Non-Markovian quantum state diffusion

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A nonlinear stochastic Schrödinger equation for pure states describing non-Markovian diffusion of quantum trajectories and compatible with non-Markovian master equations is presented. This provides an unraveling of the evolution of any quantum system coupled to a finite or infinite number of harmonic oscillators without any approximation. Its power is illustrated by several examples, including measurementlike situations, dissipation, and quantum Brownian motion. Some examples treat this environment phenomenologically as an infinite reservoir with fluctuations of arbitrary correlation. In other examples the environment consists of a finite number of oscillators. In such a quasiperiodic case we see the reversible decay of a macroscopic quantum-superposition (''Schrödinger cat''). Finally, our description of open systems is compatible with different positions of the ''Heisenberg cut'' between system and environment. [S1050-2947(98)01409-7]

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I. INTRODUCTION

In quantum mechanics, a mixed state, represented by a density matrix ρ_t, describes both an ensemble of pure states and the (reduced) state of a system entangled with some other system, here consistently called ''the environment.'' In both cases the time evolution of ρ_t is given by a linear map

$$\rho_t = \mathcal{L}_t \rho_0, \tag{1}$$

which describes the generally non-Markovian evolution of the system under consideration. Such equations describe both an open system in interaction with infinite reservoirs, or a system entangled with a finite environment. In almost all cases, the general Eq. (1) cannot be solved analytically. Even numerical simulation is most often beyond today's algorithms and computer capacities, and thus, the solution of Eq. (1) remains a challenge.

In the Markov limit, Eq. (1) simplifies and reduces to a master equation of Lindblad form [1]

$$\frac{d}{dt}\rho_t = -i[H,\rho_t] + \frac{1}{2}\sum_m ([L_m\rho_t, L_m^\dagger] + [L_m, \rho_t L_m^\dagger]), \tag{2}$$

where H is the system's Hamiltonian and the operators L_m describe the effect of the environment in the Markov approximation. This approximation is often very useful because it is valid for many physically relevant situations and because analytical or numerical solutions can be found.

In recent years, a breakthrough in solving the Markovian master equation (2) has been achieved through the discovery of *stochastic unravelings* of the density operator dynamics. An unraveling is a stochastic Schrödinger equation for states $|\psi_t(z)\rangle$, driven by a certain noise z_t such that the mean of the solutions of the stochastic equation equals the density operator

$$\rho_t = M[|\psi_t(z)\rangle\langle\psi_t(z)|]. \tag{3}$$

Here $M[\cdots]$ denotes the ensemble mean value over the classical noise z_t according to a certain distribution functional $P(z)$.

The simplest stochastic Schrödinger equations unraveling the density matrix evolution are linear and do not preserve the norm of $\psi_t(z)$. Such an unraveling is merely a mathematical relation. To be truly useful, one should derive unravelings in terms of the corresponding normalized states

$$\tilde{\psi}_t(z) = \frac{\psi_t(z)}{\|\psi_t(z)\|}, \tag{4}$$

where now relation (3) can be interpreted as an unraveling of the mixed state ρ_t into an ensemble of pure states. Of course, using the normalized states $\tilde{\psi}_t(z)$ requires a change of the distribution $P(z)\to\tilde{P}_t(z)$ in order to ensure the correct ensemble mean, with

$$\tilde{P}_t(z) \equiv \|\psi_t(z)\|^2 P(z) \tag{5}$$

so that the Eq. (3) remains valid for the normalized solutions,

$$\rho_t = \tilde{M}_t[|\tilde{\psi}_t(z)\rangle\langle\tilde{\psi}_t(z)|]. \tag{6}$$

We refer to this change (5) of the probability measure as a Girsanov transformation [2]—other authors refer to ''cooking the probability'' or to ''raw and physical ensembles'' [3], or to ''*a priori* and *a posteriori* states'' [4].

In the case of Markovian master equations of Lindblad form (2), several such unravelings (6) are known. Some unravelings involve jumps at random times, others have continuous solutions. The Monte Carlo wave-function method [5], sometimes called quantum jump trajectories [6,7], is the best known example of the first class, whereas the quantum state diffusion (QSD) unraveling [8] is typical of the second class. All these unravelings have been used extensively over recent years, as they provide useful insight into the dynamics of continuously monitored (individual) quantum processes [9,10]. In addition, they provide an efficient tool for the numerical solution of master equations. It is thus desirable to extend the powerful concept of stochastic unravelings to the more general case of non-Markovian evolution. First attempts towards this goal using linear equations can be found in [11], other authors have tackled this problem by adding fictitious modes to the system in such a way as to make the enlarged, hypothetical system's dynamics Markovian again [12–14]. In our approach, by contrast, the system remains as small as possible and thus the corresponding stochastic Schrödinger equation becomes genuinely non-Markovian.

Throughout this paper we assume a normalized initial state $\psi_0(z)\equiv\psi_0$ of the system, independent of the noise at $t=0$. Such a choice corresponds to a pure initial state $\rho_0=|\psi_0\rangle\langle\psi_0|$ for the quantum ensemble and correspondingly, to a factorized initial state $\rho_{\rm tot}=\rho_0\otimes\rho_{\rm env}$ of the total density operator of system and environment.

In this paper we present the nonlinear non-Markovian stochastic Schrödinger equation that unravels the dynamics of a system interacting with an arbitrary ''environment'' of harmonic oscillators, finite or infinite in number. For a brief overview of the underlying microscopic model see Appendix C. In the Markov limit, this unraveling reduces to QSD [8] and will therefore be referred to as *non-Markovian quantum state diffusion*. Our results are based on the linear theories presented in [15,16], where the problem of non-Markovian unravelings was tackled from two quite different approaches. The linear version of the non-Markovian stochastic Schrödinger equation relevant for this paper, unifying these first attempts, was presented in [17] for unnormalized states.

Here we present examples of the corresponding normalized and thus more relevant theory. We include cases where the environment is treated phenomenologically, represented by an exponentially decaying bath correlation function, and cases where the ''environment'' consists of only a finite, small number of oscillators—in Sec. V of even just a single oscillator. The latter case corresponds to periodic (or quasiperiodic) systems, that is, to extreme non-Markovian situations. Before presenting examples in Secs. III, IV, and V, all the basic equations are summarized in Sec. II. Several open problems are discussed in Sec. VII, while the concluding Sec. VIII summarizes the main achievements.

II. BASIC EQUATIONS

In this section we summarize all the basic equations. Let us start by recalling the case of Markov QSD, providing an unraveling of the Lindblad master equation (2).

A. Markov case

The linear QSD equation for unnormalized states reads

$$\frac{d}{dt}\psi_t=-iH\psi_t+L\psi_t\circ z_t-\frac{1}{2}L^\dagger L\psi_t, \tag{7}$$

where z_t is a white complex-valued Wiener process of zero mean and correlations

$$M[z_t^* z_s]=\delta(t-s),\quad M[z_t z_s]=0, \tag{8}$$

and $\circ$ denotes the Stratonovich product [18].

The solutions of Eq. (7) unravel the density matrix evolution according to the master equation (2) through the general relation (3). Here, Eq. (7) is written for a single Lindblad operator L, but it can be straightforwardly generalized by including a sum over all Lindblad operators L_m, each with an independent complex Wiener process z_m.

The simple linear equation (7) has two drawbacks. First, its physical interpretation is unclear because unnormalized state vectors do not represent pure states. Next, its relevance for numerical simulation is severely reduced by the fact that the norm $\|\psi_t(z)\|$ of the solutions tends to 0 with probability 1 (and to infinity with probability 0, so that the mean square norm is constant). Hence, in practically all numerical simulations of Eq. (7) the norm tends to 0, while the contribution to the density matrix in Eq. (3) is dominated by very rare realizations of the noise z.

Introducing the normalized states (4) removes both these drawbacks. As a consequence, the linear Eq. (7) is transformed into a nonlinear equation for $\tilde\psi_t(z)$. In this Markov case, the result of Girsanov transforming the noise according to Eq. (5) and normalizing the state is well known [2,3], it is the following QSD evolution equation for the normalized states

$$\frac{d}{dt}\tilde\psi_t=-iH\tilde\psi_t+(L-\langle L\rangle_t)\tilde\psi_t\circ(z_t+\langle L^\dagger\rangle_t)$$
$$-\tfrac{1}{2}(L^\dagger L-\langle L^\dagger L\rangle_t)\tilde\psi_t, \tag{9}$$

where $\langle L\rangle=\langle\tilde\psi_t|L|\tilde\psi_t\rangle$. This equation is the standard QSD equation for the Markov case written as a Stratonovich stochastic equation. Notice that it appears in its Itô version in Ref. [8]. The effect of the Girsanov transformation is the appearance of the shifted noise

$$z_t+\langle L^\dagger\rangle_t, \tag{10}$$

entering Eq. (9), where z_t is the original process of Eq. (7). The effect of the normalization is the subtraction of the operator's expectation values.

