Asymptotic Floquet states of a periodically driven spin-boson system in the nonperturbative coupling regime

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Being an exemplary model of open quantum system, the spin-boson model is widely employed in theoretical and experimental studies. Beyond the weak coupling limit, the spin-boson dynamics can be described by a time-nonlocal generalized master equation with a memory kernel accounting for the dissipative effects induced by the bosonic environment. When the spin is in addition modulated by an external time-periodic electromagnetic field, the interplay between dissipation and forcing provides a spectrum of nontrivial asymptotic states, especially so in the regime of nonlinear response. Here we implement the method for evaluating the dissipative Floquet dynamics of non-Markovian systems introduced in Magazzù *et al.* [Phys. Rev. A **96**, 042103 (2017)] to obtain these nonequilibrium asymptotic states.

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I. INTRODUCTION

The spin-boson model [1] has been—and still remains—the subject of extensive studies, as it constitutes an archetype of open quantum system [2–7]. This model describes a single spin (qubit) coupled to a dissipative environment consisting of an infinite number of bosonic modes. The spin-boson model is of relevance for a great many applications in physics and chemistry, such as, for example, electron tunneling [2,3], driving assisted transport in biological complexes [4,5], and superconducting qubit technologies [6,7], to name but a few.

In the regime of weak coupling to a bosonic environment, the dynamics of the spin can be described by a master equation derived within the Born-Markov approximation [8] together with various improvements over this approximation scheme; see, for example, Refs. [9,10]. Different techniques have been developed to deal with the more challenging strong coupling regime, which goes beyond the perturbative limit. The current toolbox includes stochastic Schrödinger [11] and Liouville [12] equations, different variational approaches [13–16], numerical renormalization group methods [17], sparse polynomial approach [18], extended reaction coordinate schemes [19–21], and combined thermofield/chain [22] mappings.

Within the path integral approach, the influence of the environment on the evolution of an open system (described with a reduced density matrix) is captured by the Feynman-Vernon influence functional [23]. This formulation is suitable for numerically precise treatments, such as quantum Monte Carlo methods [24–26], the quasiadiabatic propagator path-integral method [4,27,28], or the hierarchical equations of motion (HEOM) [29–32]. Furthermore, the path integral approach allows for analytical schemes addressing the limits of both weak [33] and strong coupling [1], together with approximation schemes that bridge these two regimes [34,35].

In experiments, different coupling regimes, corresponding to different spin dynamics (coherent or incoherent), have been attained with superconducting qubits [6,7,36,37], constituting one of the most popular platforms for quantum computing and quantum simulations [38–41]. In particular, a setup based on a flux qubit coupled to a transmission line has been proposed to cover coupling strengths ranging from weak to ultrastrong [37]. The same setup has recently been employed to investigate the impact of a monochromatic driving on the qubit dynamics in different regimes of dissipation and driving [42]. Experimental results have been appropriately accounted for by the path integral approach within an approximation scheme that is nonperturbative with respect to the coupling strength. In this approach, the driven spin-boson dynamics is described by means of a generalized master equation (GME) for the spin, where a memory kernel constructed on a microscopical basis accounts for both the driving and dissipation [43].

While this GME for the spin dynamics cannot be evaluated within the standard Floquet formalism (because of the inherent *time-nonlocal* character of the dynamics), the unitary evolution of the spin-boson system in the *full* Hilbert space is governed by a time-periodic Hamiltonian and consequently can be, though only in principle, handled within standard Floquet theory. The latter also applies to the reduced dynamics when the time evolution can be approximated on physical grounds by time-local equations. This occurs typically in the weak coupling regime, as in the case of the Markovian Bloch-Redfield or Lindblad master equations [43–47]. Further, in the limit of a high frequency driving, the Floquet approach can also be implemented beyond the weak coupling limit [48] by using the inverse frequency of modulations as a perturbation parameter.

In the present work we apply to the GME for the periodically driven spin-boson model the method presented in Ref. [49]. This method allows one to find the asymptotic Floquet states of systems whose evolution is described by a generalized master equation, i.e., an integrodifferential equation characterized by a memory kernel. The method is based on a so-called "embedding" procedure. The embedding is performed by coupling the system to a set of nonphysical auxiliary variables, so that the resulting evolution equations governing the dynamics in the enlarged space of variables are rendered time-local. This system of equations has time-periodic coefficients and is therefore tractable with the standard Floquet theory. The projected solution in the physical subspace assumes the form predicted by a generalization of the Floquet theorem [50] for systems with memory. We next demonstrate that the method allows one to investigate the spin dynamics in different dissipation regimes under periodical modulations with no restrictions on their amplitude or frequency.

II. EMBEDDING AND THE GENERALIZED FLOQUET THEORY

We outline a generalization of the Floquet theorem [51,52] to systems exhibiting a memory dynamics [49]. Consider a periodically driven physical system described by the n-dimensional vector $\mathbf{x}(t)$ and governed by the time-nonlocal evolution equation,

$$\dot{\mathbf{x}}(t) = \int_{t_0}^{t} dt' \mathbf{K}(t,t')\mathbf{x}(t') + \mathbf{z}(t), \tag{1}$$

with integrable memory kernel $\mathbf{K}(t,t')$. Assume that the inhomogeneous term vanishes asymptotically, i.e., $\lim_{t\to\infty} \mathbf{z}(t) = \mathbf{0}$, and that the kernel matrix is biperiodic, namely, $\mathbf{K}(t+\mathcal{T}, t'+\mathcal{T}) = \mathbf{K}(t,t')$, where $\mathcal{T}$ is the period of the driving. Under these conditions, in the limit $t \to \infty$, the action of $\mathcal{L}\{\mathbf{x}, t\}$, given by the right-hand side of Eq. (1), commutes with that of the time-translation operator $\mathcal{S}_{\mathcal{T}}\{\mathbf{x}(t)\} = \mathbf{x}(t+\mathcal{T})$. Then, according to the generalized Floquet theory [50], the solution $\mathbf{x}(t)$ is formally expressed by

$$\mathbf{x}(t) = \mathbf{S}(t,t_0)e^{(t-t_0)\mathbf{F}}\mathbf{v}(t_0)\ , \tag{2}$$

with $\mathbf{S}(t,t_0)$ a $\mathcal{T}$-periodic $n \times p$ matrix, $\mathbf{F}$ a constant $p \times p$ matrix, and $\mathbf{v}(t_0)$ a p-dimensional constant vector, where $p \leqslant +\infty$.

