Dressed quantum trajectories: novel approach to the non-Markovian dynamics of open quantum systems on a wide time scale

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Abstract

A new approach to theory and simulation of the non-Markovian dynamics of open quantum systems is presented. It is based on identification of a parameter which is uniformly bounded on wide time intervals: the occupation of the virtual cloud of quanta. By ‘virtual’ we denote those bath excitations which were emitted by the open system, but eventually will be reabsorbed before any measurement of the bath state. A useful property of the virtual cloud is that the number of its quanta is expected to saturate on long times, since physically this cloud is a (retarded) polarization of the bath around the system. Therefore, the joint state of open system and virtual cloud (we call it dressed state) can be accurately represented in a truncated basis of Fock states, on a wide time scale. At the same time, there can be an arbitrarily large number of the observable quanta (which survive up to measurement), especially if the open system is under driving. However, it turns out that the statistics of the bath—measurement outcomes is classical (in a suitable measurement basis): one can employ a Monte Carlo sampling of these outcomes. Therefore, it is possible to efficiently simulate the dynamics of the observable quantum field. In this work we consider the bath measurement with respect to the coherent states, which yields the Husimi function as the positive (quasi)probability distribution of the outcomes. The joint evolution of the dressed state and the corresponding outcome is called the dressed quantum trajectory. The Monte Carlo sampling of these trajectories yields a stochastic simulation method with promising convergence properties on wide time scales.

1. Introduction

The model of a finite quantum system coupled to an infinite harmonic bath (the open quantum system, abbreviated as OQS) is of a great importance for numerous branches of quantum physics. It is this model on which the concepts of measurement and decoherence have been worked out [1, 2], from the fundamental questions of the emergence of classical world [3–7], to the modern protocols of adaptive quantum control [8–13] and information processing [14–17]. In physical chemistry the concept of OQS is applied to describe the transfer of phononic or electronic energy in the molecular complexes [18]. Finally, in the condensed matter physics, a special type of OQS, the Anderson impurity model within a self-consistent environment, is a central component of the dynamical mean-field theory calculations [19–22]. Theoretical and experimental advances in all these branches continuously raise the challenging questions about how to properly characterize the physical state of an open system, and how to simulate its dynamics in various regimes.

In the Markovian regime, when the environment recovers instantly after the OQS disturbances, it is fairly well understood how to characterize and propagate the state of an open system: its state is represented either by a reduced density matrix, which is governed by a master equation [23]; or by a wavefunction, which is governed by a stochastic Schrödinger equation [23–33]. Closely related to these methods is the input–output formalism [34–36], which allows one to take into account the properties of the incident and scattered excitations of the bath.
On the contrary, the non-Markovian regime [18, 23, 37], when the bath has the memory of the OQS disturbances, is still lacking a clear physical description [38, 39]. The main challenge of the non-Markovian regime is the entanglement: as the time goes, the OQS and the bath continuously exchange the quanta between themselves. The number of emitted bath quanta \( n(t) \) and the number of the involved bath modes \( N(t) \) grow with time. The dimension \( d(t) \) of the resulting joint entangled state grows with the time approximately as the number of partitions (for boson bath)

\[
\dim(t) \propto \frac{(n(t) + N(t) - 1)!}{(N(t) - 1)! n(t)!},
\]

with the ensuing complexity of description and simulation. The challenge of an entanglement dimension can be subdivided into the two problems: (1) how to deal with the growth of the excitation number \( n(t) \) and (2) how to deal with the growth of the number of the involved bath modes \( N(t) \).

As for the first problem in the Markovian case the situation is rather simple: at the moment of absorption and emission, the OQS state experiences a sudden jump. Right after that, the bath forgets the disturbance [40]. However, in the non-Markovian regime, the emitted quanta maintain the entanglement with the OQS for a certain period of time. In the literature, there is an understanding that OQS cannot be entangled to the whole bath state all the time: OQS should eventually forget about the emitted quanta [41]. Therefore, it is proposed to think of the bath state \( B \) as consisting of the two parts: (i) the entangled memory part \( M \) which is occupied by \( n_B(t) \) quanta; and (ii) the ‘detector’ part \( D \) of irreversibly emitted and forgotten quanta, whose number is \( n_D(t) \), so that \( n(t) = n_B(t) + n_D(t) \). Then, one would expect that \( n_B(t) \) is asymptotically bounded with time, and \( n_D(t) \) can grow with time. However, the question of how to partition the bath state \( B \) into these two parts, \( M \) and \( D \), still has no clear answer, albeit there are investigations and proposals of possible decompositions [41–46].

The second problem, the growth of \( N(t) \), is actually related to the problem of the long-range character of the bath memory function. Roughly speaking, no matter how far the emitted quanta fly into the bath (the farther, the more bath modes are involved), the return amplitude (i.e. the memory function) decays only by the inverse power law [47]. This tail turns out to be important: whenever it is cut off (whether directly after a certain time \( \tau_{\text{cut}} \) or indirectly by truncating \( N(t) \)), a revival occurs after a finite time [48–50] so that the large-time asymptotical behavior of the observables is corrupted.

The desirable physical approach to the non-Markovian regime should naturally solve these conceptual problems, thus making the description of this regime simple. In particular, it should be immune to the growth of \( n(t) \) and \( N(t) \). This would provide a solid foundation for the development of novel computational methods on large time scales.

As for the latter, there is a large number of the numerical simulation algorithms for the non-Markovian quantum dynamics. Different algorithms achieve varying degree of success for the specific models and parameter ranges. In particular, the case of the Ohmic bath was treated in [50] by a novel variant of the matrix-product-states algorithm. This algorithm truncates the bath memory after \( t_{\text{cut}} \). They indeed found that the large-time asymptotics of the observables depends on \( t_{\text{cut}} \). However, it is argued that at least for the case of the Ohmic bath the numerical complexity scales polynomially with \( t_{\text{cut}} \). In [51] the case of the superohmic bath is considered. In that work, the technique of augmented density tensor (ADT) [52, 53] is employed. It is demonstrated that the finite-\( \tau_{\text{cut}} \) memory cutoff may lead to the non-positive OQS states and exponential instabilities. They propose an improvement for the finite memory cutoff approximation, which allows one to achieve converged results for certain parameter ranges of the superohmic model. There are also recent developments in the stochastic simulation algorithms [48, 54–58]. In particular, in [48] the hierarchy of pure states (HOPS) [54] method was applied to the case of subohmic bath. It is demonstrated that even if the absolute value of memory tail is very small, in the strong coupling regime its truncation considerably distorts the dynamics of observables. HOPS method has combinatorial complexity with respect to \( t_{\text{cut}} \). Finally, it is necessary to mention the recent advances in the diagrammatic Monte Carlo methods: the novel inchworm quantum Monte Carlo (iQMC) [59] was demonstrated to be able to achieve converged results at least up to a few dozens of the OQS scales for the spin-boson [60, 61] and for the Anderson impurity models [62], in the most part of the corresponding parameter spaces.

The purpose of this work is to propose a physical description of the non-Markovian regime which is simple both conceptually and computationally, on large time scales. We expect that it will facilitate and visualize the analysis of the non-Markovian phenomena. Also, it should shed light on the successes of the recent simulation methods (like HOPS, iQMC), and provide us with outlook for their further improvement or for the development of novel techniques.

A physical description is usually based on a certain small parameter. We identify such a small parameter on wide time scales: the population of the cloud of the virtual bath quanta \( n_{\text{cut}}(t) \). What we mean is the following. When the open quantum system interacts with the surrounding bath, it emits and absorbs the quanta (bath excitations). We classify the quanta into the following types: virtual and observable [63, 64]. By ‘virtual’ we
denote those excitations which were emitted by the OQS, but eventually will be reabsorbed before any measurement of the bath state. At the same time, the observable quanta are those which will survive up to the bath measurement time moment. We suggest that the joint state ‘OQS + virtual quanta’, also called the **dressed OQS state**, is the appropriate characterisation of the physical state of OQS in a non-Markovian regime. We take the analogies from the other branches of physics: the physical state of electron which interacts with an electromagnetic field, is the ‘bare’ electron dressed by a cloud of virtual photons; in solid state, the electron is always dressed by the cloud of virtual phonons. From these analogies, one may expect that the number of the virtual quanta should be upper bounded even at the long simulation times and in the presence of driving. On a physical grounds, we expect it to be not large for the sufficiently small coupling. That is very favorable property for numerical methods, since we will represent the dressed OQS state in a truncated $n_{\text{virt}}(t)$-particle Fock basis for the virtual quanta.