B. Non-Markovian case

In the non-Markovian case, the linear stochastic Schrödinger equation generalizing Eq. (7) was derived in Ref. [17], it reads

$$\frac{d}{dt}\psi_t=-iH\psi_t+L\psi_t z_t-L^\dagger\int_0^t\alpha(t,s)\frac{\delta\psi_t}{\delta z_s}ds. \tag{11}$$

It unravels the reduced dynamics of a system coupled to an arbitrary ''environment'' of harmonic oscillators—see Appendix C for a brief overview. Thus, Eq. (11) represents an unraveling of a certain (standard) class of general non-Markovian reduced dynamics as in Eq. (1). The structure of Eq. (11) is very similar to the Markovian linear equation (7): The isolated system dynamics is Schrödinger's equation with some Hamiltonian H. The stochastic influence of the environment is described by a complex Gaussian process z_t driving the system through the Lindblad operator L. While this is a white noise process in the Markov case, here it is a colored process with zero mean and correlations

$$M[z_t^* z_s] = \alpha(t,s), \quad M[z_t z_s] = 0, \tag{12}$$

where the Hermitian $\alpha(t,s) = \alpha^*(s,t)$ is the environment correlation function. Its microscopic expression can be found in Appendix C. In this paper, we sometimes but not always adopt a phenomenological point of view and will often choose $\alpha(t,s)$ to be an exponential $(\gamma/2)\exp[-\gamma|t-s| - i\Omega(t-s)]$, decaying on a finite environmental ''memory'' time scale γ^{-1}, and oscillating with some environmental central frequency Ω. The Markov case emerges in the limit $\gamma \to \infty$. In the most extreme non-Markovian case, when the ''environment'' consists of just a single oscillator of frequency Ω, we have the periodic $\alpha(t,s) = \exp[-i\Omega(t-s)]$. Finally, the last term of Eq. (11) is the non-Markovian generalization of the last term of the Markovian linear QSD Eq. (7). This term is highly nontrivial and reflects the origin of the difficulties of non-Markovian unravelings.

One can motivate Eq. (11) on several grounds. First, it was originally derived from a microscopic system-environment model [17]. In the original derivation the correlation function $\alpha(t,s)$ describes the correlations of environment oscillators with positive frequencies. However, as can be seen in Appendix C, any positive definite $\alpha(t,s)$ can formally be obtained from some suitably chosen environment that possibly includes negative frequency oscillators (Hamiltonian not bounded from below).

Next, as a second motivation, we sketch a direct proof that Eq. (11) defines an evolution equation (1) for density operators. This ensures that the stochastic equation is compatible with the standard description of mixed quantum states [19,20]. Let $\rho_0 = \Sigma_j p_j |\psi_0^{(j)}\rangle\langle\psi_0^{(j)}|$ be any decomposition of the density operator at the initial time 0 (recall that at time zero the system and environment are assumed uncorrelated). What needs to be proven is that ρ_t is a function of ρ_0 only, where $\rho_t \equiv \Sigma_j p_j M[|\psi_t^{(j)}\rangle\langle\psi_t^{(j)}|]$. This guarantees that ρ_t does not depend on the decomposition of ρ_0 into a mixture of pure states $\{|\psi_0^{(j)}\rangle\}$. For this purpose we notice that the solution ψ_t of Eq. (11) is analytic in z and is thus independent of z^*. Hence we find $(\delta|\psi_t\rangle/\delta z_s)\langle\psi_t| = \delta(|\psi_t\rangle\langle\psi_t|)/\delta z_s$. Accordingly, the evolution equation of $|\psi_t\rangle\langle\psi_t|$ is linear: it depends linearly on $|\psi_0\rangle\langle\psi_0|$. Since the mean M is also a linear operation, ρ_t depends linearly on ρ_0. Finally, the positivity of ρ_t is guaranteed by the existence of a pure state decomposition and its normalization follows from the fact that Eq. (11) preserves the norm in the mean, $M[\|\psi_t\|^2] = \text{const}$ as shown in Appendix B.

Third, another set of motivations for Eq. (11) is provided by the numerous examples of the next sections of this paper and by the fact that, by full analogy with the Markov case, there exists a corresponding nonlinear equation for normalized states, as will be shown in the remainder of this section.

To summarize, Eq. (11) is the basic equation for non-Markovian linear QSD. The functional derivative under the integral indicates that the evolution of the state ψ_t at time t is influenced by its dependence on the noise z_s at earlier times s. Admittedly, this functional derivative is the cause for the difficulty of finding solutions of Eq. (11) in the general case, even numerical solutions.

We tackle this problem by noting that the linear equation (11) may be simplified with the *Ansatz*

$$\frac{\delta\psi_t}{\delta z_s} = \hat{O}(t,s,z)\psi_t, \tag{13}$$

where the time and noise dependence of the operator $\hat{O}(t,s,z)$ can be determined from the consistency condition

$$\frac{d}{dt}\frac{\delta\psi_t}{\delta z_s} = \frac{\delta}{\delta z_s}\dot{\psi}_t \tag{14}$$

with the linear equation (11). The ansatz (13) is completely general and hence, once the operator $\hat{O}(t,s,z)$ is known, the linear non-Markovian QSD equation (11) takes the more appealing form

$$\frac{d}{dt}\psi_t = -iH\psi_t + L\psi_t z_t - L^\dagger \int_0^t \alpha(t,s)\hat{O}(t,s,z)ds\,\psi_t. \tag{15}$$

We are going to show in the subsequent sections how to determine $\hat{O}(t,s,z)$ for many interesting and physically relevant examples. In most of these cases, in fact, the operator $\hat{O}$ turns out to be independent of the noise z and takes a simple form.

Being the non-Markovian generalization, Eq. (11), or equivalently Eq. (15) suffers from the same drawbacks as its Markov limit (7): the norm of its solutions tend to 0 with probability 1. And the cure will be similar. One introduces the normalized states (4) and substitutes the linear stochastic Schrödinger equation (15) by the corresponding nonlinear one. Its explicit form can be rather involved as will be demonstrated in the following sections.

The derivation of the desired evolution equation of the normalized states $\tilde{\psi}_t$ requires two steps: taking into account the Girsanov transformation of the noise (5) and normalization. In Appendix B we prove that the non-Markovian Girsanov transformation for the noise probability distribution $\tilde{P}_t(z)$ (5) corresponds to a time-dependent shift of the original process z_t,

$$\tilde{z}_t = z_t + \int_0^t \alpha(t,s)^* \langle L^\dagger\rangle_s ds. \tag{16}$$

This shift and the normalization of the state ψ_t results, as shown in Appendix B, in the nonlinear, non-Markovian QSD equation for the normalized state vectors $\tilde{\psi}_t$, which takes the ultimate form

$$\begin{aligned}\frac{d}{dt}\tilde{\psi}_t = &-iH\tilde{\psi}_t + (L - \langle L\rangle_t)\tilde{\psi}_t\tilde{z}_t \\ &- \int_0^t \alpha(t,s)[(L^\dagger - \langle L^\dagger\rangle_t)\hat{O}(t,s,\tilde{z}) \\ &- \langle (L^\dagger - \langle L^\dagger\rangle_t)\hat{O}(t,s,\tilde{z})\rangle_t]ds\,\tilde{\psi}_t,\end{aligned} \tag{17}$$

where $\tilde{z}_t$ is the shifted noise (16).

Equation (17) is the central result of this paper, the non-Markovian, normalized stochastic Schrödinger equation that unravels the reduced dynamics of a system in interaction with an arbitrary ''environment'' of harmonic oscillators—

encoded by the properties of the environment correlation function $\alpha(t,s)$. In the following sections we will give many interesting examples of this *non-Markovian quantum state diffusion* equation (17).

III. SPIN-$\frac{1}{2}$ EXAMPLES

In this section we use spin-$\frac{1}{2}$ examples to illustrate general methods to solve the non-Markovian QSD equations (11) [or (15)] and (17), respectively. These are generally numerical, though sometimes analytical, solutions, which illustrate certain features of non-Markovian QSD, unknown in the Markov theory. Throughout this section $\vec{\sigma}$ denote the Pauli matrices.

A. Measurementlike interaction

This is the simplest example, hence we present it in some detail. Let $H=(\omega/2)\sigma_z$, $L=\lambda\sigma_z$ with λ a real number parametrizing the strength of the interaction. The harmonic oscillator environment is encoded by its correlation function $\alpha(t,s)$, which is left arbitrary in this section. First, in order to eliminate the functional derivative in Eq. (11), we assume as an *Ansatz*

$$\frac{\delta\psi_t}{\delta z_s}=\lambda\sigma_z\psi_t, \tag{18}$$

i.e., we choose $\hat{O}(t,s,z)=\lambda\sigma_z$ independent of t, s, and z in Eq. (13). It is straightforward to show that, indeed, this ansatz is compatible with Eq. (14), i.e., it solves the fundamental linear equation (11).

The corresponding nonlinear, non-Markovian QSD Eq. (17) for the normalized state $\tilde{\psi}_t$ reads

$$\frac{d}{dt}\tilde{\psi}_t=-i\frac{\omega}{2}\sigma_z\tilde{\psi}_t+\lambda(\sigma_z-\langle\sigma_z\rangle_t)\tilde{\psi}_t \times\left(z_t+\lambda\int_0^t\alpha(t,s)^*\langle\sigma_z\rangle_s ds+\lambda\int_0^t\alpha(t,s)ds\langle\sigma_z\rangle_t\right). \tag{19}$$

This equation is the generalization of the Markov QSD equation (9) for general environment correlations $\alpha(t,s)$. Notice that, indeed, Eq. (19) reduces to the corresponding Markov QSD equation (9) in the limit of a delta-correlated environment [one has $\int_0^t\alpha(t,s)f(s)ds\rightarrow\frac{1}{2}f(t)$ for any function $f(t)$].

Equation (19) shows the effect of the non-Markovian Girsanov transformation (5). It induces not only the shifted noise (16), but also leads to an additional shift due to the implicit z_t dependence of $\tilde{\psi}_t$, as explained in detail in Appendix B. Numerical simulations of Eq. (19) are shown below.