In Ref. [49], we presented a method to find the asymptotic solution of Eq. (1). The method is based on the enlargement of the system state space obtained by coupling $\mathbf{x}$ to an auxiliary nonphysical variable $\mathbf{u}$. The resulting extended system is described by the vector $\mathbf{v}^{\mathsf{T}} = (x_1, \dots, x_n, u_1, u_2, \dots)$, which obeys a time-local equation. This equation is then subjected to the standard Floquet treatment [52]. By projecting the solution $\mathbf{v}(t)$ into the physical subspace, we find the solution for the original vector $\mathbf{x}(t)$.

We assume that the $n \times n$ kernel matrix in Eq. (1) can be expressed as (or approximated by) the following sum of complex matrices,

$$\mathbf{K}(t,t') = \sum_{j=1}^{k} \Gamma_j e^{-\gamma_j (t-t')}\mathbf{E}_j(t)\mathbf{F}_j(t')\ , \tag{3}$$

with $\Gamma_j, \gamma_j \in \mathbb{C}$ and $\mathbf{E}_j(t) = \mathbf{E}_j(t+\mathcal{T})$, $\mathbf{F}_j(t) = \mathbf{F}_j(t+\mathcal{T})$ complex $n \times n$ matrices. This form is flexible enough to reproduce—at lest approximatively, as we do below—a variety of memory kernels, including oscillatory ones [53].

With the kernel in the form of Eq. (3), the time evolution of the physical variable $\mathbf{x}$, Eq. (1), can be obtained by solving the following set of time-local equations [54]:

$$\dot{\mathbf{x}}(t) = -\mathbf{H}(t)\mathbf{u}(t), \tag{4}$$

$$\dot{\mathbf{u}}(t) = -\mathbf{G}(t)\mathbf{x}(t) - \mathbf{A}\mathbf{u}(t), \tag{5}$$

where the n-dimensional vector $\mathbf{x}$ is coupled to the auxiliary variable $\mathbf{u}$. Here we have introduced the matrices

$$\mathbf{H}(t) = (\Gamma_1\mathbf{E}_1(t) \quad \dots \quad \Gamma_k\mathbf{E}_k(t)), \quad \mathbf{G}(t) = \begin{pmatrix} \mathbf{F}_1(t) \\ \vdots \\ \mathbf{F}_k(t) \end{pmatrix},$$

$$\text{and} \quad \mathbf{A} = \mathrm{diag}(\gamma_1 \mathbf{1}^{n\times n}, \dots, \gamma_k \mathbf{1}^{n\times n})\ . \tag{6}$$

These definitions entail that the vector of auxiliary variables has dimension $n \cdot k$.

Without loss of generality, we set $t_0 = 0$ from now on. To prove that Eqs. (4)-(5) are equivalent to Eq. (1), as far as the physical variable is concerned, we define $\mathbf{G}(t)\mathbf{x}(t) \equiv \mathbf{w}(t)$. Laplace transform of Eq. (5) yields $\mathbf{u}(\lambda) = [\lambda\mathbf{1} + \mathbf{A}]^{-1}\mathbf{u}(0) - [\lambda\mathbf{1} + \mathbf{A}]^{-1}\mathbf{w}(\lambda)$. Transforming back to the time domain, multiplying to the left by $-\mathbf{H}(t)$, and using Eq. (4), we recover Eq. (1) with

$$\mathbf{K}(t,t') = \mathbf{H}(t)e^{-\mathbf{A}(t-t')}\mathbf{G}(t'), \tag{7}$$

[this expression is equivalent to Eq. (3)] provided that

$$\mathbf{z}(t) = -\mathbf{H}(t)e^{-\mathbf{A}t}\mathbf{u}(0). \tag{8}$$

This requirement fixes the initial condition for the auxiliary vector $\mathbf{u}(t)$.

Equations (4) and (5) can be cast in the compact form

$$\dot{\mathbf{v}}(t) = \mathbf{M}(t)\mathbf{v}(t), \tag{9}$$

where $\mathbf{v}^{\mathsf{T}} = (x_1, \dots, x_n, u_1, \dots, u_{nk})$ is the p-dimensional state vector associated to the enlarged system, with $p = n + nk$, and $\mathbf{M}(t)$ is a $p \times p$ matrix with block structure

$$\mathbf{M}(t) = \begin{pmatrix} \mathbf{0} & -\mathbf{H}(t) \\ -\mathbf{G}(t) & -\mathbf{A} \end{pmatrix}, \tag{10}$$

where $\mathbf{0} \in \mathbb{R}^{n\times n}$. Note that having $\mathcal{T}$-periodic $\mathbf{H}(t)$ and $\mathbf{G}(t)$ entails $\mathcal{T}$-periodicity of $\mathbf{M}(t)$. Then, according to the Floquet theorem, Eq. (9) with initial condition $\mathbf{v}(t_0)$ has a formal solution whose projection in the physical subspace yields the form of Eq. (2) [49,50]. The asymptotic Floquet state of the original system at stroboscopic instances of time $t = s\mathcal{T}$, $s \in \mathbb{Z}$, is then given by the $\mathbf{x}$ component of the extended vector $\mathbf{v}^{as}$, which is an invariant of the Floquet propagator $\mathbf{U}_{\mathcal{T}} = \hat{T}\exp[\int_0^{\mathcal{T}} dt\, \mathbf{M}(t)]$, i.e., $\mathbf{U}_{\mathcal{T}}\mathbf{v}^{as}(s\mathcal{T}) = \mathbf{v}^{as}(s\mathcal{T})$ [46,52]; here, $\hat{T}$ denotes the time-ordering operator.