At the same time, the observable quantum field may contain arbitrarily high number $n_{\text{obs}}(t)$ of the quanta at large time scales, especially if there is a driving, or the coupling contains the terms beyond the rotating-wave approximation (RWA). Fortunately, the physical properties of the observable field provide us with the escape from the ensuing complexity: the observable field is always measured. If a suitable basis is chosen (in this paper, the coherent states, the measurement statistics turns out to be classical. We can employ a Monte Carlo sampling of the measurement outcomes in order to simulate the dynamics of the observable field. Then, the quantum observable fields are replaced by the classical fluctuating fields, resulting in the **dressed** non-Markovian quantum state diffusion (shortly dressed NMQSD) equation of motion.

This way we solve the first problem of the entanglement dimension challenge (equation (1)): the growth of $n(t)$ is eliminated. The second problem, the growth of $N(t)$, is solved by considering of what would be a natural description of the virtual quanta state. The virtual quanta are never observed at any spatial or frequency mode: the only allowed ‘event’ for them is to be reabsorbed after a certain delay time. Therefore, we introduce the **delay time amplitudes** and derive the equations of motion for them. It turns out that the discretization of delay times provides us with a ‘soft’ coarsegraining of the bath memory, so that the exponentially large simulation times become accessible without revivals.

The presented approach also provides a solution to the aforementioned bath-state decomposition problem: the entangled memory $M$ is the dressed OQS state, and the detector part $D$ is the observable quanta.

In order to confirm our ideas, we perform simulations for a particular type of the open system: a two-state system coupled to a bosonic transmission line (the spin-boson model), in which the bath is bilinearly coupled to OQS. In this work we consider the case of a small coupling, but of strong memory (narrow bandwidth of the transmission line).

The proposed approach is based on many partial results in the literature. In particular, the idea of how to sample stochastically the observable state of the bath was first introduced in the NMQSD [65]. Another idea, that the correct non-Markovian description of the physical state of OQS should involve additional degrees of freedom (besides the reduced density matrix), is repeatedly expressed in literature in various contexts [41–46, 54, 66, 67]. The distinction between the two types of photons (the bath quanta)—those which will be eventually absorbed by the detector, and those which will be reabsorbed by the OQS—was first discussed in the works of Jack et al [38, 68].

Our paper is organized as follows. In section 2.1 we introduce the model of open quantum system and then in 2.2 we outline the technical realization of our approach. In 2.3 we derive the stochastical description of the observable field by considering the Husimi function of the bath. Then, the notion of a dressed OQS state corresponding to a fixed measurement outcome for the bath is introduced in section 2.4. In section 2.5 we define the dressed quantum trajectory as a joint self-consistent evolution of the measurement outcome and the corresponding dressed state. Summary of the simulation algorithm for the dressed wavefunction is provided in section 2.6, and the example calculation is performed in section 2.7. The problem of the long-range bath memory tails is discussed and solved in section 3, with the resulting numerical scheme and example calculation in sections 3.8 and 3.9 correspondingly. In section 4 the case of a bath at finite temperature is discussed with an illustrating calculation. How to deal with multiple baths, with the example of a heat current through OQS, is the content of section 5. We conclude in section 6.

## 2. Dressed quantum trajectories: eliminating the growth of the number of involved excitations

In this section, we present our approach to the description and simulation of open quantum system dynamics. Also, the first part of the entanglement challenge is solved: the growth of the number of involved excitations $n(t)$ is eliminated.
2.1. Model of open system and definitions

We consider a system which is linearly coupled to the bath of harmonic oscillators. The Hamiltonian is

$$\tilde{H} = \tilde{H}_s + \tilde{z}^\dagger \tilde{z} + \tilde{b}^\dagger \tilde{b} + \tilde{H}_b,$$

where $\tilde{H}_s$ is the OQS, $\tilde{H}_b$ is the bath

$$\tilde{H}_b = \int_0^{+\infty} d\omega \omega \tilde{a}^\dagger (\omega) \tilde{a} (\omega).$$

The bosonic annihilation operators $\tilde{a} (\omega)$ obey to the canonical commutation relations

$$[\tilde{a} (\omega), \tilde{a}^\dagger (\omega') ] = \delta (\omega - \omega').$$

The coupling is through the operator $\tilde{z}$ which is in the OQS Hilbert space, and through the operator $\tilde{b}$ which is in the Hilbert space of bath,

$$\tilde{b} = \int_0^{+\infty} d\omega \omega \tilde{a} (\omega).$$

In our representation, the frequency dependence of the density-of-states is transferred to the coupling coefficient $c (\omega)$. In the interaction picture with respect to the free bath, the Hamiltonian (2) becomes

$$\tilde{H} (t) = \tilde{H}_s + \tilde{z}^\dagger (t) \tilde{z} + \tilde{b}^\dagger (t) \tilde{b},$$

with

$$\tilde{b} (t) = \int_0^{+\infty} d\omega \omega \tilde{a} (\omega) \exp (-i\omega t).$$

Properties of the bath are defined in terms of its memory function

$$M(t - t') = [\tilde{b}^\dagger (t), \tilde{b} (t') ] = \int_0^{+\infty} d\omega |c (\omega)|^2 \exp (-i\omega (t - t')).$$

In the following, we will distinguish between the open system Hilbert space $\mathcal{H}_s$, the bath Hilbert space $\mathcal{H}_b$, and the joint Hilbert space $\mathcal{H}_{sb} = \mathcal{H}_s \otimes \mathcal{H}_b$. The membership to the corresponding space will be denoted by a lower subscript e.g. $\psi_t (z | x) \in \mathcal{H}_s$ and $|\varphi_t \rangle_b$ is a ket vector from $\mathcal{H}_b$. The presence of the two subscripts, e.g. $|\psi_t \rangle_{sb}$, will designate that the state belongs to the joint Hilbert space.

We will also need the notion of the conditional states. For this purpose, given any two states $|\psi_t \rangle_{sb}$ and $|z \rangle_b$, we define the contraction of them along a common pair of subscripts as

$$b_t (z | \psi_t )_{sb} \equiv \text{Tr}_b [ |\psi_t \rangle_{sb} \langle z | ] = \int \langle \tilde{z} | (z ) |\psi_t \rangle_{sb} = \sum_q |q \rangle_b \langle q | \otimes \langle z |_{b} \langle \psi_t \rangle_{sb},$$

where $|q \rangle_b$ is an arbitrary basis of OQS states and $\tilde{z}$ is the identity in $\mathcal{H}_b$. The contraction removes common subscripts (like in tensor calculus), so that $b_t (z | \psi_t )_{sb}$ is a ket vector which lies in the open system Hilbert space $\mathcal{H}_s$. The state $b_t (z | \psi_t )_{sb}$ has the physical meaning of unnormalized conditional wavefunction of OQS provided the bath is observed in $|z \rangle_b$.

In the following sections we assume that the initial joint state $|\psi (t = 0) \rangle_{sb}$ corresponds to the open system in a pure state $|\psi (0) \rangle_s$, and the environment in its ground state $|0 \rangle_b$ (no initial entanglement):

$$|\psi (t = 0) \rangle_{sb} = |\psi (0) \rangle_s \otimes |0 \rangle_b.$$

2.2. Outline of the proposed approach

Conventional theoretical description of the OQS evolution is based on the sequential application of the two stages: (i) the full joint state $|\psi (t) \rangle_{sb}$ is evolved during the time interval $[0, \ t]$ according to the (interaction picture) Schrodinger equation

$$\partial_t |\psi (t) \rangle_{sb} = -i \tilde{H} (t) |\psi (t) \rangle_{sb},$$

and only after then (ii) at the time moment $t$ the bath is subjected to the non-selective measurement (which is the underlying physical meaning of the partial trace $\text{Tr}_b$), so that the corresponding reduced state of OQS is

$$\tilde{\rho}_s (t) = \text{Tr}_b [ |\psi (t) \rangle_{sb} \langle \psi (t) | ] .$$

In this conventional approach we immediately face the trouble: as the involved bath size grows (and the time goes on), the state $|\psi (t) \rangle_{sb}$ contains a combinatorially large coherent superposition of the potential measurement outcomes, which renders the long-time computations intractable.

In order to overcome this problem of large superpositions, we devise an equivalent theoretical description in which a single bath measurement outcome $z$ is pre-selected and propagated in time, together with its conditional OQS wavefunction $b_t (z | \psi_t )_{sb}$. The expected merit of this approach is that most members of the coherent
superposition will die out since they are not compatible with $w$, thus reducing the complexity of the long time computations. Putting it other way, we want to develop a stochastic simulation of the observable bath quantum field. We call quantum trajectory the resulting joint self-consistent evolution of $z$ and $b_z(z)\rho_{ab}$.