In order to find the reduced density matrix of this model, we solve analytically the linear non-Markovian QSD equation (15). Using Eq. (18) we find

$$\frac{d}{dt}\psi_t=-i\frac{\omega}{2}\sigma_z\psi_t+\lambda\sigma_z\psi_t z_t+\lambda^2\int_0^t\alpha(t,s)^*ds\,\psi_t. \tag{20}$$

From the explicit solution of this equation we obtain the expression for the ensemble mean

$$\rho(t)\equiv M[|\psi_t\rangle\langle\psi_t|]=\begin{pmatrix}\rho_{11}(0) & \rho_{12}(0)e^{-F(t)}\\ \rho_{21}(0)e^{-F(t)^*} & \rho_{22}(0)\end{pmatrix}, \tag{21}$$

with $F(t)=i\omega t+2\lambda^2\int_0^t ds\int_0^s du[\alpha(s,u)+\alpha^*(s,u)]$. Taking the time derivative, one can show that this density matrix is the solution of the following non-Markovian master equations:

$$\dot{\rho}_t=-i\frac{\omega}{2}[\sigma_z,\rho_t] -\frac{\lambda^2}{2}\int_0^t[\alpha(t,s)+\alpha^*(t,s)]ds[\sigma_z,[\sigma_z,\rho_t]] \tag{22}$$

$$=-i\frac{\omega}{2}[\sigma_z,\rho_t]+\int_0^t\mathcal{K}(t,s)\rho_s ds, \tag{23}$$

where the "memory superoperator" $\mathcal{K}(t,s)$ acts as follows on any operator A:

$$\mathcal{K}(t,s)A=-\frac{\lambda^2}{2}[\alpha(t,s)+\alpha(t,s)^*] \times e^{-2\lambda^2\int_s^t du\int_0^u dv[\alpha(u,v)+\alpha(u,v)^*]}[\sigma_z,[\sigma_z,A]]. \tag{24}$$

Let us now turn to actual simulations of this example. In Fig. 1(a) we show non-Markovian QSD trajectories from solving Eq. (19) numerically with $\lambda^2=2\omega$ and an exponentially decaying environment correlation function $\alpha(t,s)=(\gamma/2)\exp(-\gamma|t-s|)$ with $\gamma=\omega$ (solid lines). For this exponentially decaying environment correlation function the asymptotical solution is either the up state or the down state ($\langle\sigma_z\rangle=\pm1$), while the ensemble mean $M[\langle\sigma_z\rangle]$ remains constant (dashed line). Thus, as in the standard Markov QSD case, the two outcomes "up" or "down" appear with the expected quantum probability: $\mathrm{Prob}(\lim_{t\rightarrow\infty}\psi_t=|\uparrow\rangle)=|\langle\uparrow|\psi_0\rangle|^2$. Notice that for these non-Markovian situations, the quantum trajectories are far smoother than their white-noise counterparts of Markov QSD [8]. We emphasize that if the environment consists of only a finite number of oscillators, represented by a quasiperiodic correlation function $\alpha(t,s)$, no such reduction to an eigenstate will occur.

In Fig. 1(b) we compare the average over 10 000 trajectories of the non-Markovian QSD equation (19) with the analytical ensemble mean (21) and see very good agreement. This confirms that indeed both the memory integrals in Eq. (19) arising from the Girsanov transformation of the noise are needed to ensure the correct ensemble mean.

B. Dissipative interaction

This is the simplest example with a non-self-adjoint Lindblad operator. Again we set $H=(\omega/2)\sigma_z$, but now we choose $L=\lambda\sigma_-\equiv\lambda\frac{1}{2}(\sigma_x-i\sigma_y)$ describing spin relaxation.

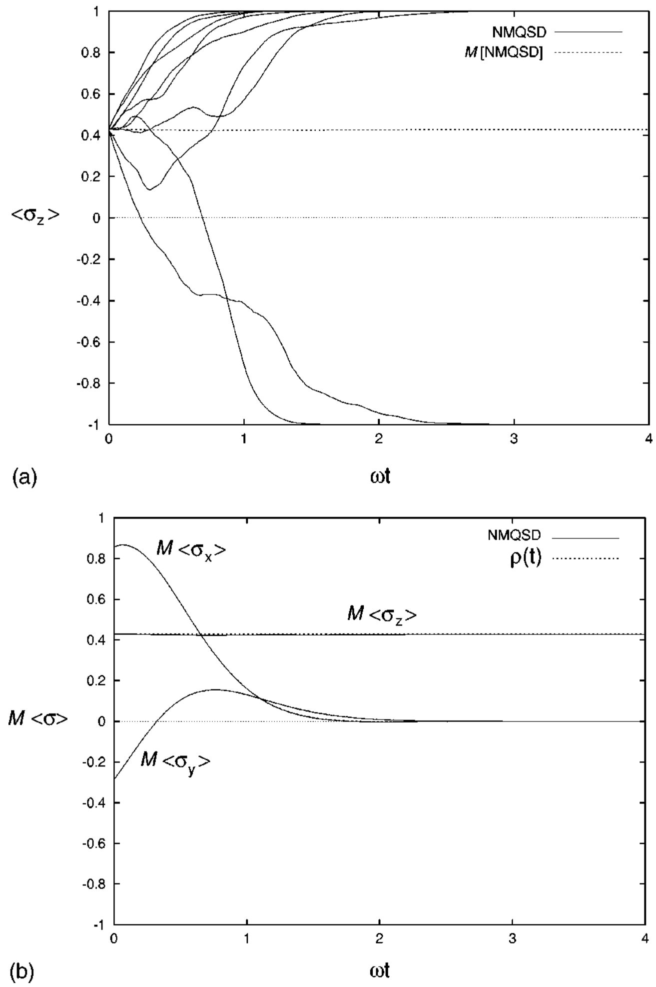

FIG. 1. Quantum trajectories of the non-Markovian QSD equation for the ''measurement''-like case $H=(\omega/2)\,\sigma_z$, $L=\lambda\sigma_z$ and an exponentially decaying bath correlation function $\alpha(t,s)=(\gamma/2)\exp(-\gamma|t-s|)$. We choose $\lambda^2=2\omega$, $\gamma=\omega$ and an initial state $|\psi_0\rangle=(1+2i)|\uparrow\rangle+(1+i)|\downarrow\rangle$. Displayed is the expectation value $\langle\sigma_z\rangle$ of several solutions of the non-Markovian QSD equation (solid lines) and their ensemble average (dashed line). (b) Same parameters as in (a). Here we compare the ensemble average of the Bloch vector using 10 000 quantum trajectories of non-Markovian QSD (solid lines), with the analytical result (dashed lines).

Also, the environmental correlation function $\alpha(t,s)$ and thus the quantum harmonic oscillator environment can be chosen arbitrary.

First we have to replace the functional derivative in Eq. (11), and we try an ansatz (13) of the form

$$\frac{\delta\psi_t}{\delta z_s}=f(t,s)\sigma_-\psi_t, \tag{25}$$

with $f(t,s)$ a function to be determined. The consistency condition (14) of our ansatz (25) leads to the condition on $f(t,s)$:

$$\partial_t f(t,s)\sigma_-\psi_t=\left[-i\frac{\omega}{2}\sigma_z-\lambda F(t)\sigma_+\sigma_-,f(t,s)\sigma_-\right]\psi_t \tag{26}$$

$$=[i\omega+\lambda F(t)]f(t,s)\sigma_-\psi_t \tag{27}$$

with

$$F(t)\equiv\int_0^t\alpha(t,s)f(t,s)ds. \tag{28}$$

Hence, if $\sigma_-\psi_t\neq 0$, the function $f(t,s)$ must satisfy the following equation:

$$\partial_t f(t,s)=[i\omega+\lambda F(t)]f(t,s) \tag{29}$$

with initial condition $f(s,s)=\lambda$. The corresponding non-Markovian QSD equation (17) for normalized state vectors $\tilde{\psi}_t$ reads

$$\begin{aligned}\frac{d}{dt}\tilde{\psi}_t=&-i\frac{\omega}{2}\sigma_z\tilde{\psi}_t-\lambda F(t)(\sigma_+\sigma_--\langle\sigma_+\sigma_-\rangle_t)\tilde{\psi}_t\\&+\lambda(\sigma_--\langle\sigma_-\rangle_t)\tilde{\psi}_t\\&\times\left(z_t+\lambda\int_0^t\alpha(t,s)^*\langle\sigma_+\rangle_s ds+\langle\sigma_+\rangle_t F(t)\right),\end{aligned} \tag{30}$$

with $F(t)$ determined from Eqs. (28) and (29). For a given $\alpha(t,s)$, the non-Markovian QSD equation (30) can be solved numerically, having $F(t)$ determined numerically from Eq. (29). Note that in the Markov limit, the correlation function $\alpha(t,s)$ tends to the Dirac function $\delta(t-s)$. Consequently, $F(t)$ tends to the constant $\frac{1}{2}f(t,t)=\lambda/2$ and one recovers the standard Markov QSD, Eq. (9).

It turns out that non-Markovian QSD can exhibit remarkable properties, unknown in the Markov theory. In order to highlight these features, we proceed analytically and assume exponentially decaying environment correlations $\alpha(t,s)=(\gamma/2)\,e^{-\gamma|t-s|-i\Omega(t-s)}$. Then we see from Eqs. (28) and (29) that the relevant function $F(t)$ in Eq. (30) satisfies

$$\dot{F}(t)=-\gamma F(t)+i(\omega-\Omega)F(t)+\lambda F(t)^2+\frac{\lambda\gamma}{2} \tag{31}$$

with initial condition $F(0)=0$. With $\tilde{\gamma}\equiv\gamma-i(\omega-\Omega)$ the solution reads

$$\begin{aligned}F(t)=&\frac{\tilde{\gamma}}{2\lambda}-\frac{\sqrt{\tilde{\gamma}^2-2\tilde{\gamma}\lambda^2}}{2\lambda}\\&\times\tanh\left[\frac{t}{2}\sqrt{\tilde{\gamma}^2-2\tilde{\gamma}\lambda^2}+\operatorname{arctanh}\left(\frac{\tilde{\gamma}}{\sqrt{\tilde{\gamma}^2-2\tilde{\gamma}\lambda^2}}\right)\right].\end{aligned} \tag{32}$$

For the remainder of this section we assume exact resonance: $\Omega=\omega$ and thus $\tilde{\gamma}=\gamma$. Let us first consider the case of short memory or weak coupling, $\gamma>2\lambda^2$. For long times, $F(t)$ tends to $(\gamma-\sqrt{\gamma^2-2\gamma\lambda^2})/(2\lambda)$. For large γ this asymptotic value tends to $\lambda/2$, which corresponds to the Markov limit (7), as it should.