III. THE PERIODICALLY DRIVEN SPIN-BOSON MODEL

Now we apply the method described in the previous section to a periodically modulated spin-boson model. In this model [1], a two-state system, the spin (or qubit), interacts with a dissipative environment represented by a set of independent bosonic modes of frequencies ω_i ("heat bath"). The strength of the coupling between the ith mode and the two-state system is quantified by the frequency λ_i. According to the Caldeira-Leggett model [55], to which we include a time-dependent driving term, the full Hamiltonian reads [43]

$$H(t) = -\frac{\hbar}{2}[\Delta\sigma_x + \varepsilon(t)\sigma_z] - \frac{\hbar}{2}\sigma_z \sum_i \lambda_i (a_i^\dagger + a_i) + \sum_i \hbar\omega_i a_i^\dagger a_i, \quad (11)$$

where Δ is the bare transition amplitude per unit time between the eigenstates $|\pm 1\rangle$ of the spin operator σ_z, and a_i ($a_i^\dagger$) is the annihilation (creation) operator of the ith bosonic mode.

Following Ref. [43], we consider a monochromatic driving of amplitude ε_d and frequency Ω, resulting in a time-dependent bias of the form

$$\varepsilon(t) = \varepsilon_0 + \varepsilon_d \cos(\Omega t). \quad (12)$$

This setting corresponds to the setup used in recent experiments [42].

The bath and its coupling to the two-state system can be fully specified by the spin-boson spectral density function $G(\omega) := \sum_i \lambda_i^2 \delta(\omega - \omega_i)$. For the bosonic heat bath, we assume the continuous Ohmic spectral density with a Drude cutoff [23]

$$G(\omega) = 2\alpha\omega\left(1 + \omega^2/\omega_c^2\right)^{-1}, \quad (13)$$

where the dimensionless parameter α quantifies the overall system-bath coupling and ω_c is the cutoff frequency. In a physical system where the spin dynamics occurs through tunneling transitions between sites at distance q_0, the spin position operator is given by $\sigma_z q_0/2$.

Let $\rho(t)$ denote the spin density matrix. For a factorized system-bath initial condition at $t = 0$, with the heat bath in the canonical thermal state, the exact dynamics of the population difference $\langle\sigma_z(t)\rangle = P_{+1}(t) - P_{-1}(t)$, where $P_{\pm 1} \equiv \langle \pm 1|\rho(t)| \pm 1\rangle$, is governed by the following GME:

$$\frac{d}{dt}\langle\sigma_z(t)\rangle = \int_0^t dt'[K^a(t,t') - K^s(t,t')\langle\sigma_z(t')\rangle], \quad (14)$$

where the symmetric (s) and antisymmetric (a) kernels—with respect to $\varepsilon(t)$—have in general intricate path integral expressions [23,43].

In the path integral picture, the Feynman-Vernon influence functional for the reduced system dynamics displays bath-induced, time-nonlocal interactions among the two-state transitions building-up the paths. These interactions are mediated by the so-called pair interaction [23],

$$Q(t) = Q'(t) + iQ''(t) = \int_0^\infty d\omega\, \frac{G(\omega)}{\omega^2} \times \left\{\coth\left(\frac{\beta\hbar\omega}{2}\right)[1 - \cos(\omega t)] + i\sin(\omega t)\right\}, \quad (15)$$

which is proportional to the second time integral of the bath correlation function. In terms of Matsubara frequencies $\nu_k = 2\pi k/\beta\hbar$ (with $k = 1, 2, \dots$), we get for the real part of the bath correlation function (see Ref. [31])

$$\frac{d^2}{dt^2}Q'(t) = \int_0^\infty d\omega\, G(\omega)\coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(\omega t) = c_0 e^{-\omega_c t} + \sum_{k=1}^\infty c_k e^{-\nu_k t}, \quad (16)$$

and thus

$$Q(t) = \sum_{k=0}^\infty \frac{c_k}{\nu_k}\left[t - \frac{1 - e^{-\nu_k t}}{\nu_k}\right] + i\pi\alpha(1 - e^{-\omega_c t}), \quad (17)$$

where $\nu_0 \equiv \omega_c$ and where

$$\frac{c_k}{\nu_k} = 4\pi\alpha\frac{\omega_c^2}{\nu_k^2 - \omega_c^2} \qquad (k \geqslant 1), \quad (18)$$

$$\text{and} \quad \frac{c_0}{\nu_0} = \pi\alpha\omega_c \cot\left(\frac{\beta\hbar\omega_c}{2}\right). \quad (19)$$

For the Ohmic case considered here, sufficiently large values of temperature and cutoff frequency, $k_B T, \hbar\omega_c \gtrsim \hbar\Delta$, cause the real part $Q'(t)$ to become a linear function of time and the imaginary part $Q''(t)$ to become constant on a rather small time scale. In the path integral picture, this entails the decoupling of transitions which are distant in time. In this regime of temperatures and cutoff frequencies, the noninteracting blip approximation (NIBA), an approximation scheme where only local-in-time correlations are retained [1,23], well describes the dynamics of the population difference $\langle\sigma_z(t)\rangle$ beyond the weak coupling regime, as we demonstrate below. The NIBA is nonperturbative with respect to the coupling α. It is also valid down to low temperatures in the limit of strong coupling, when the spin dynamics is fully incoherent. Finally, provided that the bias is zero, $\varepsilon(t) = 0$, this approximation scheme is accurate for every α, again down to low temperatures [56].

Within the NIBA, the kernels $K^{s/a}(t,t')$ in Eq. (14) read [43]

$$K^s(t,t') = h^s(t - t')\cos[\zeta(t,t')]$$
$$K^a(t,t') = h^a(t - t')\sin[\zeta(t,t')], \quad (20)$$

with

$$h^s(t - t') := \Delta^2 e^{-Q'(t-t')}\cos[Q''(t - t')]$$
$$h^a(t - t') := \Delta^2 e^{-Q'(t-t')}\sin[Q''(t - t')]. \quad (21)$$

The function $\zeta(t,t') = \int_{t'}^t dt''\varepsilon(t'') = \xi(t) - \xi(t')$, where

$$\xi(t) = \varepsilon_0 t + \frac{\varepsilon_d}{\Omega}\sin(\Omega t), \quad (22)$$

takes into account the modulations of the bias. Note that, in the absence of a time-dependent driving, i.e., $\varepsilon_d = 0$, the GME (14) with the NIBA kernels given by Eq. (20) acquires the character of a convolution, namely the kernels depend exclusively on the difference $t - t'$.