It is worth noting that the outlined approach is similar in spirit to the non-Markovian quantum state diffusion methods [48, 54, 65] and to the modal interpretations of quantum mechanics [69, 70]. However, the way we develop it, and the resulting description of non-Markovian dynamics, is quite different.

Turning to the implementation of this idea, we need to choose a certain measurement basis $|z\rangle_b$ for the bath. For a given joint state $|\Psi(t)\rangle_{ab}$, this will yield a probability distribution of the measurement outcomes $Q(z, t)$. Then, by deriving the master equation for $Q(z, t)$ and finding its stochastic interpretation, we will obtain a closed system of equations for the quantum trajectories. The basis $|z\rangle_b$ should evolve in a simple way under the bath coupling operators ($\hat{b}(t)$ and $\hat{b}^\dagger(t)$). Otherwise, it will be difficult to derive a master equation for $Q(z, t)$.

For the system of bosonic harmonic oscillators (which $\hat{H}_b$ is), the appropriate basis is provided by coherent states [71]. Therefore, we employ the normalized multimode coherent states of the bath

$$b_z(z) = N_{z}^{-1}b_z(0) \exp\left[\int d\omega \varphi(\omega)\tilde{a}(\omega)\right] \equiv N_{z}^{-1}b_z(|z|),$$

which depend on complex functions of frequency $z(\omega)$ (our measurement outcomes). Here $b_z(|z|)$ is the unnormalized form of the coherent state, and $N_z$ is the norm of $b_z(|z|)$:

$$N_z \equiv b_z(|z|)b_z = \exp\left[\int d\omega |z(\omega)|^2\right].$$

The family of coherent states possess the resolution of unity property [71]

$$\hat{1}_b = \int d|z|N_z^{-1} \langle z|b_z \langle z| = \int d|z| |z\rangle_b \langle z|,$$

where $\hat{1}_b$ is the identity operator in the Hilbert space of the bath. We substitute the resolution of unity (15) into the reduced density matrix definition (12):

$$\tilde{\rho}_z(t) = \int d|z|N_z^{-1} b_z(|z|) \langle (|\Psi(t)\rangle_{ab})_b \langle \Psi(t)| \rangle_\Omega \langle z| b_z,$$

From this expression we identify that the probability distribution of the outcomes is the Husimi function [72]

$$Q(z, t) = N_z^{-2}\text{Tr}_{\Omega} \langle b_z(|z|)\rangle_{ab} \langle \Psi(t)| \rangle_\Omega \langle z| b_z,$$

Introducing the conditional density matrix of OQS

$$\tilde{\rho}_z(t|z) = \frac{b_z(|z|\langle (|\Psi(t)\rangle_{ab})_b \langle \Psi(t)| \rangle_{\Omega} \langle z| b_z}{||b_z|\langle \Psi(t)| \rangle_{ab}||^2},$$

we represent the reduced density matrix as the average over the bath measurement outcomes

$$\tilde{\rho}_z(t) = \int d|z|\tilde{\rho}_z(t|z)Q(z, t).$$

Now, provided we are able to sample stochastically the realizations $z^{(i)}$ of $z$ from $Q(z, t)$, we can evaluate the state of OQS as the average

$$\tilde{\rho}_z(t) = \frac{1}{M} \sum_{i=1}^{M} \tilde{\rho}_z(t|z^{(i)}),$$

where $M$ is the number of outcome samples $z^{(1)}, \ldots, z^{(M)}$.

2.3. Master equation for Husimi function and its stochastic interpretation

In this section we derive the master equation for $Q(z, t)$ which will enable us to find a stochastic (Monte Carlo) procedure for the sampling from $Q(z, t)$. We proceed by differentiating the definition (17) with respect to time:

$$\frac{\partial}{\partial t} Q(z, t) = \text{Tr}_\Omega\{[z|b_z \langle z| - i\hat{H}(t)\}, |\Psi(t)\rangle_{ab} \langle \Psi(t)|\} = \text{Tr}_\Omega\{[i\hat{H}_b(t) + 3\hat{\beta}^\dagger(t) + 3\hat{\beta}(t),] |z\rangle_b \langle z| \} |\Psi(t)\rangle_{ab} \langle \Psi(t)|\},$$

where we have employed the property $\text{Tr}\{A[B, C]\} = \text{Tr}\{[A, B]C\}$ and the fact that $\hat{H}_b$ commutes with the bath coherent state projections. Our aim is to transform the right hand side of (21) into a form which possess a stochastic interpretation. The stochastic master equation can contain the terms of the following kinds: (i) convection (drift), (ii) diffusion, and (iii) jumps. The terms of types (ii) and (iii) are not compatible with the time-reversal symmetry of the Schrodinger equation. Therefore, the desired form is

$$\int d|z|d|\omega|d\omega| = \lim_{M \to \infty} \sum_{i=1}^{M} \int d\omega_i d\omega_i \int d\omega_i \int d\omega_i \ldots \int d\omega_i d\omega_i d\omega_i d\omega_i$$

for a discretization of the frequency axis $\omega_1, \ldots, \omega_M$, and $\omega_i(\omega)$, $\omega_i(\omega)$ are understood as real and imaginary parts correspondingly of the complex number $z(\omega)$.
\[ \partial_t Q(z, t) = \partial_z \{ \mathcal{A}(z, t) Q(z, t) \} + \partial_z \{ (\mathcal{A}(z, t))^\dagger Q(z, t) \}. \]  

(22)

Then, we would say that this is just a convection in the space \( z \), with the velocity field \( \mathcal{A}(z, t) \). To obtain (22) from the right hand side of (21), we employ the fact that the creation \( \hat{a}^\dagger(\omega) \) and annihilation \( \hat{a}(\omega) \) operators act as differential operators on the normalized coherent state projections [71]:

\[
\hat{a}(\omega) \ket{z}_{b} = \hat{a}^\dagger(\omega) \ket{z}_{b}, \quad \hat{a}^\dagger(\omega) \ket{z}_{b} = (\partial_z z(\omega) + z(\omega)) \ket{z}_{b},
\]

(23)

and

\[
|z\rangle_b \bra{z} \hat{a}(\omega) = (\partial_z z(\omega) + z^*(\omega)) \ket{z}_{b} \bra{z}, \quad |z\rangle_b \bra{z} \hat{a}^\dagger(\omega) = z(\omega) \ket{z}_{b} \bra{z}. \]

(24)

Substituting these identities into the commutator in the last line of (21), and recalling the definition of the coupling operator (7), we obtain the desired convection form (22), with the velocity field

\[
\mathcal{A}(z, t) = -ie^{-i\xi(t)\omega} z^\dagger(z, t),
\]

(25)

where the normalized average \( s(z, t) \) of the system coupling operator \( \hat{s} \) is

\[
s(z, t) = \frac{\text{tr} \bra{z} \mathcal{H} \ket{z}}{\text{tr} \bra{z} \mathcal{H} \ket{z}}.
\]

(26)

Let us recapitulate that we have a fixed initial condition (10), which is propagated to a unique state \( \ket{\mathcal{H}(t)}_{sb} \) at any later time \( t \). Then, for the latter state, at each point \( z \) we evaluate the average \( s(z, t) \) and the velocity \( \mathcal{A}(z, t) \). Therefore, the velocity field in the convection equation (22) is uniquely and consistently defined for all values of its arguments \( (z, t) \).

The stochastic interpretation of the convection equation is as follows. At the time moment \( t = 0 \) we have a population of \( M \) signal samples \( z^{(1)} \ldots z^{(M)} \), which are drawn from the initial Husimi function

\[
Q(z, 0) = N_z^{-1} = \exp \left[ -\int \text{d}\omega \ |z(\omega)|^2 \right].
\]

(27)

Then, starting from \( z^{(i)} \), each sample \( i \) is evolved in time as

\[
\partial_t z^{(i)}(\omega; t) = ic(\omega) e^{-i\xi t} \hat{s}(z, t),
\]

(28)

or, equivalently,

\[
z^{(i)}(\omega, t) = z^{(i)}(\omega) + ic(\omega) \int_0^t e^{-i\xi t'} \hat{s}(z(t'), t') \text{d}t'.
\]

(29)

The resulting population of samples \( z^{(1)}(t) \ldots z^{(M)}(t) \) has the statistics of \( Q(z, t) \). Now, this population can be used to compute the time-dependent reduced OQS state according to (20).

2.4. Dressed state of open quantum system

In order to solve the convection equation (29) we need to know the conditional states \( b(z) \ket{\mathcal{H}(t)}_{sb} \). In other words, the Husimi master equation is not a closed set of equations. Some additional (virtual) degrees of freedom are coupled to the observable field dynamics. In this section we derive the equations of motion for these virtual degrees of freedom.