More interesting, let us consider the opposite case of a long memory or strong coupling, $\gamma<2\lambda^2$. In this case, $F(t)$ diverges to infinity when the time t approaches the critical time $t_c=[\pi+2\arctan(\gamma/\sqrt{2\lambda^2\gamma-\gamma^2})]\sqrt{2\lambda^2\gamma-\gamma^2}$. What

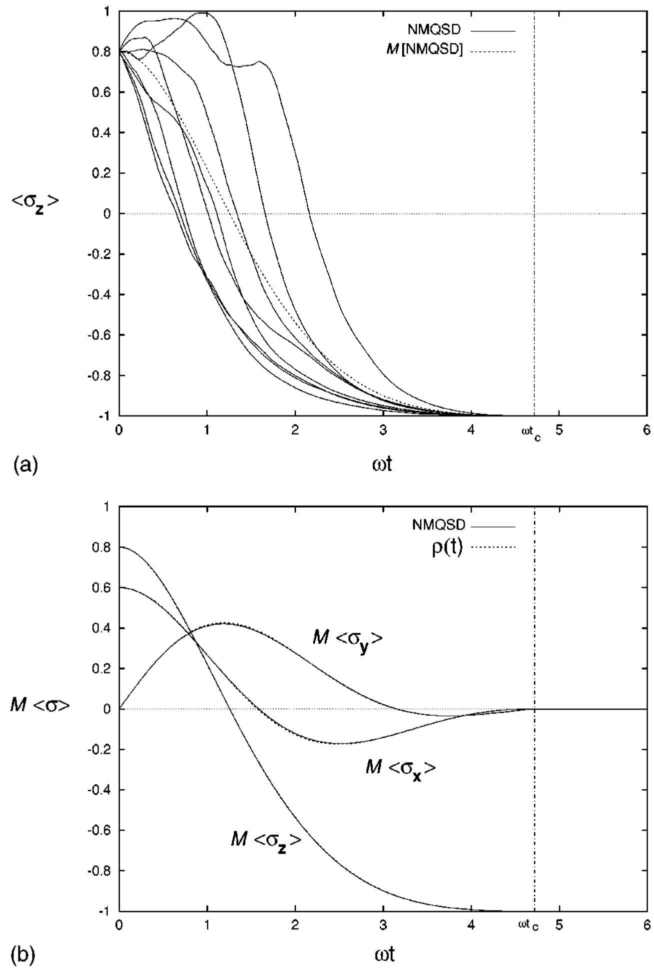

FIG. 2. (a) Quantum trajectories of the non-Markovian QSD equation for the dissipative case $H=(\omega/2)\sigma_z$, $L=\lambda\sigma_-$, and an exponentially decaying bath correlation function $\alpha(t,s) =(\gamma/2)\exp[-\gamma|t-s|-i\Omega(t-s)]$. We choose $\lambda^2=\omega$, $\gamma=\omega$ and resonance $\Omega=\omega$. As an initial state we use $|\psi_0\rangle=3|\uparrow\rangle+|\downarrow\rangle$. Displayed is the expectation value $\langle\sigma_z\rangle$ of several solutions of the non-Markovian QSD equation (solid lines) and their ensemble average (dashed line). At the finite time $\omega t_c=\frac{3}{2}\pi\approx 4.71$, all individual trajectories reach the ground state. (b) Same parameters as in (a). Here we compare the ensemble average of the Bloch vector using 10 000 quantum trajectories of non-Markovian QSD (solid lines), with the analytical result (dashed lines).

happens is that at time t_c, the first component of the vector ψ_t vanishes, hence $\sigma_-\psi_{t_c}=0$ and Eq. (29) no longer holds. Indeed, the second term of Eq. (30) becomes dominant and drives the spin to the ground state in a finite time, which we prove below in terms of the density matrix. In Fig. 2(a) (for individual trajectories) and Fig. 2(b) (for the ensemble average over 10 000 runs) we see this effect from solving the non-Markovian QSD equation numerically, where we choose $\lambda^2=\Omega=\omega$, so that $\omega t_c=\frac{3}{2}\pi\approx 4.71$. For $t>t_c$ the state ψ_t is constant. This is an example where a stationary solution is reached after a finite time. This is an example of a diffusive stochastic Schrödinger equation that is at the same time compatible with the no-signaling constraint (i.e., the evolution of mixed states depends only on the density matrix, not on a particular decomposition into a mixture of pure states) and has no "tails" (does not take an infinite time to reach a definite state); see the discussions in [21,22]. In [23] it is proven that such a feature is impossible for Markov situations. Notice that this peculiar feature holds at resonance only.

Finally, we note that for the intermediate case $\gamma=2\lambda^2$, one has $F(t)=\lambda^3 t/(1+\lambda^2 t)\to\lambda$ for $t\to\infty$, again approaching a constant value (the reader may find it helpful to adopt our convenient convention for the choice of units: $[z_t] =[\lambda]=[f(t)]=[F(t)]=[1/\sqrt{t}]$ and $[\alpha(t,s)]=[1/t]$).

In order to determine the corresponding master equation for the reduced density operator, we solve the linear QSD equation (11) where we make use of the change of variable: $\phi_t\equiv e^{-i(\omega/2)\sigma_z t+\lambda\sigma_+\sigma_-\int_0^t F(s)ds}\psi_t$. After some computation and taking the ensemble mean analytically, one gets

$$\rho_t\equiv M[|\psi_t\rangle\langle\psi_t|] =\begin{pmatrix} \rho_{11}(0)e^{-\int_0^t[F(s)+F(s)^*]ds} & \rho_{12}(0)e^{-i\omega t-\int_0^t F(s)ds} \\ \rho_{21}(0)e^{i\omega t-\int_0^t F(s)^* ds} & 1-\rho_{11}(t) \end{pmatrix}. \tag{33}$$

This proves that whenever $\mathrm{Re}[\int_0^t F(s)ds]$ diverges for a finite time, the density matrix ρ_t reaches the ground state in that finite time and thus all pure state samples have to do so as well. For the time evolution of this reduced density matrix one gets

$$\dot{\rho}_t=-i\frac{\omega}{2}[\sigma_z,\rho_t]+\lambda[F(t)+F(t)^*] \times(\sigma_-\rho_t\sigma_+-\tfrac{1}{2}\{\sigma_+\sigma_-,\rho_t\}) \tag{34}$$

$$=-i\frac{\omega}{2}[\sigma_z,\rho_t]+\int_0^t\mathcal{K}(t,s)\rho_s ds, \tag{35}$$

where the "memory superoperator" $\mathcal{K}(t,s)$ acts as follows on any operator A:

$$\mathcal{K}(t,s)A=-\frac{\lambda^2}{2}[\alpha(t,s)+\alpha(t,s)^*] \times(2e^{-\lambda\int_s^t F(u)du}\sigma_- A\sigma_+-\{\sigma_+\sigma_-,A\} -2(e^{-\lambda\int_s^t F(u)du}-1)\sigma_+\sigma_- A\sigma_+\sigma_-). \tag{36}$$

In Figs. 2(a) and 2(b) we illustrate this example ($\lambda^2=\gamma =\Omega=\omega$) for exponentially decaying correlations. All individual non-Markovian quantum trajectories reach the ground state in the critical time $\omega t_c\approx 4.71$ [Fig. 2(a)]. Taking the ensemble mean over 10 000 trajectories, we find very good agreement with the analytical result of the reduced density matrix [Fig. 2(b)].

IV. MORE EXAMPLES

A. Model of energy measurement

This case $H=L=L^\dagger$ is a straightforward generalization of Sec. III A. Again, the environment correlation $\alpha(t,s)$ can be chosen arbitrary. We find $\hat{O}=H$ in Eq. (13) and the non-Markovian QSD equation (17) for the normalized states reads

$$\frac{d}{dt}\tilde{\psi}_t=-iH\psi_t-(H^2-\langle H^2\rangle_t)\tilde{\psi}_t\int_0^t\alpha(t,s)ds+(H-\langle H\rangle_t)\tilde{\psi}_t\left(z_t+\int_0^t\alpha(t,s)^*\langle H\rangle_s ds+\int_0^t\alpha(t,s)ds\langle H\rangle_t\right). \tag{37}$$

For the corresponding master equation we find

$$\dot{\rho}_t=-i[H,\rho_t]-\int_0^t\alpha(t,s)dsH[H,\rho_t]-\int_0^t\alpha(t,s)^*ds[\rho_t,H]H, \tag{38}$$

hence $\mathrm{Tr}(H\rho_t)$ is constant, contrary to the individual expectation values $\langle H\rangle_{\tilde{\psi}_t}$.

The eigenvectors of H are stationary solutions of the non-Markovian QSD equation (37). Thus, if the noise is large enough, all initial states tend asymptotically to such an eigenstate, as in Markov QSD. However, if the noise has long memory, as for example in the extreme case of periodic systems (see Sec. V), such a reduction property clearly does not hold. The exact conditions under which Eq. (37) describes reduction (localization) to eigenstates are not known. Notice, however, that if the correlation decays smoothly such that $\int_0^t\alpha(t,s)ds$ tends for large times t to a real constant, and if $\langle H\rangle_t$ converges for large times to a fixed value, then the non-Markovian equation (37) tends to

$$\frac{d}{dt}\tilde{\psi}_t=-iH\tilde{\psi}_t-(H^2-\langle H^2\rangle_t)\tilde{\psi}_t\times\mathrm{const}+(H-\langle H\rangle_t)\tilde{\psi}_t(z_t+\mathrm{const}\times\langle H\rangle_t). \tag{39}$$

The long-time solutions of this equation are the same as the long-time solutions of the corresponding Markov approximation. The latter is the Markov QSD equation, hence the asymptotic solutions tend to eigenstates of H. Section III A provides an example of this more general statement for $H=(\omega/2)\sigma_z$.