The nonperturbative character of the NIBA with respect to the coupling α, is apparent from Eqs. (20) and (21) by noting that α is contained as a prefactor in the function $Q(t)$. However, neglecting the time-nonlocal correlations of the spin paths, as prescribed by the NIBA, entails automatically a truncation to the second order in Δ of the exact formal expression for the kernels. In general, the higher-order corrections in Δ become relevant in the presence of a nonzero bias when temperature or coupling strength are not large enough [56].

By using the definition $\langle\sigma_z(t)\rangle = P_{+1}(t) - P_{-1}(t)$ and the conservation of probability $P_{+1}(t) + P_{-1}(t) = 1$, we can cast Eq. (14) into an equation describing the evolution of the population vector $\mathbf{p}^\mathsf{T} = (P_{+1}, P_{-1})$,

$$\dot{\mathbf{p}}(t) = \int_0^t dt' \mathbf{K}(t,t')\mathbf{p}(t'), \tag{23}$$

which is of the form of Eq. (1) with dimension $n = 2$ and $\mathbf{z}(t) = 0$. This form is suitable to be generalized to the case of a multisite (tight-binding) [43,57] or multilevel systems [35,58–60]. These generalizations fall under the domain of applicability of the present treatment. The 2×2 kernel matrix $\mathbf{K}(t,t')$ in Eq. (23) has elements,

$$\begin{aligned} K_{\substack{+1-1\\-1+1}}(t,t') &= \tfrac{1}{2}[K^s(t,t') \pm K^a(t,t')],\\ K_{\substack{+1+1\\-1-1}}(t,t') &= -K_{\substack{-1+1\\+1-1}}(t,t'), \end{aligned} \tag{24}$$

and can thus be written as

$$\mathbf{K}(t,t') = \frac{1}{2}\sum_{j=s,a} h^j(t-t')\mathbf{E}_j(t)\mathbf{F}_j(t'). \tag{25}$$

The effect of the driving is encapsulated in the time-dependent matrices $\mathbf{E}_j(t)$ and $\mathbf{F}_j(t)$, reading

$$\begin{aligned} \mathbf{E}_s(t) &= \begin{pmatrix} \cos[\xi(t)] & \sin[\xi(t)] \\ -\cos[\xi(t)] & -\sin[\xi(t)] \end{pmatrix}\\ \mathbf{E}_a(t) &= \begin{pmatrix} \sin[\xi(t)] & \cos[\xi(t)] \\ -\sin[\xi(t)] & -\cos[\xi(t)] \end{pmatrix}\\ \mathbf{F}_s(t) &= \begin{pmatrix} -\cos[\xi(t)] & \cos[\xi(t)] \\ -\sin[\xi(t)] & \sin[\xi(t)] \end{pmatrix}\\ \mathbf{F}_a(t) &= \begin{pmatrix} \cos[\xi(t)] & \cos[\xi(t)] \\ -\sin[\xi(t)] & -\sin[\xi(t)] \end{pmatrix}, \end{aligned} \tag{26}$$

where the function $\xi(t)$ has been defined in Eq. (22).

To complete the embedding, we need to cast the kernel matrix in the form prescribed by Eq. (3). To this aim, we approximate the two functions $h^{s/a}(t)$ introduced in Eq. (21) as the following sums of oscillating exponentials:

$$\begin{aligned} h^s(t) &\simeq c_1 e^{-c_2 t}\cos(c_3 t) + c_4 e^{-c_5 t} \equiv 2\sum_{j=1}^{3}\Gamma_j e^{-\gamma_j t},\\ h^a(t) &\simeq e^{-d_1 t}\sin(d_2 t) + d_3(e^{-d_4 t} - e^{-d_5 t}) \equiv 2\sum_{j=4}^{7}\Gamma_j e^{-\gamma_j t}. \end{aligned} \tag{27}$$

This yields the complex coefficients Γ_j and γ_j in Eq. (3). Indeed, by comparing with Eq. (25) we find

$$\mathbf{K}(t,t') \simeq \sum_{j=1}^{7}\Gamma_j e^{-\gamma_j(t-t')}\mathbf{E}_j(t)\mathbf{F}_j(t'), \tag{28}$$

with

$$\begin{aligned} &\Gamma_1 = \Gamma_2 = c_1/4,\ \Gamma_3 = c_4/2,\ \Gamma_4 = -i/4,\\ &\Gamma_5 = +i/4,\ \Gamma_6 = +d_3/2,\ \Gamma_7 = -d_3/2,\\ &\gamma_1 = c_2 - ic_3,\ \gamma_2 = c_2 + ic_3, \gamma_3 = c_5,\ \gamma_4 = d_1 - id_2,\\ &\gamma_5 = d_1 + id_2,\ \gamma_6 = d_4,\ \gamma_7 = d_5, \end{aligned} \tag{29}$$

and

$$\begin{aligned} &\mathbf{E}_1(t) = \mathbf{E}_2(t) = \mathbf{E}_3(t) = \mathbf{E}_s(t),\\ &\mathbf{E}_4(t) = \mathbf{E}_5(t) = \mathbf{E}_6(t) = \mathbf{E}_7(t) = \mathbf{E}_a(t),\\ &\mathbf{F}_1(t) = \mathbf{F}_2(t) = \mathbf{F}_3(t) = \mathbf{F}_s(t),\\ &\mathbf{F}_4(t) = \mathbf{F}_5(t) = \mathbf{F}_6(t) = \mathbf{F}_7(t) = \mathbf{F}_a(t). \end{aligned} \tag{30}$$