Given an outcome \( z \), we associate to it the dressed state of the open system

\[
\ket{\mathcal{H}_{\text{dres}}(z, t)}_{sb} = \exp \left[ \int \text{d}\omega \hat{a}(\omega) \right] \ket{\mathcal{H}(t)}_{sb}.
\]

(30)

Then, the conditional state is a bath-vacuum projection of the dressed state:

\[
b(z) \ket{\mathcal{H}(t)}_{sb} = b(0) \ket{\mathcal{H}_{\text{dres}}(z, t)}_{sb}.
\]

(31)

Let us discuss the physical content of these two objects. The non-unitary operator

\[
\hat{S}(z) = \exp \left[ \int \text{d}\omega \hat{a}(\omega) \right],
\]

(32)

which appears at the right hand side of (30), generates the canonical transformation

\[
\hat{S}(z) \hat{a}(\omega) \hat{S}(z)^{-1} = \hat{a}(\omega), \quad \hat{S}(z) \hat{a}^\dagger(\omega) \hat{S}(z)^{-1} = \hat{a}^\dagger(\omega) + z(\omega).
\]

(33)

Then, the equation (30) means that we take the joint state \( \ket{\mathcal{H}(t)}_{sb} \) and to each quantum which was created in it by \( \hat{a}^\dagger(\omega) \), a classical signal (the outcome) \( z(\omega) \) is coherently added: that is how the dressed state \( \ket{\mathcal{H}_{\text{dres}}(z, t)}_{sb} \) is obtained. Moreover, as it follows from (31), the bath measurement results in a simple discard of all the quanta: only the outcome \( z(\omega) \) remains. These discarded (i.e. virtual) quanta do not contribute to the measurement: if they were emitted via the coupling \( \hat{b}^\dagger(\tau) \) at earlier times \( \tau \), the only way for them to contribute to the dynamics is to be reabsorbed by the open system via \( \hat{b}(\tau') \) at later times \( \tau' \).

Now we can summarize the physical picture behind our approach. As we have established in the previous section, the measurement outcomes of the observable bath field have a classical statistics. The statistics is the
same as if the measurement outcomes \( z(t) \) were pre-existing: at the initial time moment \( t = 0 \), they are distributed according to the vacuum quantum noise (27). Then, they follow the deterministic classical evolution (29). In this situation, whenever the open system emits a bath quantum, at the very emission time moment, the quantum is offered a coherent superposition of the two fates: (i) to immediately collapse to the pre-known outcome \( z(\omega, t) \), and (ii) to become a virtual quantum, which ultimately will be reabsorbed by OQS, and will never be detected. So, in this description, OQS is always dressed by the cloud of virtual quanta, hence the name for \( |\Psi_{\text{dress}}(z, t)\rangle_{\text{ab}} \).

The phenomenon of ‘dressing’, when a small system is interacting with the surrounding medium, is ubiquitous in physics. The prominent examples are: the dressing of the ‘bare’ electron in QED by a cloud of virtual photons [73]; electron in a solid crystal gets dressed by a cloud of virtual phonons, thus forming a polaron quasiparticle [74]. What is important to observe is that in all these cases the dressing and the ‘bare’ system form a single physical object, whose properties are changed (renormalized) as compared to the ‘bare’ case. Thus, in this work we also take on the view that \( |\Psi_{\text{dress}}(z, t)\rangle_{\text{ab}} \) is the most natural characterization of OQS state when the bath is non-Markovian.

For a fixed \( z \), the state \( |\Psi_{\text{dress}}(z, t)\rangle_{\text{ab}} \) evolves according to the Schrödinger equation

\[
\frac{\partial}{\partial t} |\Psi_{\text{dress}}(z, t)\rangle_{\text{ab}} = -iH_{\text{dress}}(z, t)|\Psi_{\text{dress}}(z, t)\rangle_{\text{ab}},
\]

where the dressed Hamiltonian \( H_{\text{dress}}(z, t) \) is related to \( \bar{H}(t) \) (equation (6)) by the canonical transformation (33):

\[
\bar{H}_{\text{dress}}(z, t) = \bar{S}(z)\bar{H}(t)\bar{S}(z)^{-1} = H_s + \bar{s}(\xi_{\text{vac}}(t) + \hat{b}^\dagger(t)) + \bar{s}^\dagger\hat{b}(t).
\]

Here the classical complex noise

\[
\xi_{\text{vac}}(t) = \int_{0}^{+\infty} d\omega \xi^a(\omega) z(\omega) e^{i\omega t}
\]

represents the collapsed observable quantum field.

### 2.5. Dressed non-Markovian quantum trajectory

The dressed non-Markovian quantum trajectory (or shortly the dressed trajectory) is defined as a self-consistently evolving pair of \( z(t) \) and \( |\Psi_{\text{dress}}(z(t), t)\rangle_{\text{ab}} \). Let us here derive the equations of motion for them. We proceed by differentiating the dressed state:

\[
\frac{\partial}{\partial t} |\Psi_{\text{dress}}(z(t), t)\rangle_{\text{ab}} = \left\{ \partial_t \bar{S}(z(t)) \right\} |\Psi(t)\rangle_{\text{ab}} + \bar{S}(z(t)) \partial_t |\Psi(t)\rangle_{\text{ab}}
\]

\[
= \left\{ \int d\omega 2(\omega, t) \partial_t \omega + iH_{\text{dress}}(z(t), t) \right\} |\Psi_{\text{dress}}(z(t), t)\rangle_{\text{ab}}.
\]

Now we employ the convection equation (28) in order to eliminate \( \bar{s}(\omega, t) \), and we substitute the solution (29) into the expression for the classical noise (36):

\[
\frac{\partial}{\partial t} |\Psi_{\text{dress}}(z(t), t)\rangle_{\text{ab}} = -i[H_s + \xi_{\text{vac}}(t) + \phi^a(t) + \hat{b}^\dagger(t)] (\bar{s}^\dagger - \bar{s}^a(t)\bar{s}(t)) \hat{b}(t) \] |\Psi_{\text{dress}}(z(t), t)\rangle_{\text{ab}},
\]

where the self-consistent field \( \phi(t) \),

\[
\phi(t) = -i \int_{0}^{t} dt' M(t - t') \bar{s}(t'),
\]

is a convolution of the history of per-trajectory averages \( \bar{s}(t) \) of the system operator \( \bar{s} \):

\[
\bar{s}(t) = \frac{\langle \Phi_{\text{dress}}(z(t), t) | 0 \rangle_b \bar{s}(t)}{\| \langle \Phi_{\text{dress}}(z(t), t) | 0 \rangle_b \|^2}.
\]

Here, the noise \( \xi_{\text{vac}}(t) \) represents the vacuum fluctuations of the bath (36), and \( \phi(t) \) can be interpreted as a self-consistent displacement of the bath vacuum, due to the linear coupling. The operators \( \hat{b}(t) \) and \( \hat{b}^\dagger(t) \) annihilate and create the virtual quanta correspondingly.

The expected value \( \langle \bar{s} \rangle \) of an OQS observable \( \bar{s} \) is obtained by averaging over the vacuum fluctuations of the per-trajectory values:

\[
\langle \bar{s} \rangle = \frac{\langle \Phi_{\text{dress}}(z(t), t) | 0 \rangle_b \bar{s}(t) \langle \Phi_{\text{dress}}(z(t), t) | 0 \rangle_b \bar{s}(t) \rangle_{\text{ab}}}{\| \langle \Phi_{\text{dress}}(z(t), t) | 0 \rangle_b \|^2}.
\]

We call (38) the dressed non-Markovian quantum trajectory equation of motion. Alternatively, in order to acknowledge and distinguish from the related developments in literature [65], one may call the equation (38) the dressed NMQSD.

The numerical solution of (38) is the basis of our approach. At a first glance, there is no simplification with respect to the original Schrödinger equation (11): there is still coupling to infinite dimensions via \( \hat{b}(t) \) and \( \hat{b}^\dagger(t) \).
Therefore, let us discuss why we expect to benefit from our reformulation. First of all, if the cloud of virtual quanta has the meaning of (retarded) polarization of the bath around OQS, then it is not expected to explode, or to grow without bounds, as the time increases. Instead, it is expected to saturate on a certain average number of quanta, even at large times. Therefore, we hope to achieve an accurate solution of the dressed NMQSD (38) on wide time scales, by using a Fock basis for the virtual quanta, which is truncated above certain occupation numbers. At the same time, the observable quantum fields have different complexity behavior: since OQS can continuously emit excitations, especially if it is driven, or the coupling with the bath is non-RWA, their occupation numbers can grow without bounds with time. Therefore, the observable quantum fields are the major factor which makes the real-time simulation such a hard problem. And this is the virtue of the presented approach that these complicated quantum fields are simulated stochastically through the classical field $\xi_{\text{vac}}(t)$.