B. A simple toy model

In this subsection we use a simple toy model [24] to illustrate that the non-Markovian QSD equation (17) may contain unexpected additional terms that cancel in the Markov limit. Consider $H=p$ and $L=q$ and an arbitrary environment correlation function $\alpha(t,s)$. Then the ansatz (13) for replacing the functional derivative with some operator satisfying the consistency condition (14) reads

$$\frac{\delta\psi_t}{\delta z_s}=[q-(t-s)]\psi_t. \tag{40}$$

Thus, the non-Markovian QSD Eq. (17) takes the form

$$\frac{d}{dt}\tilde{\psi}_t=-ip\tilde{\psi}_t-(q^2-\langle q^2\rangle_t)\int_0^t\alpha(t,s)ds\tilde{\psi}_t+(q-\langle q\rangle_t)\tilde{\psi}_t\times\left(z_t+\int_0^t\alpha(t,s)^*\langle q\rangle_s ds+\int_0^t\alpha(t,s)ds\langle q\rangle_t\right)+(q-\langle q\rangle_t)\tilde{\psi}_t\int_0^t(t-s)\alpha(t,s)ds. \tag{41}$$

The first two lines of this non-Markovian QSD equation could have been expected, since they have the same form as in the previous examples; see, for instance, Eq. (37). The last line of the above equation, however, has no counterpart in the previous examples. Clearly, it vanishes in the Markov limit $[\alpha(t,s)\rightarrow\delta(t-s)]$, when the non-Markovian QSD equation (41) for this model reduces to the Markov QSD equation (9).

C. Quantum Brownian motion model

In this subsection we consider the important case of quantum Brownian motion of a harmonic oscillator [25], that is, we choose $H=(\omega/2)(p^2+q^2)$, $L=\lambda q$, and arbitrary environmental correlation $\alpha(t,s)$. As shown in Appendix C, the basic linear non-Markovian QSD equation for this quantum Brownian motion case is again the fundamental linear equation (11).

It turns out that the functional derivative in Eq. (11) is more complicated in this case, because $\hat{O}(t,s,z)$ depends explicitly on the noise z. However, fortunately, this dependence is relatively simple. Indeed, let

$$\frac{\delta\psi_t}{\delta z_s}\equiv\hat{O}(t,s,z)\psi_t=\left[f(t,s)q+g(t,s)p+i\int_0^t ds'j(t,s,s')z_{s'}\right]\psi_t. \tag{42}$$

The consistency condition (14) leads to the following equations for the unknown functions $f(t,s)$, $g(t,s)$, and $j(t,s,s')$ in Eq. (42):

$$\partial_t f(t,s)=\omega g(t,s)+i\lambda f(t,s)\int_0^t ds'[\alpha(t,s')g(t,s')]-2i\lambda g(t,s)\int_0^t ds'[\alpha(t,s')f(t,s')]-i\lambda\int_0^t ds'[\alpha(t,s')j(t,s',s)], \tag{43}$$

$$\partial_t g(t,s)=-\omega f(t,s)-i\lambda g(t,s)\int_0^t ds'[\alpha(t,s')g(t,s')], \tag{44}$$

$$j(t,s,t)=\lambda g(t,s), \tag{45}$$

$$\partial_t j(t,s,s') = -i\lambda g(t,s)\int_0^t ds''[\alpha(t,s'')j(t,s'',s')]. \tag{46}$$

These equations have to be solved together with the non-Markovian QSD equation (17).

If, for simplicity, we assume exponentially decaying environment correlations $\alpha(t,s)=(\gamma/2)\,e^{-\gamma|t-s|}$ and introducing capital letters for the integrals, $X(t)\equiv\int_0^t\alpha(t,s)x(t,s)ds$, for $x=f,g,j$, one obtains the simpler closed set of equations

$$\dot{F}(t)=\frac{\lambda\gamma}{2}-\gamma F(t)+\omega G(t)-i\lambda F(t)G(t)-i\lambda\tilde{J}(t), \tag{47}$$

$$\dot{G}(t)=-\gamma G(t)-\omega F(t)-i\lambda G(t)^2, \tag{48}$$

$$\dot{\tilde{J}}(t)=\frac{\lambda\gamma}{2}G(t)-2\gamma\tilde{J}(t)-i\lambda G(t)\tilde{J}(t), \tag{49}$$

where $\tilde{J}(t)\equiv\int_0^t\alpha(t,s')J(t,s')ds'$. The initial conditions read $F(0)=G(0)=\tilde{J}(0)=0$. Finally, $J(t,s)$ can be determined from the solutions of the above equations, we get

$$J(t,s)=\lambda G(s)e^{-\int_s^t[\gamma+i\lambda G(s')]ds'}. \tag{50}$$

Hence, the non-Markovian QSD equation for quantum Brownian motion becomes

$$\begin{aligned}\frac{d}{dt}\tilde{\psi}_t=&-iH\tilde{\psi}_t-(q^2-\langle q^2\rangle_t)\tilde{\psi}_tF(t)\\&-(qp-\langle qp\rangle_t-p\langle q\rangle_t+\langle p\rangle_t\langle q\rangle_t)\tilde{\psi}_tG(t)\\&+(q-\langle q\rangle_t)\tilde{\psi}_t\bigg(z_t+\int_0^t\alpha(t,s)^*\langle q\rangle_s ds+\langle q\rangle_tF(t)\\&-i\int_0^tJ(t,s')\bigg(z_{s'}+\int_0^{s'}\alpha(s',s)^*\langle q\rangle_s ds\bigg)ds'\bigg).\end{aligned} \tag{51}$$

Let us make some comments about this non-Markovian QSD equation. First, recall that it corresponds to the exact solution of the quantum Brownian motion problem [25] of a harmonic oscillator. Next, this example shows a new feature that we did not encounter in the previous examples: the noise z_t enters the equation nonlocally in time. Third, terms involving the operator qp appear, although there are no such terms either in the Hamiltonian or in the Lindblad operator $L=\lambda q$. Finally, since this equation is exact, it is a good starting point to tackle the quantum Brownian motion problem using this approach and to find its proper Markov limit. In connection with this last point, we emphasize that the master equation corresponding to Eq. (51) necessarily preserves positivity [26] because it provides a decomposition of the density operator into pure states at all times. However, these questions and numerical simulations are left for future work.

D. Harmonic oscillator at finite temperature

As another important example of an open quantum system we briefly sketch the case of a harmonic oscillator $H=\omega a^\dagger a$ coupled to a finite temperature environment through $L_-=\lambda_-a$. As explained in detail in Appendix C, the finite temperature also induces absorption from the bath, which has to be described by a second environment operator $L_+=\lambda_+a^\dagger$. Hence, the linear non-Markovian QSD equation (11) has to be modified and involves two independent noises, z_t^- and z_t^+,

$$\begin{aligned}\frac{d}{dt}\psi_t=&-iH\psi_t+\lambda_-a\psi_tz_t^--\lambda_-a^\dagger\int_0^t\alpha^-(t,s)\frac{\delta\psi_t}{\delta z_s^-}ds\\&+\lambda_+a^\dagger\psi_tz_t^+-\lambda_+a\int_0^t\alpha^+(t,s)\frac{\delta\psi_t}{\delta z_s^+}ds,\end{aligned} \tag{52}$$

see Eq. (C5) in Appendix C. This equation can be solved with the following *Ansätze*:

$$\frac{\delta\psi_t}{\delta z_s^-}=\left[f_-(t,s)a+\int_0^t ds'j_-(t,s,s')z_{s'}^+\right]\psi_t, \tag{53}$$

$$\frac{\delta\psi_t}{\delta z_s^+}=\left[f_+(t,s)a^\dagger+\int_0^t ds'j_+(t,s,s')z_{s'}^-\right]\psi_t. \tag{54}$$

Using similar techniques as in the previous subsection the evolution equations for $f_\pm(t,s)$ and $j_\pm(t,s,s')$ can be obtained and thus the resulting non-Markovian QSD equation can be written in closed form. A new feature of this example, again unknown in the Markov case, is that each of the two environment operators L_- and L_+, is coupled to both noises.

V. HARMONIC OSCILLATOR COUPLED TO A FEW OSCILLATORS: DECAY AND REVIVAL OF SCHRÖDINGER CAT STATES

The case of a harmonic oscillator coupled to a finite or infinite number of harmonic oscillators all of which are initially in their ground state (zero temperature), $H=\omega a^\dagger a$, $L=\lambda a$, is very similar to the damped spin-$\frac{1}{2}$ example treated in Sec. III B. The *Ansatz* $\delta\psi_t/\delta z_s=f(t,s)a\psi_t$ similar to Eq. (25) holds with $f(t,s)$ and $F(t)$ satisfying the same equations (29) and (28). Thus, the non-Markovian QSD equation (17) for this situation reads

$$\begin{aligned}\frac{d}{dt}\tilde{\psi}_t=&-i\omega a^\dagger a\tilde{\psi}_t+(a-\langle a\rangle_t)\tilde{\psi}_t\\&\times\left(z_t+\int_0^t\alpha^*(t,s)\langle a^\dagger\rangle_s ds+\lambda F(t)\langle a^\dagger\rangle_t\right)\\&-\lambda F(t)(a^\dagger a-\langle a^\dagger a\rangle_t)\tilde{\psi}_t.\end{aligned} \tag{55}$$

Again, this non-Markovian QSD equation reduces to the Markov equation (9) for $\alpha(t,s)=\delta(t-s)$ since in this case $F(t)=\lambda/2$ according to Eq. (28). As in the case of a dissipative spin (Sec. III B), for exponentially decaying bath cor-