Once the physical parameters of the problem are fixed, the coefficients $c_j, d_j \in \mathbb{R}$ can be obtained upon a fitting procedure, see Appendix B, by using the approximated Eqs. (27) as fitting functions. The coefficients, in turn, produce the complex coefficients γ_j and Γ_j through Eq. (29). Applying to the present case the general rule, the dimension of the embedded system is $n + nk = 16$ with $n = 2$, the dimension of the physical variable $\mathbf{p}$, and $nk = 14$ the dimension of the auxiliary variable $\mathbf{u}$, being $k = 7$ [see Eq. (28)]. The extended system is thus described by $\mathbf{v}^\mathsf{T} = (P_{+1}, P_{-1}, u_1, \dots, u_{14})$. Its asymptotic state is invariant under the action of the Floquet propagator $\mathbf{U}_\mathcal{T}$. The latter is in practice constructed as follows. Its columns are the one-period propagated elements of the canonical basis of $\mathbb{R}^{16}$ $(1,0,\dots,0),\ (0,1,\dots,0),\dots,(0,0,\dots,1)$. The propagation is performed via the time-local matrix Eq. (9) by using a fourth-order Runge-Kutta scheme with the rather small time step $\delta = \mathcal{T}/10^4$, where $\mathcal{T} = 2\pi/\Omega$. The invariant vector $\mathbf{v}^{as}$ is the eigenvector of $\mathbf{U}_\mathcal{T}$ corresponding to eigenvalue 1. The asymptotic Floquet state on a time span of one period is then obtained by propagating for one period the extended system, with $\mathbf{v}^{as}$ as initial condition.

In concluding the present section we note that if the driving period Ω is a multiple of the static bias ε_0, then the extended system has the period $\mathcal{T} = 2\pi/\Omega$ of the driving. Moreover, if the ratio Ω/ε_0 is a rational number, then the periodicity of the extended system is $\mathcal{T} = m2\pi/\varepsilon_0$, where m is the minimum integer such that the ratio $m\Omega/\varepsilon_0$ is also an integer. However, if the frequencies ε_0 and Ω are not commensurate, then the embedding procedure still yields a time-local system but with nonperiodic coefficients; such systems do not allow for a Floquet treatment. Note, however, that the above considerations hold for the extended system: The physical degrees of freedom have, asymptotically, the periodicity of the driving, independently of the values of static bias and driving frequency.

IV. RESULTS

In the present section we evaluate numerically the asymptotic states of the driven spin-boson model for three values of coupling strength, $\alpha = 0.05,\ 0.2$, and 0.6, and for different values of static bias ε_0, driving amplitude ε_d, and frequency Ω. All physical parameters are scaled with the frequency Δ, the bare transition amplitude per unit time of the two-state system; see Eq. (11). The results presented are obtained for the temperature $T = 0.7\hbar\Delta/k_B$ and Drude cutoff frequency

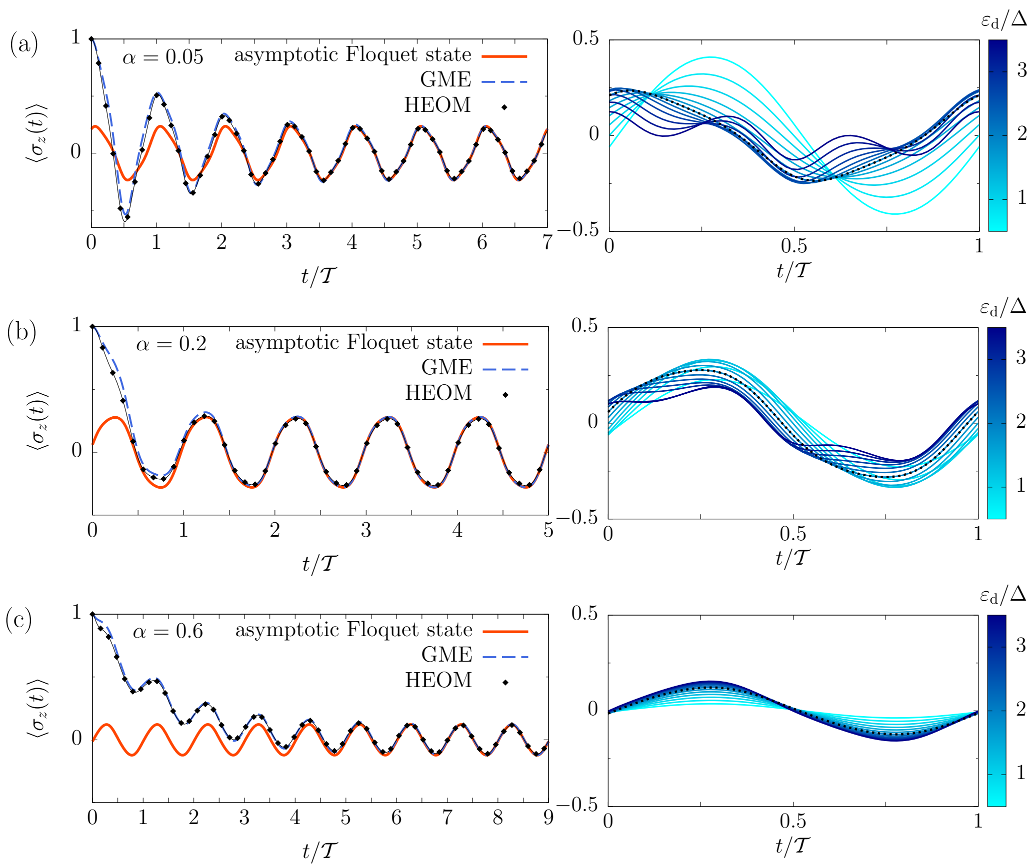

FIG. 1. Asymptotic Floquet states of the driven spin-boson model, Eq. (11), for different coupling strengths and modulation amplitudes. Left panels—Asymptotic population difference $\langle\sigma_z(t)\rangle = P_{+1}(t) - P_{-1}(t)$ vs. time at fixed driving amplitude $\varepsilon_d = 2\Delta$. The populations $P_{\pm 1}(t)$ are the physical components of the extended system obeying the time local Eq. (9) (solid lines). A comparison is made with the corresponding propagated solutions of the GME (14) (dashed lines) and the converged numerically exact HEOM (diamonds), starting with $P_{+1}(0) = 1$. Right panels—Asymptotic Floquet states for different values of the drive amplitude ε_d evaluated for the same coupling strengths α as in the corresponding left panels. The dotted lines depict the same asymptotic dynamics as the thick solid lines in the corresponding left panels. Note that, for different values of the spin-boson coupling strength α, the maximum amplitude of the oscillations is reached at a different driving amplitude ε_d. Fixed parameters are: Static bias $\varepsilon_0 = 0$, driving frequency $\Omega = \Delta$, temperature $T = 0.7\hbar\Delta/k_B$, and Drude cutoff $\omega_c = 5\Delta$. Time is in units of the driving period $\mathcal{T} = 2\pi/\Omega$.