2.6. Numerical scheme for wavefunction

For a given open quantum system (2), (3), (5), the bath frequency range $[0, \omega_{\text{max}}]$ is chosen, and is discretized in a certain way $\omega_1, \ldots, \omega_N$. The bath mode operators are approximated as

$$\hat{a}_i \approx \sqrt{\Delta \omega} \hat{a}(\omega_i),$$

with the resulting commutation relations $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$, so that the bath Hamiltonian and coupling operator are approximated as

$$H_b \approx \sum_{i=1}^{N} \omega_i \hat{a}_i^\dagger \hat{a}_i \quad \text{and} \quad \hat{b} \approx \sum_{i=1}^{N} \sqrt{\Delta \omega} \epsilon(\omega_i) \hat{a}_i.$$

In a numerical simulation, we draw $M$ samples of the discretized signal $z^{(1)}, \ldots, z^{(M)}$, where now the $j$th sample $z^{(j)}$ is the complex vector of $N$ components:

$$z^{(j)} = \begin{bmatrix} z_1^{(j)} \\ \vdots \\ z_N^{(j)} \end{bmatrix},$$

and the component $z_i^{(j)}$ corresponds to the frequency $\omega_i$. The distribution of samples is complex Gaussian, with the statistics

$$z_i = \bar{z}_i = \bar{z}_i \bar{z}_k = \bar{z}_i \bar{z}_k = 0, \quad \bar{z}_i \bar{z}_k = \delta_{ik}.$$

For each sample $z^{(j)}$, we solve for the dressed quantum trajectory,

$$|\Psi_{\text{dressed}}(z^{(j)}(t), t)\rangle_{\text{sh}} = -i \hat{H}_{\text{dressed}}^{(j)}(t) |\Psi_{\text{dressed}}(z^{(j)}(t), t)\rangle_{\text{sh}},$$

where $\hat{H}_{\text{dressed}}^{(j)}(t)$ is obtained from discretization of equation (38) in the Schrödinger picture:

$$\hat{H}_{\text{dressed}}^{(j)}(t) = H_t + \sum_{i=1}^{N} \sqrt{\Delta \omega} \sum_{j=1}^{N} \epsilon(\omega_j) z_j^{(j)} e^{i \omega_j t} + \phi^*(t) + \hat{b}^\dagger + (\hat{b}^{\dagger} - \hat{b}^\dagger t) \hat{b} + \hat{H}_b.$$

Here the Hamiltonian $\hat{H}_{\text{dressed}}^{(j)}(t)$ depends self-consistently on the average of the system operator

$$\bar{s}(t) = \frac{\langle \langle \Psi_{\text{dressed}}(z^{(j)}(t), t) | 0 \rangle_{\text{sh}} \langle 0 | \Psi_{\text{dressed}}(z^{(j)}(t), t) \rangle_{\text{sh}} \rangle_{\text{sh}}}{\langle \langle 0 | \Psi_{\text{dressed}}(z^{(j)}(t), t) \rangle_{\text{sh}} \rangle_{\text{sh}}^2},$$

and on the retarded field $\phi(t)$

$$\phi(t) = -i \int_{0}^{t} dt' M(t - t') \bar{s}(t').$$

The initial condition for the trajectory $|\Psi_{\text{dressed}}(z^{(j)}(t), t)\rangle_{\text{sh}}$ is

$$|\Psi_{\text{dressed}}(z^{(j)}(t), t)\rangle_{\text{sh}} = |0\rangle_b \otimes |\psi(0)\rangle_s.$$
In this section we deal with the second problem of the entanglement dimension challenge: how to eliminate the growth of the number of involved bath degrees of freedom.

3.1. Revivals on large time scales

The spin is coupled to the bath through the spin lowering operator $\hat{\mathbf{s}} \cdot \mathbf{\hat{a}}$. The bath is represented by a semiinfinite chain of boson sites with the on-site energy $\varepsilon_0$ and the hopping between the sites $h$. The bath frequency spectrum is represented by a band $[\varepsilon_0 - 2h, \varepsilon_0 + 2h]$, which is discretized as

$$\omega_i = \varepsilon_0 + 2h \cos \left( \frac{i\pi}{N+1} \right), \quad \varepsilon(\omega_i) = h \sqrt{\frac{2}{\pi}} \sin \left( \frac{i\pi}{N+1} \right)$$

for $i = 1 \ldots N$. In this model, the spin can be interpreted as a qubit coupled to a finite-band-width waveguide. Therefore, hereinafter we will refer to it as the qubit. For calculations, we use the following values of parameters of the bath: $\varepsilon_0 = 1$, $h = 0.05$, $N = 20$. In figure 1 we present the convergence of stochastic simulation with $n = 0$ (only the spin Hilbert space, no virtual quanta), $n = 1$ (the spin Hilbert space and one virtual bath quantum), and $n = 2$ (the spin Hilbert space and two virtual bath quanta), towards the ED solution (the full Schrödinger equation in the truncated Fock space). From the presented results we see that the convergence on the whole time interval is achieved with only two virtual quantum, whereas ED required us to include the states with 8 excitations of the bath. This result confirms our idea that the virtual cloud saturates on long times, so that this approach is indeed promising for the development of efficient long-time simulation algorithms. The advantage of the algorithm is that it is parallelizable: different trajectories can be computed on different CPU cores of the cluster.

3. Delay-time amplitudes: eliminating the growth of the number of involved bath modes

2.7. Example calculation

We test the proposed approach on the spin-boson model,

$$\hat{H} = \varepsilon \hat{a} \hat{a}^\dagger + \hat{a}^\dagger \hat{a} f(t) + \hat{a}^\dagger f^*(t),$$

with $\varepsilon = 1$ and the driving field

$$f(t) = 0.1 \cos t.$$  

The spin is coupled to the bath through the spin lowering operator

$$\hat{s} = \hat{a}^\dagger \hat{a}.$$

The bath is represented by an infinite chain of bose sites with the on-site energy $\varepsilon_0$ and the hopping between the sites $h$. The bath frequency spectrum is represented by a band $[\varepsilon_0 - 2h, \varepsilon_0 + 2h]$, which is discretized as

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Figure 1. Time dependence of the qubit occupation. The qubit energy level is at the center of bath’s energy band. The average occupation of the qubit is computed by exact diagonalization (in the truncated full Fock space), which required us to take into account 8 bath excitations to achieve the convergence up to the time $t_e = 180$ (black dashed line). Beyond $t_e$, a higher number of bath excitations is required, but the combinatorially large memory and time requirements did not allow us to continue the exact calculation further. At the same time, the results for the dressed quantum trajectory method (numerical scheme for wavefunction, section 2.6) at $n = 0$ (blue), $n = 1$ (brown), and $n = 2$ (green), show that we reach convergence up to the stationary regime with only 2 virtual excitations. The number of retained bath modes for virtual quanta $N = 20$. The averaging was done over $M = 1.6 \times 10^5$ trajectories. Here are the times needed to compute 1000 trajectories sequentially on a single core of Intel Xeon CPU E5-2680: 7 min for $n = 0$, 9 min for $n = 1$; 40 min for $n = 2$.  

2.7. Example calculation

We test the proposed approach on the spin-boson model,

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The spin is coupled to the bath through the spin lowering operator

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The bath is represented by a semiinfinite chain of bose sites with the on-site energy $\varepsilon_0$ and the hopping between the sites $h$. The bath frequency spectrum is represented by a band $[\varepsilon_0 - 2h, \varepsilon_0 + 2h]$, which is discretized as

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for $i = 1 \ldots N$. In this model, the spin can be interpreted as a qubit coupled to a finite-band-width waveguide. Therefore, hereinafter we will refer to it as the qubit. For calculations, we use the following values of parameters of the bath: $\varepsilon_0 = 1$, $h = 0.05$, $N = 20$. In figure 1 we present the convergence of stochastic simulation with $n = 0$ (only the spin Hilbert space, no virtual quanta), $n = 1$ (the spin Hilbert space and one virtual bath quantum), and $n = 2$ (the spin Hilbert space and two virtual bath quanta), towards the ED solution (the full Schrödinger equation in the truncated Fock space). From the presented results we see that the convergence on the whole time interval is achieved with only two virtual quantum, whereas ED required us to include the states with 8 excitations of the bath. This result confirms our idea that the virtual cloud saturates on long times, so that this approach is indeed promising for the development of efficient long-time simulation algorithms. The advantage of the algorithm is that it is parallelizable: different trajectories can be computed on different CPU cores of the cluster.

