBA works for weak dissipation and is valid only for the symmetric case at the Toulouse limit.

By applying iteration to the IFE, we arrived at an infinite series, which is identical to the celebrated known result from the influence functional method. For the biased case at the Toulouse limit we find that the spontaneous fields result in blip-blip interactions with a local real part plus a treatable nonlocal imaginary part. By exploiting this specialty we were able to obtain the single-blip dynamics. The exact dynamics thus is feasibly solved by virtue of the equation of motion. Summing up the perturbative series, we also reproduced the exact result obtained by Sassetti and Weiss using the path-integral method.

We analyzed the decay of quantum coherence $\tilde{x}(t)$ as well as the population difference $\tilde{z}(t)$ and revealed a damped oscillation. In addition, we demonstrated the difference between the reduced equilibrium state and the Boltzmann distribution at the Toulouse limit. It can be large at low temperature and becomes negligible only at high temperature. For a fixed frequency cutoff, the reduced equilibrium values $\tilde{x}(\infty)$ and $\tilde{z}(\infty)$ are univariate functions of ϵ/Δ at low temperature. At high temperature $\tilde{x}(\infty)$ and $\tilde{z}(\infty)$ depend on only $k_BT/\hbar\Delta$ and $k_BT/\hbar\epsilon$, respectively. By contrast, the temperature dependence of the Boltzmann distribution always follows $\hbar\sqrt{\Delta^2 + \epsilon^2}/k_BT$.

The FIE may be established for solving both the dynamics and thermodynamics of quantum impurity systems. It is also expected that our method may directly be extended to the case with external fields, which may clarify the interplay between dissipation and driving and help us to understand nonequilibrium quantum features for strong coupling. Moreover, for strong dissipation, the asymptotic behavior of those functions determining the interaction between the blips and sojourns is worth exploring, and the FIE might be applicable for revealing the dynamical feature for $K > \frac{1}{2}$.

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