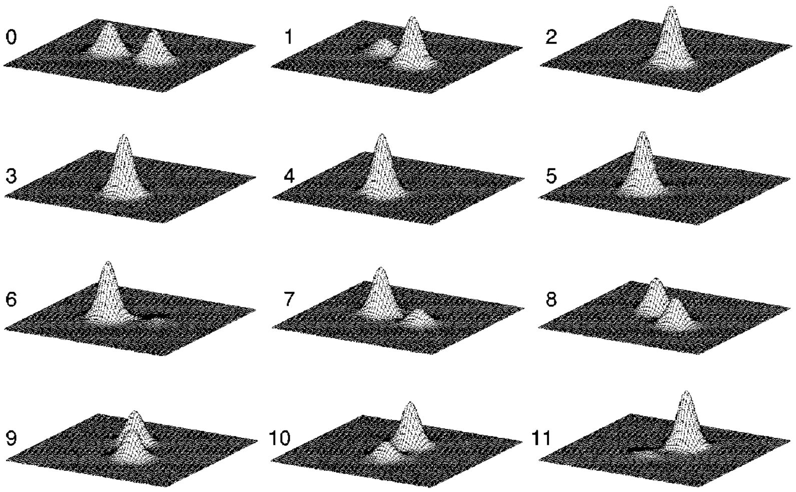

FIG. 3. Reversible decay of an initial Schrödinger cat state $|\psi_0\rangle = |\alpha\rangle + |-\alpha\rangle$ with $\alpha = 2$. We show the Q function of a non-Markovian quantum trajectory of a harmonic oscillator (ω), coupled to just a single ''environment'' oscillator ($\Omega = 0.5\omega$), initially in its ground state. The coupling strength between the two oscillators is 0.1ω, and the time step between two successive plots is $0.47/\omega$.

relations at resonance, the system oscillator may reach its ground state in a finite time, provided the correlation time γ^{-1} is long enough.

Notice also that Eq. (55) preserves coherent states $|\beta\rangle$. The time evolution of the complex number β_t labeling these coherent states is given by

$$\dot{\beta}_t = [-i\omega - F(t)]\beta_t . \tag{56}$$

More interesting than a coherent state initial condition is the case of a superposition $|\beta\rangle + |-\beta\rangle$ of two symmetric coherent states, known as a ''Schrödinger cat'' [27]. If the correlation decays, so does the Schrödinger cat state. If, in contrast, the environment consists only of a finite number of oscillators, then the cat state will first decay, due to the localization property of QSD, but since the entire system is quasiperiodic, the cat state will then revive.

As an illustration, we simulate the extreme case where the ''environment'' consists of only a single oscillator. It thus models the decay and revival of a field cat state in a cavity that is isolated from the outside, but coupled to a second cavity, to which it may decay reversibly. Such an experiment on reversible decoherence was proposed recently in [28]. In this simple case, the environment correlation function reads

$$\alpha(t,s) = e^{-i\Omega(t-s)}, \tag{57}$$

where Ω is the frequency of the single ''environment'' oscillator. Figure 3 shows the time evolution of the Q function of such a ''Schrödinger cat'' in phase space for $\Omega = 0.5\omega$ and a coupling strength between the two oscillators of 0.1ω. Apart from an overall oscillatory motion due to the ''system'' Hamiltonian $\omega a^\dagger a$, we see how the cat first decays but later becomes alive again. Further investigations of stochastic state vector descriptions of such reversible decoherence processes are left for future investigations. It is worth mentioning that depending on the stochastic process, the cat my subsequently decay into either of its two components.

VI. SHIFTING THE SYSTEM-ENVIRONMENT BOUNDARY

In this section we consider a situation where the ''Heisenberg cut'' between the system and the environment is not obvious. Since the non-Markovian QSD equation provides the exact solution of the total system-environment dynamics, the description of the system does not depend on this cut. This is in contrast to the usual Markov approximation, where the position of the cut is crucial. As an example, let us consider a system consisting of one spin-$\frac{1}{2}$ and one harmonic oscillator, the two subsystems being linearly coupled. Assume moreover that the spin $\frac{1}{2}$ is coupled to a heat bath at zero temperature, see Fig. 4. The total Hamiltonian reads

$$H_{\text{total}} = H_1 + H_2 + H_{12} + H_{\text{env}} + H_I \tag{58}$$

with

$$H_1 = \frac{\omega_1}{2}\sigma_z , \tag{59}$$

$$H_2 = \omega_2 a^\dagger a, \tag{60}$$

$$H_{12} = \chi(\sigma_- a^\dagger + \sigma_+ a), \tag{61}$$

$$H_{\text{env}} = \sum_\omega \omega a_\omega^\dagger a_\omega , \tag{62}$$

$$H_I = \sum_\omega \chi_\omega (\sigma_- a_\omega^\dagger + \sigma_+ a_\omega). \tag{63}$$

We can either consider the spin-oscillator system coupled to a heat bath, or consider only the spin coupled to a heat bath and coupled to an auxiliary oscillator, as illustrated in

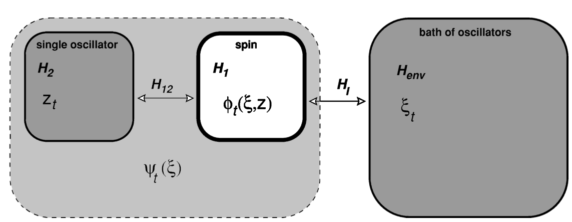

FIG. 4. Shifting the ''system-environment'' boundary. First, we consider the ''spin-single oscillator'' system with state $\psi_t(\xi)$, coupled to a heat bath with noise ξ_t. Alternatively, we can consider the ''spin'' only as the ''system'' $\phi_t(\xi,z)$, coupled to the ''single oscillator + heat bath'' environment (noises ξ_t, z_t). In non-Markovian QSD, both descriptions are possible and lead to the same reduced spin state.

Fig. 4. In the first case, we can consider the Markov QSD description, i.e., a family of spin-oscillator state vectors $\psi_t(\xi)$ indexed by the complex Wiener processes ξ_t. In the second case, using non-Markovian QSD we have a family of spin-$\frac{1}{2}$ state vectors $\phi_t(\xi,z)$ indexed by the same ξ_t plus the non-Markovian noise z_t with correlations

$$M[z_t^* z_s]=e^{-i\omega_2(t-s)}. \tag{64}$$

The (linear) stochastic equations (11) governing ψ_t and ϕ_t read

$$\dot{\psi}_t=-i(H_1+H_2+H_{12})\psi_t+\lambda\sigma_-\psi_t\xi_t-\frac{\lambda^2}{2}\sigma_+\sigma_-\psi_t, \tag{65}$$

$$\dot{\phi}_t=-iH_1\phi_t+\lambda\sigma_-\phi_t\xi_t-\frac{\lambda^2}{2}\sigma_+\sigma_-\phi_t+\chi\sigma_-\phi_t z_t-\chi\sigma_+\int_0^t e^{-i\omega_2(t-s)}\frac{\delta\phi_t}{\delta z_s}ds, \tag{66}$$

where λ is a function of the χ_ω's, that is of the strength of the spin–heat-bath coupling.

A natural question in the present framework is to study the ''Heisenberg cut'': compare the states of the spin $\frac{1}{2}$ averaged over the noise z with the mixed state obtained by tracing out the second oscillator (Tr_2) from the one-oscillator-spin states, i.e., we ask whether the equality

$$M_z[|\phi_t(\xi,z)\rangle\langle\phi_t(\xi,z)|]\overset{?}{=}\mathrm{Tr}_2(|\psi_t(\xi)\rangle\langle\psi_t(\xi)|) \tag{67}$$

holds. According to the general non-Markovian QSD theory presented in this paper, the spin-$\frac{1}{2}$ state should be independent of the position of the Heisenberg cut. Below we illustrate this feature using the present example.

By assumption the oscillator starts in the ground state: $\psi_0=\phi_0\otimes|0\rangle$. Hence, the state ψ_t can be expanded as

$$\psi_t=c_0(t)|\downarrow,0\rangle+c_1(t)|\uparrow,0\rangle+c_2(t)|\downarrow,1\rangle, \tag{68}$$

where

$$\dot{c}_0=\lambda\xi(t)c_1+i\frac{\omega_1}{2}c_0, \tag{69}$$

$$\dot{c}_1=-\left(i\frac{\omega_1}{2}+\frac{\lambda^2}{2}\right)c_1-i\chi c_2, \tag{70}$$

$$\dot{c}_2=-i\left[\left(\omega_2-\frac{\omega_1}{2}\right)c_2+\chi c_1\right]. \tag{71}$$

Tracing out the single harmonic oscillator, one obtains the spin-$\frac{1}{2}$ state (in the $\uparrow\downarrow$ basis)

$$\rho_1\equiv\mathrm{Tr}_2(|\psi_t(\xi)\rangle\langle\psi_t(\xi)|)=\begin{pmatrix}|c_1|^2 & c_0^*c_1\\ c_0c_1^* & |c_0|^2+|c_2|^2\end{pmatrix}. \tag{72}$$

We now turn to the alternative description of the same situation, but with the ''cut'' between the spin $\frac{1}{2}$ and the oscillator. In order to solve Eq. (66) we make the usual *Ansatz*

$$\frac{\delta\phi_t}{\delta z_s}=f(t,s)\sigma_-\phi_t, \tag{73}$$

where the consistency condition (14) leads to $\partial_t f(t,s)=[i\omega_1+\lambda^2/2+\chi F(t)]f(t,s)$, where $f(t,t)=\chi$ and $F(t)=\int_0^t\alpha(t,s)f(t,s)ds$. Consequently,

$$\dot{F}(t)=\chi+\left(i\omega_1-i\omega_2+\frac{\lambda^2}{2}+\chi F(t)\right)F(t). \tag{74}$$