3. Delay-time amplitudes: eliminating the growth of the number of involved bath modes

3.1. Revivals on large time scales

In this section we deal with the second problem of the entanglement dimension challenge: how to eliminate the growth of the number of involved bath degrees of freedom $N(t)$. In order to illustrate the necessity of this component, let us simulate the system described in the previous section for a longer period of time. In figure 2 we present the results for zero ($n = 0$) and one ($n = 1$) virtual quantum. We see that for zero virtual quanta the simulation is stable and reaches the stationary non-equilibrium state. At the same time, for one virtual quantum we observe the spurious revival around $t = 400$. The reason for this revival is common to all the numerical methods in the regime when the bath memory is important: when there is at least one quantum, it involves...
already an infinite number of the bath degrees of freedom. Then, in order to make the simulation tractable, ones usually retains only a finite number of degrees of freedom. Conventionally, this is done by either a finite discretization of the bath frequency modes; or by keeping only a finite number of the sites of the equivalent semiinfinite chain [75–77]; finally, the methods which directly deal with the memory functions, such as path integral-based methods (QUAPI and beyond) and HOPS, directly truncate the memory tails. In all the cases, the result of such a truncation is the same: large-time asymptotics of the observables is corrupted. And in order to delay the onset of the corrupted behavior, the number of the retained degrees should be at least linearly increased as the desired simulation time is enlarged. Therefore, it turns out that the large-time asymptotical behavior stems from a certain collective motion of the whole infinity of degrees of motion. This fact is expressed more concisely in terms of the memory function: it has inverse-power law tails which determine the large-time dynamics of OQS.

Now the question arises: is there any representation for the bath wavefunction, so that the correct large-time asymptotics is reproduced, and at the same time the dimension of the wavefunction can be kept asymptotically constant? For the joint state \( |\psi(t)\rangle_\text{sb} \), there is still no known answer. However, for the dressed state \( |\psi_{\text{dressed}}(z, t)\rangle_\text{sb} \) there is one. In the following sections, we gradually introduce the answer by discussing the questions: (i) how the memory tails arise; (ii) how the memory is lost in a classical non-Markovian system; (iii) what is the appropriate ‘configurational space’ for the virtual quanta. We consider them sequentially in the following sections.

### 3.2. Memory function tails

In a general (structured) environment, the bath spectral density \( |c(\omega)|^2 \) can be considered as being smooth except a finite number of frequencies \( \omega_1, \ldots, \omega_B \) where \( |c(\omega)|^2 \) (or its derivatives) is changing sharply. As we approach the frequency \( \omega_k \) from below (or from above), the discontinuous part of spectral density \( |c(\omega)|^2 \) behaves as a certain power,

\[
|c(\omega_k + \delta\omega)|^2 \propto \delta\omega^{\alpha \theta(\pm\delta\omega)}, \tag{56}
\]

where \( \theta \) is the Heavyside function. Since the memory function \( (8) \) is a Fourier transform of the spectral density, each singularity point \( (56) \) contributes an inverse-power law term

\[
e^{-i\omega_k t}M_k(t) \propto e^{-i\omega_k t(\pm it)^{-\alpha-1}}, \tag{57}
\]

and the memory function can be represented as a sum of these contributions,

\[
M(t) = \sum_{k=1}^{B} e^{-i\omega_k t}M_k(t). \tag{58}
\]

We call \( M_k(t) \) the memory channel. There is always at least one memory channel, since the physical spectral density does not have negative frequencies, thus it should vanish below a certain frequency. At the same time, in a structured environment where the spectral density is composed of bands (e.g. photonic crystals), each band edge yields a separate memory channel.
Recalling our model of the semiinfinite bosonic lattice \( (55) \), we have the memory function
\[
M(t) = e^{-i\omega_0 t} \frac{J_1(2ht)}{ht}.
\] (59)

There are two band edges, \( \omega_1 = \omega_0 - 2h \) and \( \omega_2 = \omega_0 + 2h \), and the corresponding memory channels are
\[
M_1(t) = e^{-i\omega_1 t} \left( \frac{H_{11}^{(1)}(2ht)}{2ht} + iR(2ht) \right) \propto t^{-\frac{3}{2}},
\] (60)
\[
M_2(t) = e^{+i\omega_2 t} \left( \frac{H_{12}^{(2)}(2ht)}{2ht} - iR(2ht) \right) \propto t^{-\frac{3}{2}},
\] (61)
and \( R(z) \) is a certain fast-decaying real-valued function, which fixes the \( t = 0 \) divergence of the Hankel functions. See appendix for the details about \( R(z) \).

### 3.3. How the memory is lost in a classical non-Markovian system

Here we consider the classical non-Markovian system. It will turn out that the results for this case can be directly transferred to the quantum case. Usually the classical non-Markovianity appears as the convolution integral. As an example, let us recall the self-consistent field \( \phi(39) \):
\[
\phi(t) = -i \int_0^t dt' M(t - t') \tilde{\tau}(t') = -i \sum_k e^{-i\omega_k t} \int_0^t dt' M_k(t - t') e^{-i\omega_k t} \tilde{\tau}(t'),
\] (62)
where we have substituted the channel decomposition \( (58) \). Were the memory finite (vanish for \( t > t_{\text{cut}} \)), the memory loss mechanism would be simply to forget instantly everything that happened \( t_{\text{cut}} \) units of time ago. However, in the presence of tails, the memory loss happens gradually. It is important to understand its mechanism in order to construct an efficient numerical coarse-graining of the memory.

Let us consider a single memory channel \( M_k(t) \). It has a crucial property that its local spectrum gradually becomes more and more narrowed to the frequency \( \omega_k \) as the time argument \( t \) is increased. Equivalently, one may say that as \( t \) is increased, there is an increasingly large time scale \( \Delta(t) \) over which \( M_k(t) \) can be considered as being effectively constant. Therefore, starting from \( t \) every spectral component outside the frequency range \( \approx \omega_k - \Delta(t)^{-1}, \omega_k + \Delta(t)^{-1} \) will be averaged to zero by convolving with the memory channel \( (57) \) in \( (62) \).

Physically this means that in the remote past, the spectral memory about the OQS behavior \( \tau(t) \) is completely averaged out (forgotten), except a progressively small vicinity of these singular frequencies \( \omega_k \).

To make profit from these considerations, we need to transform the equation \( (62) \). This is because it has one disadvantage for the analysis: it couples together different time scales. One scale is that of the laboratory times \( t \) and \( t' \), which is fixed by OQS energies and the singular frequencies \( \omega_k \). The other scale \( \Delta(t) \) is that of the memory delay time \( \tau = t - t' \), which as we have just discussed will dominate for the remote past. We decouple these scales by introducing the delay-time amplitudes \( \phi^{(k)}(\tau; t) \), which are defined to satisfy the system of delay-time equations
\[
\partial_\tau \phi^{(k)}(\tau; t) = \partial_t \phi^{(k)}(\tau; t) - iM_k(\tau) e^{-i\omega_k \tau} \tilde{\tau}(t).
\] (63)
The delay-time variable \( \tau \) ranges in \([0, +\infty)\). The initial condition for \( \phi^{(k)}(\tau; t) \) is
\[
\phi^{(k)}(\tau; t) = 0.
\] (64)
By an explicit solution it can be shown that the delay-time amplitudes \( \phi^{(k)}(\tau; t) \) are related to the original \( \phi(t) \) of \( (62) \) as
\[
\phi(t) = \sum_k e^{-i\omega_k \tau} \phi^{(k)}(0; t).
\] (65)
Therefore, \( (62) \) and \( (63) \) are equivalent to each other.

To grasp the meaning of the equation \( (63) \), imagine that the \( \tau \)-variable axis is a conveyor belt: the values of \( \phi^{(k)}(\tau; t) \) for \( \tau \geq 0 \) are transported along the \( \tau \)-variable axis with a unit speed towards the end of conveyor at \( \tau = 0 \), where they are ‘eaten’ forming the value of \( \phi(t) \) according to \( (65) \). Therefore, the farther we move from the conveyor end \( (\tau = 0) \), the more retarded influence is represented by \( \phi^{(k)}(\tau; t) \). At every time moment \( t \), the conveyor belt is populated at different positions \( \tau \) through the source term in \( (63) \), which depends on \( \tau \) only through \( M_k(\tau) \). This means that the local spectral properties of \( \phi^{(k)}(\tau; t) \) are similar to those of \( M_k(\tau) \): its characteristic delay-time scale \( \Delta(\tau) \) increases with \( \tau \).