$\omega_c = 5\Delta$. For each value of α, the coefficients of the embedding are determined by numerically optimizing the approximated expressions for $h^{s/a}(t)$, Eq. (27), against the numerical evaluations of the corresponding exact expressions in Eq. (21) (see Appendix B).

In Fig. 1, we depict the physical part of the asymptotic Floquet states of the extended system, namely the population difference $\langle\sigma_z(t)\rangle$ of the two-state system, at zero static bias, $\varepsilon_0 = 0$, and at fixed driving frequency $\Omega = \Delta$. This is done for the three values of coupling strength considered and by changing the drive amplitude. In the left panels we show, for $\varepsilon_d = 2\Delta$, the asymptotic Floquet states over multiple driving periods along with the transient dynamics, as obtained by integrating the NIBA generalized master equation (14) (see Appendix A for details) with initial condition $\langle\sigma_z(0)\rangle = 1$. This provides information on the time scales of relaxation to the asymptotic, time-periodic dynamics at different dissipation regimes and also certifies that the embedding procedure renders correctly the dynamics obtained from the GME. We note that, in the asymptotic limit, the results of the integration of the GME and of the Floquet solutions coincide perfectly, notwithstanding that the decomposition of the memory kernel employed in the embedding is only approximate, thus confirming the flexibility of the embedding method described in Sec. II. We benchmark the NIBA results with the numerically exact approach of hierarchical equations of motion (HEOM) (see Appendix A), obtaining reasonable agreement, even for $\varepsilon(t) \neq 0$, in all of the dissipation regimes.

The right panels of Fig. 1 depict the asymptotic Floquet states over a single driving period for driving strengths ε_d in the range $[0.5\Delta, 3.5\Delta]$. Note that the maximum amplitude of the oscillations is reached at different strengths for different values of α and that, in general, a large value of the coupling tends to suppress the higher harmonics which are most clearly visible for $\alpha = 0.05$ in the nonlinear driving regime, i.e., when the condition $\varepsilon_d/\Omega \ll 1$ is not met [43].

The same behavior is displayed by the spin system also in the presence of a finite bias, as depicted in the right panels of Fig. 2, where the Floquet asymptotic states over a time span of one diving period are shown with $\varepsilon_0 = \Delta$, for driving strengths

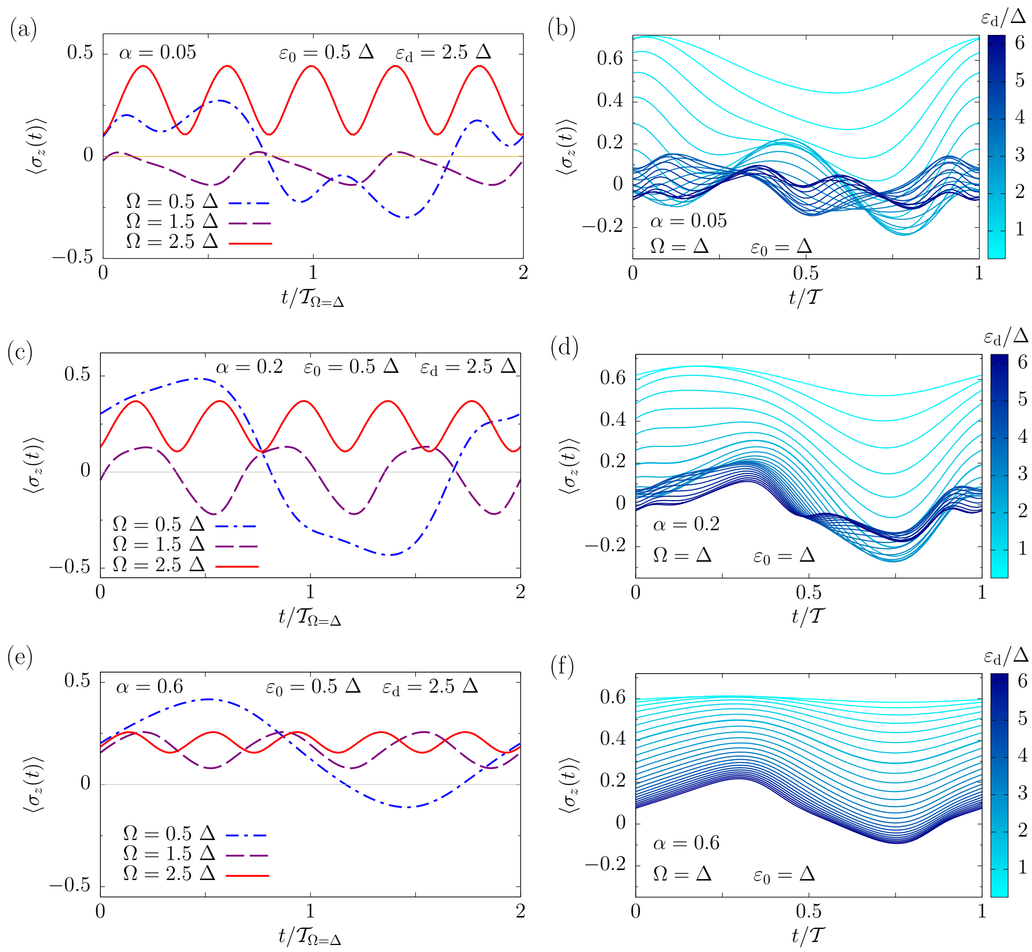

FIG. 2. Asymptotic Floquet states of the driven spin-boson model, Eq. (11), with finite static bias. For each of the three values of the coupling strength α, on the left panels the driving frequency Ω is varied at fixed driving strength $\varepsilon_d = 2.5\Delta$ and for $\varepsilon_0 = 0.5\Delta$, while the right panels show the asymptotic states at fixed frequency and constant static bias $\Omega = \varepsilon_0 = \Delta$ for different driving amplitudes. Temperature and Drude cutoff are $T = 0.7\hbar\Delta/k_B$ and $\omega_c = 5\Delta$, respectively. Time is in units of the driving period $\mathcal{T} = 2\pi/\Omega$ with $\Omega = \Delta$.