Using the notations $\phi_t=v_0(t)|\downarrow\rangle+v_1(t)|\uparrow\rangle$ one gets

$$\dot{v}_0=i\frac{\omega_1}{2}v_0+(\lambda\xi_t+\chi z_t)v_1, \tag{75}$$

$$\dot{v}_1=-\left(i\frac{\omega_1}{2}+\frac{\lambda^2}{2}+\chi F(t)\right)v_1. \tag{76}$$

Note that since $\dot{v}_1$ is independent of z_t, $v_1(t)$ is itself independent of z, hence,

$$\frac{d}{dt}M_z[v_0]=i\frac{\omega_1}{2}M_z[v_0]+\lambda\xi_t v_1. \tag{77}$$

Averaging over the z noise, one obtains the spin-$\frac{1}{2}$ state (in the $\uparrow\downarrow$ basis)

$$\rho_2\equiv M_z[|\phi_t(\xi,z)\rangle\langle\phi_t(\xi,z)|]=\begin{pmatrix}|v_1|^2 & M_z[v_0^*]v_1\\ M_z[v_0]v_1^* & M_z[|v_0|^2]\end{pmatrix}. \tag{78}$$

Finally, a straightforward comparison of Eqs. (69)–(71) and (74)–(76) shows that $c_0=M_z[v_0]$, $c_1=v_1$, and $c_2=-iFv_1$. Hence, 3 of the 4 entries of the matrices ρ_1 and ρ_2 are equal. The equality of the fourth entry follows from the general feature that linear non-Markovian QSD preserves the mean of the square norm.

This completes the proof that $\rho_1=\rho_2$: the spin-$\frac{1}{2}$ state is independent of the position of the Heisenberg cut, for all times and all realizations of the heat-bath-induced noise ξ. This illustrates the general fact that non-Markovian QSD attributes stochastic pure states to systems in a way that depends on the position of the Heisenberg cut, but that is consistent for all possible choices of the cut. See Fig. 4 for the illustration of these relationships. This is in opposition to the case prevailing in Markovian unravelings.

VII. OPEN PROBLEMS

This paper is the first presentation of non-Markovian QSD. Admittedly, there remain many open questions and a lot of work has still to be done to exploit all the possibilities opened up by this new approach. In this section we list some of the open problems:

(1) The ultimate goal would be to develop a general pur-

pose numerical simulation program. However, at present no general recipe is known.

(2) When do the long time limit and the Markov limit commute? This is a question that is of particular interest for quantum Brownian motion.

(3) If the initial condition is not factorized, the present approach must be generalized.

(4) In the Markov case unravelings exist both with continuous trajectories and with quantum jumps, and the connection between the two is well understood [6,7]. In the non-Markovian case, the only unraveling known at present is the continuous non-Markovian QSD described in this paper. What about non-Markovian unravelings with quantum jumps?

(5) In the Markov case, continuous QSD unravelings exist for real or pure imaginary noise, as well as for complex noise. What about the non-Markovian case? It seems that in the present case complex noise is essential.

(6) Note that most of the non-Markovian master equations used in this paper have known analytical solutions. In these cases, the general Zwanzig form [29] of the master equation:

$$\dot{\rho}_t = \int_0^t \mathcal{K}(t-s)\rho_s ds \tag{79}$$

with the memory kernel $\mathcal{K}(t-s)$ could be rewritten as a Lindblad type master equation with time-dependent coefficients. Then, the master equation can also be simulated using Markov QSD with time-dependent coefficients. However, if the solution of the master equation is not known explicitly, or does not lead to a Lindblad type equation, then numerical simulation has to use the non-Markovian QSD theory. It would be interesting to illustrate non-Markovian QSD for more of such examples and to study the conditions under which a non-Markovian problem can be treated with Markovian unravelings.

(7) How does non-Markovian QSD compare with consistent histories [30] and other approaches? For instance, it was shown in [31] that the solutions of the non-Markovian equation (17) can be considered as conditional states in the framework of a ''hybrid'' representation of the fully quantized microscopic system, allowing a clear physical interpretation of the stochastic states.

(8) What is the perturbation expansion of the non-Markovian QSD equation (17) in terms of the memory time γ^{-1}? The zeroth-order term would be the Markov QSD equation (9), what about the higher orders?

(9) Finally, non-Markovian QSD should be applied to open problems in physics, where non-Markovian effects are relevant, such as semiconductor lasers [12], or atom lasers [32].

VIII. CONCLUSION

We present a stochastic equation for pure states describing non-Markovian quantum state diffusion, compatible with non-Markovian master equations. We illustrate its power with several examples. In essence, we show that quantum (finite or infinite) harmonic oscillator environments can be modeled by classical, complex Gaussian processes, entering the non-linear, non-Markovian stochastic Schrödinger equation for the ''system'' state that we derive in this paper.

Several authors have proposed stochastic pure-state descriptions of such non-Markovian situations using fictitious modes added to the system in such a way as to make to dynamics of the enlarged hypothetical system Markovian [12,13]. Others [14] treat a non-Markovian problem with an explicitly time-dependent Markov unraveling. In our approach, by contrast, there are no additional modes, hence the system is as small as possible, and the stochastic Schrödinger equation becomes genuinely non-Markovian. This is of interest for efficient numerical simulation and high-focus insight into the relevant physical processes. Also, non-Markovian quantum trajectories are in general much smoother than those of Markov processes, which might even help to reduce further the numerical effort.

Let us stress an important conceptual difference between Markov QSD and non-Markovian QSD. In the Markov case, one starts from a master equation for mixed states and associates to it a stochastic Schrödinger equation. The master equation may either be derived from a microscopic model, or merely be based on phenomenological motivations [8]. In the non-Markovian case, on the contrary, one starts from the stochastic Schrödinger equation (11). The existence of a master equation is guaranteed by the microscopic model summarized in Appendix C. In general, however, the explicit form of this master equation is not known. Nevertheless, this existence ensures that the corresponding stochastic Schrödinger equation for normalized states (17) does not allow arbitrary fast signaling, despite its nonlinearity [20].

From a pragmatic point of view, the Hamiltonian and Lindblad operators in the basic linear stochastic Schrödinger equation (11) can either be derived from a microscopic theory, or be merely based on phenomenological motivations. Non-Markovian master equations are almost always exceedingly difficult to treat, even numerically. However, one can always start from the non-Markovian QSD approach of this paper, which appears thus more fundamental than the master equation approach.

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APPENDIX A: FREQUENCY REPRESENTATION

It is sometimes useful to express the noise by frequency components z_ω:

$$z_t = \sum_\omega z_\omega e^{i\omega t}, \tag{A1}$$

where the frequencies ω can take positive as well as negative values. Also the correlation function can be written in Fourier representation:

$$\alpha(t,s)=\alpha(t-s)=\sum_\omega \alpha_\omega e^{-i\omega(t-s)}, \quad \alpha_\omega>0. \tag{A2}$$

The correlation of the Fourier components of the noise is trivial: $M[z_\omega^\star z_\lambda]=\delta_{\omega\lambda}\alpha_\omega$. In this representation the distribution functional becomes a simple Gaussian distribution over all z_ω's:

$$P(z)=\mathcal{N}\exp\left(-\sum_\omega \frac{|z_\omega|^2}{\alpha_\omega}\right) \tag{A3}$$

and the states ψ_t become functions of the frequency amplitudes z_ω of the noise. We can then write the fundamental linear non-Markovian QSD equation (11) in terms of them:

$$\frac{d}{dt}\psi_t=-iH\psi_t+\sum_\omega \left(Le^{i\omega t}z_\omega-L^\dagger\alpha_\omega e^{-i\omega t}\frac{\partial}{\partial z_\omega}\right)\psi_t. \tag{A4}$$

This frequency representation is a helpful tool to discuss the mathematical properties of the non-Markovian stochastic Schrödinger equation (17), as we do in Appendixes B and C. Remember that in Eq. (A4) we assume the initial condition to be independent of the noise: $\psi_0(z)=\psi_0$.

APPENDIX B: GIRSANOV TRANSFORMATION FOR NON-MARKOVIAN QSD

As time goes by, Girsanov transformation distorts the distribution $P(z)$ (A3) of the complex noise into $\tilde{P}_t(z)$ according to Eq. (6). In frequency representation, we have

$$\tilde{P}_t(z)=\mathcal{N}\|\psi_t(z)\|^2\exp\left(-\sum_\omega \frac{|z_\omega|^2}{\alpha_\omega}\right). \tag{B1}$$

We assume that at $t=0$ the state ψ_0 is normalized and does not depend on z. So, initially, $\tilde{P}_0(z)$ is identical with $P(z)$.