The last fact allows us to perform the coarse-graining of the remote past memory by making an exponential substitution of variable
\[
\tau = \tau(\zeta).
\] (66)
The specific form of $\tau (\varsigma)$ will depend on $M_k (\tau)$ e.g. $\tau = \exp (\varsigma) - 1$. This will compress the memory tails, thus eliminating their long-range character. The delay-time equation (63) will assume the form:

$$\partial_t \phi^{(k)} (\varsigma ; t) = [\partial_\varsigma \tau (\varsigma)]^{-1} \partial_\varsigma \phi^{(k)} (\varsigma ; t) - i M_k (\tau (\varsigma)) e^{i \varsigma / 2} \xi (t).$$

(67)

This equation is very favorable from a numerical viewpoint: (i) $\phi^{(k)} (\varsigma ; t)$ is exponentially decreasing when $\varsigma$ is increased because so is the source $M_k (\tau (\varsigma))$; (ii) the conveyor velocity $[\partial_\varsigma \tau (\varsigma)]^{-1}$ is also exponentially decreasing; (iii) $\phi^{(k)} (\varsigma ; t)$ is always moving towards the $\tau = 0$ while stretching due to (66). Due to the property (iii), $\phi^{(k)} (\varsigma ; t)$ always remains bounded both temporally and spectrally, which allows for numerically stable solutions. Therefore, a finite $\varsigma$-grid $\varsigma_1, \ldots, \varsigma_m$ can be used to carry out the numerically exact simulations of long-range memory effects on exponentially large time scales.

We would like to draw the reader’s attention that the presented procedure has more content than just a numerical trick: it has certain features of an impurity renormalization group (RG) in the time domain. Let us recall that the conventional impurity RG is done in the frequency domain: in order to obtain a large separation of energy scales, the bath spectral density is logarithmically discretized near $\omega = 0$. Then, a semiinfinite Wilson chain is obtained by tridiagonalizing the resulting discrete bath. By keeping only the entanglement between the neighboring energy scales (i.e. employing the matrix product state (MPS) ansatz), the problem is solved in a finite truncated Hilbert space. In our procedure we also perform the logarithmic discretization of the delay-time axis $\tau$, but in a numerically exact way: the discarded memory states have negligible overlap with the spectrum of $M_k (\tau)$ (to be compared with the conventional impurity RG, where the discretization is a severe approximation).

Moreover, we also have a hierarchy of time scales: only the low-frequency part of the remote past survives. The neighboring sites of the $\varsigma$-grid have exponentially-separated scales. Therefore, in the quantum case (treated in the following section) we could also consider the delay-time matrix-product states. However, currently we believe it to be not necessary since the virtual cloud is expected to have a bounded population at all times.

3.4. Memory channels in the quantum case

Our procedure for the memory coarsegraining is based on the channel decomposition (58). To extend this procedure to the quantum case, we need to make the channel decomposition of the bath Hamiltonian $\tilde{H}_b$ (3) and of the bath coupling operator $\hat{b}$. We do this decomposition by a formal substitution

$$\tilde{H}_b + \hat{b}^\dagger + \hat{b} + \tilde{H}_b \rightarrow \tilde{H}_b + \sum_{k=1}^B \{ \hat{b}^{\dagger (k)} e^{i \omega \varsigma} + \hat{b}^{(k)} e^{-i \omega \varsigma} + \tilde{H}_b^{(k)} \},$$

(68)

where the channel-wise free bath Hamiltonian is

$$\tilde{H}_b^{(k)} = \int_0^\infty d\omega \tilde{\omega} \hat{a}^\dagger (k, \omega) \hat{a} (k, \omega),$$

(69)

with $[\hat{a} (k, \omega), \hat{a}^\dagger (k', \omega')] = \delta_{k k'} \delta (\omega - \omega')$, and the corresponding coupling operators

$$\tilde{b}_k = \int_0^\infty d\omega \tilde{\omega} \hat{a} (k, \omega)$$

(70)

are defined so that their commutator reproduces exactly one memory channel:

$$[\tilde{b}^{(k)} (t), \tilde{b}^{(k')} (t')] = M_k (t - t') \delta_{k k'}.$$  

(71)

The decomposed Hamiltonian (68) leads to the same vacuum–vacuum averages of the bath observables as the original Hamiltonian (2). This is because according to the Wick theorem these averages are determined by the bath-coupling commutator (8), and this commutator is preserved by our substitution. Therefore, for virtual quanta such a decomposition is legitimate.

3.5. Delay-time amplitudes for virtual quanta

For the quantum case, the delay-time amplitude $\phi^{(k)}_1 (\tau ; t)$ is defined as the amplitude of event that exactly one quantum in the $k$th channel will be reabsorbed at the time moment $t + \tau$:

$$| \phi^{(k)}_1 (\tau ; t) \rangle_s = b (0) \tilde{b}^{(k)} (\tau) | \Psi_{\text{dress}} (z, t) \rangle_{sb},$$

(72)

where $| \Psi_{\text{dress}} (z, t) \rangle$ is now assumed to be in the Schrodinger picture, and $\tilde{b}^{(k)} (\tau)$ is in its Heisenberg form

$$\tilde{b}^{(k)} (\tau) = \int_0^{+\infty} d\omega \omega q (\omega) \hat{a} (k, \omega) \exp (-i \omega \tau).$$

(73)

We extend this definition to the many-quanta case by introducing a hierarchy of delay-time amplitudes

$$| \phi^{(k)}_{\text{vac}} (t) \rangle_s = b (0) | \Psi_{\text{dress}} (z, t) \rangle_{sb},$$

(74)

$$| \phi^{(k)}_2 (\tau_1, \tau_2 ; t) \rangle_s = b (0) \tilde{b}^{(k)} (\tau_1) \tilde{b}^{(k)} (\tau_2) | \Psi_{\text{dress}} (z, t) \rangle_{sb},$$

(75)
Here in $\phi_n^{(k_1 \ldots k_n)}(\tau_1 \ldots \tau_n; t)$ we use the semicolon in order to distinguish the external (laboratory) time $t$ from the dynamical variables—the delay times $\tau_k$. The amplitude $\phi_n^{(k_1 \ldots k_n)}(\tau_1 \ldots \tau_n; t)$ is symmetric under simultaneous permutations of $k$’s and $\tau$’s.

3.6. Equations of motion in the delay-time picture

Now let us write the equation for the dressed quantum trajectory (38)–(39) in terms of the delay-time amplitudes. We proceed by differentiating with respect to time the definition (76):

$$
\partial_1 |\phi_n^{(k_1 \ldots k_n)}(\tau_1 \ldots \tau_n; t)\rangle = \nu(0) |\dot{\theta}^{(k_n)}(\tau_n) \ldots \dot{\theta}^{(k_1)}(\tau_1)\rangle |\Psi_{\text{dress}}(z, t)\rangle_{\text{ab}}.
$$

Here $\dot{H}_{\text{dress}}(z, t)$ is the right hand side of equation (38). After the term $\dot{H}_{\text{dress}}(z, t)$ is commuted to the left and employing the properties (71) and

$$
[\dot{\theta}^{(k)}(\tau), \dot{H}_{\text{ab}}] = i\partial_1 \dot{\theta}^{(k)}(\tau),
$$

we arrive at the equations (on the two-virtual-quanta level):

$$
\partial_1 |\phi_1^{(k_1)}(\tau_1, t)\rangle = -i\dot{H}_{\text{stoch}}(t) |\phi_1^{(k_1)}(\tau_1, t)\rangle - i(\xi^\dagger - \xi^*) |\phi_1^{(0)}(0; t)\rangle,
$$

$$
\partial_2 |\phi_2^{(k_1, k_2)}(\tau_1, \tau_2, t)\rangle = -i\dot{H}_{\text{stoch}}(t) |\phi_2^{(k_1, k_2)}(\tau_1, \tau_2; t)\rangle + \partial_1 |\phi_1^{(k_1)}(\tau_1, t)\rangle + iM_k(\tau)|\phi_1^{(k_1)}(0; t)\rangle,
$$

$$
\partial_3 |\phi_3^{(k_1, k_2)}(\tau_1, \tau_2; t)\rangle = -i\dot{H}_{\text{stoch}}(t) |\phi_3^{(k_1, k_2)}(\tau_1, \tau_2, t)\rangle + [\partial_1 + \partial_2] |\phi_2^{(k_1, k_2)}(\tau_1, \tau_2; t)\rangle + i\xi e^{-i\omega_0^1 M_k(\tau_1)} |\phi_1^{(k_1, k_2)}(\tau_1, \tau_2; t)\rangle + i\xi^* e^{i\omega_0^1 M_k(\tau_2)} |\phi_1^{(k_1, k_2)}(\tau_1, \tau_2; t)\rangle.
$$