ε_d in the range $[0.25\Delta, 6.25\Delta]$. We note that, as ε_d dominates over the static bias, the symmetry of the oscillations around $\langle\sigma_z\rangle = 0$ tends to be restored. However, an increase of the coupling α tends to localize the spin state in the energetically more favorable state $|+1\rangle$, thus counteracting the effect of the time-periodic component of the driving.

Figure 2 also depicts the asymptotic states at finite static bias (left panels), $\varepsilon_0 = 0.5\Delta$, for three values of the frequency Ω. Note that, for $\alpha = 0.05$, Fig. 2(a), even if the bias is positive, at the intermediate value of frequency, $\Omega = 1.5\Delta$, the population difference mostly assumes negative values. This can be accounted for in terms of a negative effective bias $\varepsilon_{\rm eff}$, implicitly defined by the detailed balance relation [42,43] $K^f = K^b \exp(\beta\hbar\varepsilon_{\rm eff})$, where $K^{f(b)} = (1/\mathcal{T})\int_0^{\mathcal{T}} dt\ \int_0^{\infty} d\tau\ K_{\substack{+1-1\\(-1+1)}}(t, t-\tau)$ are the static rates obtained by averaging over the driving period the time-integrated kernel matrix elements.

V. CONCLUSIONS AND OUTLOOK

In this work, we applied to the periodically driven spin-boson model beyond the weak coupling regime the method developed in Ref. [49] for calculating the asymptotic Floquet states of systems governed by memory-kernel master equations.

The method rests on reshaping the memory kernel into a specific form, suitable to model memory kernels which decay monotonically or with oscillations. This representation allows us to embed the system's dynamics into an enlarged state space by coupling the actual physical variables to a set of auxiliary nonphysical variables. The dynamics of the so-obtained enlarged system is governed by a time-local equation to which the standard Floquet formalism applies.

We considered temperature and coupling regimes where the noninteracting blip approximation of the path integral expression for the reduced dynamics describes quite satisfactorily the driven spin-boson model, as we demonstrate upon comparing the results of this approximation scheme with those of converged hierarchical equations of motions. In particular, the probabilities associated to the spin states are given by a generalized master equation displaying a memory kernel that accounts for the effects of the environment and of the driving. By using an optimization procedure, we performed an approximate embedding and found the asymptotic Floquet states of the spin dynamics as the projection of the Floquet states of the enlarged system onto the physical subspace. The idea was exemplified by applying the method in different dissipation and driving regimes, both for the unbiased and biased system.

Our results substantiate, see Fig. 1, that the proposed method still performs well in the cases where the expression in Eq. (3) is employed with a finite number of terms in approximating the memory kernel. Finally, the study of the driven dynamics of the spin-boson model performed in the present work can readily be generalized to multisite or multilevel systems subjected to time-periodic modulations [35,43,57,59,60].

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APPENDIX A: HEOM AND DETAILS OF THE SIMULATIONS

Consider an open system of effective mass M coupled to a heat bath with an Ohmic-Drude spectral density function and cutoff frequency ω_c,

$$J(\omega) = \eta\omega\left(1 + \omega^2/\omega_c^2\right)^{-1}, \tag{A1}$$

where $\eta = M\gamma$ is the viscosity parameter and γ the friction parameter with dimensions of frequency. Specialization to a two-state system characterized by tunneling between sites separated by the distance $q_0 = 2d$ yields [23]

$$\alpha = \frac{\eta q_0^2}{2\pi\hbar} = \frac{2}{\pi}\eta\frac{d^2}{\hbar}. \tag{A2}$$

We set $d = 1$, in units of $(M\Delta/\hbar)^{-1/2}$, so that the position eigenvalues are identified with the eigenvalues of σ_z.

In the HEOM approach [29–31], the time evolution of an open system interacting through the operator V (in the present case $V \equiv \sigma_z$) with a harmonic heat bath is governed by a set of coupled time-local evolution equations for a set of density matrices $\{\rho_{n,\mathbf{j}}(t)\}$ of which only $\rho_{0,\mathbf{0}}(t)$ describes the actual physical system, while the others are auxiliary, nonphysical density matrices. This approach exploits the fact that, for a Ohmic spectral density with Drude cutoff, the bath correlation function,

$$L(t) = \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\left[\coth\left(\frac{\beta\hbar\omega}{2}\right)\cos(\omega t) - i\sin(\omega t)\right], \tag{A3}$$

can be expressed as a series over the Matsubara frequencies $\nu_k = 2\pi k/(\hbar\beta)$, as done in Eq. (16). The Padé spectrum decomposition allows for an efficient truncation of this series to the first M terms [61], even when the temperature is not much larger than the characteristic frequency Δ of the system,

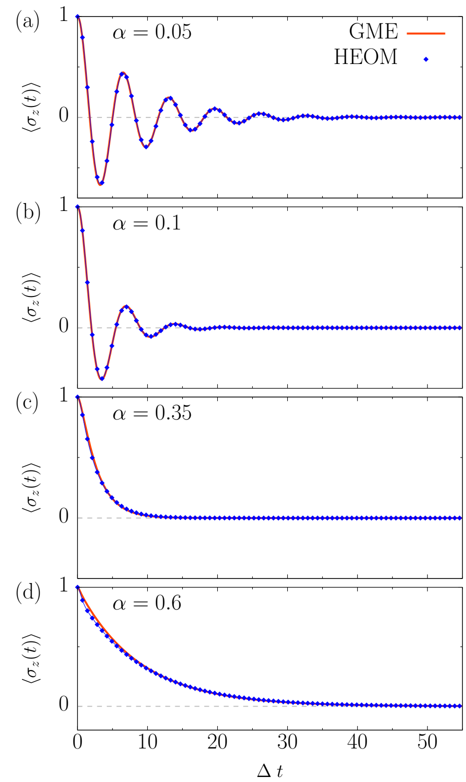

FIG. 3. Comparison between the results of the GME (14) (solid lines) and the converged HEOM (small diamonds) in the unbiased, static case $\varepsilon(t) = 0$, for different values of the coupling strength α. Temperature and cutoff frequency are $T = 0.7\hbar\Delta/k_B$ and $\omega_c = 5\Delta$, respectively.