We find the time evolution of $\tilde{P}_t(z)$ from the linear non-Markovian Schrödinger equation (11) in frequency representation (A4). Using Eq. (B1), we find

$$\frac{d}{dt}\tilde{P}_t(z)=\mathcal{N}\left\langle \psi_t(z)\middle|\frac{d}{dt}\psi_t(z)\right\rangle\exp\left(-\sum_\omega \frac{|z_\omega|^2}{\alpha_\omega}\right)+\text{c.c.} \tag{B2}$$

Now we make a crucial observation. The solution $\psi_t(z)$ of Eq. (A4), with initial condition $\psi_t(z)=\psi_0$, is analytic in all z_ω's. Then it follows that $\partial|\psi_t(z)\rangle/\partial z_\omega^\star=\partial\langle\psi_t(z)|/\partial z_\omega=0$ for all z_ω. Hence, when inserting Eq. (A4) into Eq. (B2), we can substitute

$$\left\langle \psi_t(z)\middle|L^\dagger\frac{\partial}{\partial z_\omega}\psi_t(z)\right\rangle=\frac{\partial}{\partial z_\omega}\langle L^\dagger\rangle_t\|\psi_t(z)\|^2, \tag{B3}$$

and we obtain

$$\frac{d}{dt}\tilde{P}_t(z)=-\sum_\omega \alpha_\omega e^{-i\omega t}\frac{\partial}{\partial z_\omega}\langle L^\dagger\rangle_t\tilde{P}_t(z)+\text{c.c.} \tag{B4}$$

This is a remarkable result. It shows that the Girsanov transformation is equivalent to a drift of the random variable z. We read off the drift velocities directly from Eq. (B4):

$$\frac{d}{dt}z_\omega=\alpha_\omega e^{-i\omega t}\langle L^\dagger\rangle_t. \tag{B5}$$

One can see that the Girsanov transformation preserves the normalization of the distribution $\tilde{P}_t(z)$. This has the immediate consequence that the non-Markovian stochastic Schrödinger equation (11) preserves the mean norm of the quantum state:

$$M[\|\psi_t\|^2]\equiv\int \|\psi_t\|^2P(z)dz=\int \tilde{P}_t(z)dz=1. \tag{B6}$$

Now we are going to derive the stochastic non-Markovian Schrödinger equation for the normalized states $\tilde{\psi}_t(z)=\psi_t(z)/\|\psi_t(z)\|$, where $\psi_t(z)$ is the unnormalized solution of the linear stochastic equation (11). First, we solve the drift Eq. (B5) for the trajectories $z_\omega(t)$, with the initial conditions $z_\omega(0)=z_\omega$ for all ω:

$$\tilde{z}_\omega(t)=z_\omega+\int_0^t\alpha_\omega e^{-i\omega s}\langle L^\dagger\rangle_s ds, \tag{B7}$$

where $\langle L^\dagger\rangle_t=\langle\psi_t(\tilde{z}(t))|L^\dagger|\psi_t(\tilde{z}(t))\rangle/\langle\psi_t(\tilde{z}(t))|\psi_t(\tilde{z}(t))\rangle$. The Girsanov transformation (5) leaves invariant the probability of the noise z along the above trajectories:

$$\tilde{P}_t(\tilde{z}(t))d\tilde{z}(t)\equiv P(z)dz \tag{B8}$$

for all z_ω. Hence, we can write the stochastic unraveling (6) as follows:

$$\rho_t=\tilde{M}_t[|\tilde{\psi}_t(z)\rangle\langle\tilde{\psi}_t(z)|]=M[|\tilde{\psi}_t(\tilde{z}(t))\rangle\langle\tilde{\psi}_t(\tilde{z}(t))|]. \tag{B9}$$

The mean value on the very right refers to the simple undistorted distribution $P(z)$. To calculate it, one has to express $\psi_t(\tilde{z}(t))$ as a function of the initial amplitudes $z_\omega=\tilde{z}_\omega(0)$. Remember that $\psi_t(z)$ is the solution of the linear non-Markovian equation (11) or (A4) with initial condition $\psi_t(z)=\psi_0$. The additional time dependence of $\psi_t(\tilde{z}(t))$ through $\tilde{z}(t)$ appends a new term to the evolution equation of these "Girsanov-shifted" states, so that we find the following stochastic evolution equation:

$$\frac{d}{dt}\psi_t(\tilde{z}(t))=\frac{\partial}{\partial t}\psi_t+\sum_\omega \dot{z}_\omega\frac{\partial}{\partial z_\omega}\psi_t \tag{B10}$$

$$=-iH\psi_t+\sum_\omega Le^{i\omega t}\tilde{z}_\omega-(L^\dagger-\langle L^\dagger\rangle_t)\times\int_0^t\alpha(t,s)\hat{O}(t,s,\tilde{z})ds\,\psi_t, \tag{B11}$$

where we used Eqs. (13), (15), and (B5). Finally, these states have to be normalized. The resulting evolution equation for the normalized states $\tilde{\psi}_t$ is our central result, given by Eq. (17). In the time domain, the shifted noise (B7) takes the form (16).

APPENDIX C: REVIEW OF THE LINEAR NON-MARKOVIAN THEORY

Here we briefly review the microscopic origin of the linear non-Markovian stochastic Schrödinger equation (11)—see [15–17]. The linear non-Markovian QSD equation results from a standard model of a system interacting with an environment of harmonic oscillators, represented by a set of bosonic annihilation and creation operators $a_\omega, a_\omega^\dagger$. The interaction term H_I between system and environment is chosen to be linear in the a_ω's and arbitrary in the system operator L: $H_I=\Sigma_\omega \chi_\omega (L a_\omega^\dagger + L^\dagger a_\omega)$, with some coupling constants χ_ω. Thus, the model is defined by

$$H_{\rm tot}=H_{\rm syst}+H_I+H_{\rm env} \tag{C1}$$

$$=H_{\rm syst}+\sum_\omega \chi_\omega (L a_\omega^\dagger + L^\dagger a_\omega)+\sum_\omega \omega a_\omega^\dagger a_\omega . \tag{C2}$$

Solving this total closed system in a clever way leads to the linear non-Markovian stochastic Schrödinger equation (11) for the system state $\psi_t(z)$. As an initial condition we assume a factorized form $\rho_{\rm tot}=|\psi_0\rangle\langle\psi_0|\otimes\rho_T$ for the total density operator, with all bath oscillators initially in some thermal state $\rho_T=\otimes_\omega \rho_\omega(T)$.

1. Zero temperature

In [17] it was shown that if all the environment oscillators are initially in their ground state $(T=0)$, the dynamics of the reduced density operator $\rho_t=\mathrm{tr}_{\rm env}\rho_{\rm tot}(t)$ of the model (C1) can be unraveled $(\rho_t=M[|\psi_t(z)\rangle\langle\psi_t(z)|])$ using the linear stochastic Schrödinger equation (11),

$$\frac{d}{dt}\psi_t=-iH\psi_t+L\psi_t z_t - L^\dagger\int_0^t \alpha(t,s)\frac{\delta\psi_t}{\delta z_s}ds, \tag{C3}$$

where the colored complex stochastic processes z_t with zero mean satisfy

$$M[z_t^* z_s]=\sum_\omega \chi_\omega^2 e^{-i\omega(t-s)}\equiv\alpha(t,s), \quad M[z_t z_s]=0. \tag{C4}$$

We see the microscopic origin of the bath correlation function $\alpha(t,s)$ at zero temperature. For real physical systems we have $\omega>0$ in Eq. (C4). To model an arbitrary time-translation-invariant correlation function, one needs environment oscillators with negative frequencies as well.

2. Finite temperature

In order to derive the linear non-Markovian QSD equation at finite temperatures, we use a simple mathematical trick, well known in field theory [33]: the nonzero temperature density operator ρ_T of the heat bath can be canonically mapped onto the zero-temperature density operator (the vacuum) of a larger (hypothetical) environment. The problem at $T>0$ is thus reduced to the problem at $T=0$, whose linear non-Markovian QSD equation (C3) we already know. The resulting finite-temperature linear non-Markovian QSD equation is

$$\frac{d}{dt}\psi_t=-iH\psi_t+L\psi_t z_t^- - L^\dagger\int_0^t \alpha^-(t,s)\frac{\delta\psi_t}{\delta z_s^-}ds$$
$$+L^\dagger\psi_t z_t^+ - L\int_0^t \alpha^+(t,s)\frac{\delta\psi_t}{\delta z_s^+}ds. \tag{C5}$$

It thus depends on two independent processes z_t^-, z_t^+ with zero means and with temperature-dependent correlations

$$M[z_t^{-*}z_s^-]=\sum_\omega (\bar{n}_\omega+1)\chi_\omega^2 e^{-i\omega(t-s)}\equiv\alpha^-(t,s),$$
$$M[z_t^- z_s^-]=0 \tag{C6}$$

and

$$M[z_t^{+*}z_s^+]=\sum_\omega \bar{n}_\omega \chi_\omega^2 e^{i\omega(t-s)}\equiv\alpha^+(t,s), \quad M[z_t^+ z_s^+]=0. \tag{C7}$$

Here, $\bar{n}_\omega=(\exp\hbar\omega/kT-1)^{-1}$ denotes the average thermal number of quanta in the mode ω. We identify these terms as describing the stimulated $(\bar{n})$ and spontaneous $(+1)$ emissions (Lz^-) and the stimulated absorptions $(\bar{n})$ from the bath $(L^\dagger z^+)$. Notice also that for $T\to 0$, all the $\bar{n}_\omega$ tend to zero and Eq. (C5) reduces to Eq. (C3), as it should.

3. Finite temperature and $L=L^\dagger$

In the case of a self-adjoint coupling operator $L=L^\dagger\equiv K$, the finite temperature result can be simplified considerably by introducing the sum process $z_t=z_t^-+z_t^+$ having zero mean and correlations

$$M[z_t^* z_s]=\alpha^+(t,s)+\alpha^-(t,s)\equiv\alpha(t,s)$$
$$=\sum_\omega \chi_\omega^2[(2\bar{n}_\omega+1)\cos\omega(t-s)-i\sin\omega(t-s)],$$
$$M[z_t z_s]=0. \tag{C8}$$

Notice that $(2\bar{n}_\omega+1)=\coth(\hbar\omega/2kT)$ so that $\alpha(t,s)$ is nothing but the well-known bath correlation kernel of the so-called quantum Brownian motion model [25]. In terms of this single process z_t, the linear non-Markovian QSD equation at finite temperature (C5) takes the simple form of the zero-temperature equation (C3) involving just one noise z_t

$$\frac{d}{dt}\psi_t=-iH\psi_t+K\psi_t z_t - K\int_0^t \alpha(t,s)\frac{\delta\psi_t}{\delta z_s}ds, \tag{C9}$$

with the temperature-dependent $\alpha(t,s)$ of Eq. (C8). For $K=q$ the position operator, this unraveling was first introduced in [16], derived from the exact Feynman-Vernon path integral propagator of this model.

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