as in our case where $k_B T < \hbar\Delta$. The hierarchy of equations reads

$$\begin{aligned}\dot{\rho}_{n,\mathbf{j}}(t) = &-\Bigg[\frac{i}{\hbar}H(t)^\times + n\omega_c + \sum_{k=1}^{M} j_k\nu_k \\ &+\left(g - \sum_{k=1}^{M} f_k\right)V^\times V^\times\Bigg]\rho_{n,\mathbf{j}}(t) \\ &- iV^\times\rho_{n+1,\mathbf{j}}(t) - n\omega_c(\theta V^\circ + i\varphi V^\times)\rho_{n-1,\mathbf{j}}(t) \\ &- i\sum_{k=1}^{M} V^\times\rho_{n,\mathbf{j}_{k+}}(t) - i\sum_{k=1}^{M} j_k\nu_k f_k V^\times\rho_{n,\mathbf{j}_{k-}}(t),\end{aligned} \tag{A4}$$

where $\mathcal{O}^\times\rho := [\mathcal{O},\rho]$ and $\mathcal{O}^\circ\rho := \{\mathcal{O},\rho\}$, for a given operator $\mathcal{O}$, and where the following quantities have been introduced:

$$\theta = \frac{\eta\omega_c}{2}, \quad \varphi = \theta\cot\left(\frac{\beta\hbar\omega_c}{2}\right), \quad g = \frac{\eta}{\hbar\beta} - \varphi,$$

$$\text{and} \quad f_k = \frac{\eta}{\hbar\beta}\frac{2\omega_c^2}{\nu_k^2 - \omega_c^2}. \tag{A5}$$

It is understood that the contributing density matrices have both n and all of the components of the vector index

$\mathbf{j} = (j_1, \ldots, j_k, \ldots, j_M)$ nonnegative. Moreover $\mathbf{j}_{k\pm}$ is a shorthand notation for $(j_1, \ldots, j_k \pm 1, \ldots, j_M)$. The terminators of the hierarchy of Eq. (A4) are identified by the condition $n + \sum_{k=1}^{M} j_k = N$, for some $N \gg \omega_0/\min(\omega_c, \nu_1)$, and read

$$\dot{\rho}_{n,\mathbf{j}}(t) \simeq -\left[\frac{i}{\hbar}H(t)^\times + \left(g - \sum_{k=1}^{M} f_k\right)V^\times V^\times\right]\rho_{n,\mathbf{j}}(t). \tag{A6}$$

In Figs. 1 and 3, NIBA results for the reduced dynamics are compared with those from converged HEOM for the driven and nondriven case, respectively. Simulations performed by implementing the HEOM with Padé spectrum decomposition of the bath correlation function are converged with $M = 3$ and $N = 10$, for all the parameters considered. The propagation of the HEOM is obtained by using a second order Runge-Kutta scheme with time step $\delta t = 5 \times 10^{-4}\Delta^{-1}$. The GME (14) is propagated by using the trapezoid rule for the integral and the forward finite difference for the time derivative, according to the simple implicit scheme described in Ref. [60] for a multilevel generalization of the spin-boson model. The chosen time step is $\delta t = 5 \times 10^{-3}\Delta^{-1}$.

APPENDIX B: FITS TO KERNELS

In Fig. 4 we show the optimized curves corresponding to the approximate expressions in Eq. (27) with coefficients extracted by fitting the numerically exact evaluations of the functions in Eq. (21). Note that, as these functions do not depend on the driving, the results shown in the present work required three sets of coefficients, corresponding to the three panels in Fig. 4.

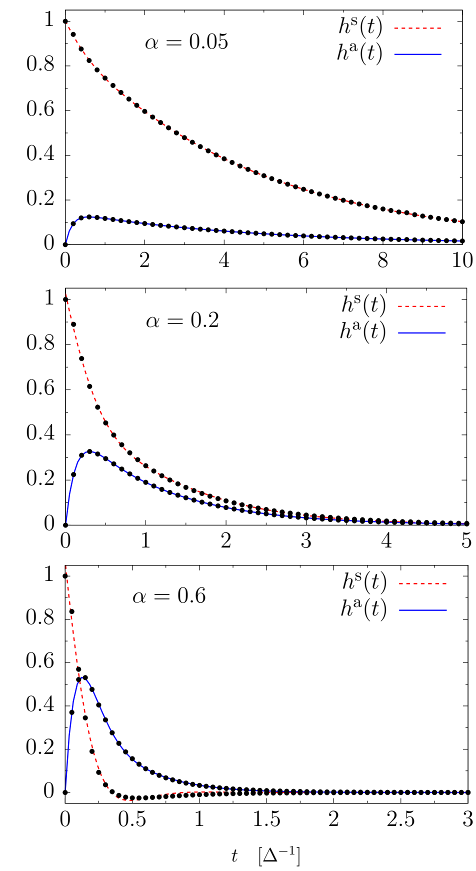

FIG. 4. Numerical fits of the functions $h^{s/a}(t)$ defined in Eq. (21) performed by using the approximated expressions in Eq. (27). The coefficients of these approximated expressions (solid lines) are determined by fitting the numerically exact evaluations (bullets). The latter are performed by truncating the sum for $Q'(t)$ to the first 4000 terms [see Eq. (17)]. Temperature and Drude-cutoff frequency are chosen as $T = 0.7\hbar\Delta/k_B$ and $\omega_c = 5\Delta$, respectively.

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