Here we have grouped into $\dot{H}_{\text{stoch}}$ all the terms which belong to the Hilbert space of OQS:

$$
\dot{H}_{\text{stoch}}(t) = \dot{H} + 3(\xi_{\text{vac}}(t) + \phi^*(t)).
$$

The field $\phi(t)$ is still defined by the formula (39), where the per-trajectory average $\bar{\xi}(t)$ is computed for the vacuum amplitude:

$$
\bar{\xi}(t) = \frac{\langle \phi_{\text{vac}}(t) | \bar{\xi} | \phi_{\text{vac}}(t) \rangle}{\| \phi_{\text{vac}}(t) \|^2},
$$

3.7. Numerical coarsegraining of the delay-time equations

For each memory channel, we make the exponential substitution (66) into the delay-time equations of motion (79)–(81). In principle, for different channels one may choose different $\tau(\zeta)$. The net effect is that the arguments are changed $\tau_i \rightarrow \zeta_i$, and the derivative term becomes $\partial_1 \rightarrow [\partial_1 \tau(\zeta)]^{-1} \partial_2$. The one-quantum equation (80) becomes

$$
\partial_1 |\phi_1^{(k_1)}(s, t)\rangle = -i\dot{H}_{\text{stoch}}(t) |\phi_1^{(k_1)}(s, t)\rangle + iM_k(\tau(\zeta)|\phi_1^{(k_1)}(s, 0; t)\rangle + i\xi e^{1/2 M_k(\tau_1)} |\phi_1^{(0)}(s, 0; t)\rangle.
$$

The higher order amplitudes are changed similarly. Inspecting the resulting equations, we find that they have the same properties as their classical counterpart (64). In particular: (i) the delay-time amplitudes are exponentially decreasing in each of their arguments $\zeta_i$; (ii) these amplitudes move towards $\zeta_i = 0$ for each $i$, and stretch at the same time; (iii) velocity of movement along $\zeta_i$ decreases exponentially as $\zeta_i$ is increased. All these features ensure that the solution of these equations is always bounded both temporally and spectrally, therefore it can be efficiently simulated on long times.

We solve the equations like (84) by introducing a finite $\zeta$-grid $\zeta_1, \ldots, \zeta_m$ with $\zeta_1 = 0$. Then, a piecewise polynomial interpolation is employed. On the $\zeta$-grid we consider the values $\phi_1^{(k_1)}(s_p; t), p = 1 \ldots m$, and the values of the first $K$ derivatives $\partial_1^k \phi_1^{(k_1)}(s, t), q = 1 \ldots K$. The equations of motion for the latter are obtained by taking the partial derivatives with respect to $\zeta$ of the both sides of (84). Introducing the notation

$$
\phi_{pq}^k(t) \equiv \partial_1^p \partial_2^q \phi_1^{(k_1)}(s, t) |_{s = \zeta, s' = \zeta'},
$$

$$
\phi_{pq}^k(t) = \partial_1^p \partial_2^q \phi_1^{(k_1)}(s, t) |_{s = \zeta, s' = \zeta'},
$$

(85)
where the complex random numbers \( t_{pq} \) and the derivative \( \frac{\partial}{\partial t} \) are obtained by differentiating the term \([\partial_t \tau (\zeta)]^{-1} \partial_t \phi^{(k)} (\zeta; t)\). It is seen that the derivative \( \left\{ \partial \phi^{(k)} (t) \right\} \) is coupled to the derivative \( \left\{ \partial \phi^{(k)} (\tau_{k+1})(t) \right\} \). In order to truncate these equations, the latter is approximated by \( \partial_{\tau_{k+1}} P(\zeta) \), where \( P(\zeta) \) is a polynomial of order \( 2K + 1 \) that interpolates between the \( (K + 1) \) values of \( \phi^{(k)} (\zeta; t) \) and its derivatives on the boundaries of the interval \([\zeta_p, \zeta_{p+1}]\). The higher order delay-time equations for \( \phi^{(k)}_{i=1} (\tau_1, \tau_2; t) \) etc. are discretized in the same way:

\[
\begin{align*}
\partial_t |\phi^{(k)}_{i=1} (\tau_{k+1}; t)\rangle &= -i \hat{H}_{\text{stoch}} \langle t | \phi^{(k)}_{i=1} (\tau_{k+1}; t)\rangle + \sum_{l=1}^n M^{(k)}_{p,kl} e^{i \omega_{l} \tau_{k+1} / \hbar} |\phi^{(k)}_{i=1} (\tau_{k+1}; t)\rangle
\end{align*}
\]

The resulting system of ordinary differential equations is solved by the implicit midpoint method.

The functional form of \( \tau (\zeta) \) was guessed by eye: that the memory function is not too compressed near \( \zeta = 0 \) and at the same time, that the power-law tails are sufficiently pure. We have checked the numerical accuracy of \( \epsilon \)-grid at a given order \( K \) by computing the response of the classical delay-time equations (67) on the delta-input \( r (t) = \delta(t) \). In this latter case we should have \( \phi^{(k)} (\tau; t) = -i M_{k} (t + \tau) \), and we required the relative error for the numerical \( \phi^{(k)} (\tau; t) \) to be less than \( 10^{-5} \) on the whole simulation range.

### 3.8. Numerical scheme for the delay-time amplitudes

The numerical scheme for the delay-time equation introduced in section 2.6 will be modified as follows. For the classical field of vacuum fluctuations \( \xi_{\text{vac}} (t) \) we still have the discretized form

\[
\xi_{\text{vac}} (t) = \sqrt{\Delta \omega} \sum_{i=1}^{N} C^{p} (\omega_i) z_i e^{i \omega_i t},
\]

where the complex random numbers \( z_i \) have the Gaussian statistics

\[
\mathbb{E}[z_i] = \bar{z} = \bar{z} \bar{z}^* = 0, \quad \mathbb{E}[z_i z_j^*] = \delta_{ij}.
\]

For each realization of \( \xi_{\text{vac}} (t) \), we solve the delay-time equation for vacuum

\[
\begin{align*}
\partial_t |\phi_{\text{vac}} (t)\rangle &= -i \hat{H}_{\text{stoch}} \langle t | \phi_{\text{vac}} (t)\rangle - i (\vec{\tau}^* - \vec{\tau}^* (t)) \sum_{l=1}^n e^{-i \omega_l t} |\phi^{(l)}_{i=1} (\tau; t)\rangle,
\end{align*}
\]

the equation for one quantum (87), and the equations for higher number of quanta (88) which are truncated after some order \( n \). The self-consistent field \( \phi (t) \in \hat{H}_{\text{stoch}} (t) \) was also computed by the numerical discretization of the delay-time equations (64), (65) and (67). The initial conditions are \( \langle \phi_{\text{vac}} (0) | \xi_{\text{vac}} (0) \rangle = |\psi(0)\rangle \), and \( |\phi^{(k)}_{i=1} (\zeta_p, \zeta_{p+1}) (0)\rangle = 0 \). The reduced density of OQS is computed as

\[
\rho_{i=1} = \frac{1}{M} \sum_{j=1}^{M} \frac{|\phi^{(j)}_{i=1} (\zeta_p, \zeta_{p+1})\rangle \langle \phi^{(j)}_{i=1} (\zeta_p, \zeta_{p+1})|}{\| \phi^{(j)}_{i=1} (\zeta_p, \zeta_{p+1}) \|^2},
\]

where \( |\phi^{(j)}_{i=1} (\zeta_p, \zeta_{p+1})\rangle \) is a solution \( \phi_{\text{vac}} (t) \rangle \) of the delay-time equations for the \( j \)th sample of \( \xi_{\text{vac}} (t) \).

### 3.9. Example calculation

Now we return to the spin-boson model (52)–(53), and repeat the long-time calculation of section 3.1 (figure 2) by solving the delay-time equations (79)–(81) using the numerical procedure described in the previous section. In figure 3 we present the results for the time dependence of the qubit occupations. We see that the system successfully reaches the stationary non-equilibrium state. There is no revivals or other deterioration of the accuracy of observables. An equidistant \( \epsilon \)-grid of \( m = 7 \) nodes was used, with the maximal node at \( \zeta_m = 2.8525 \). The order of smoothness \( K = 3 \) was sufficient to achieve a stable long-time propagation of delay-time amplitudes. We have employed the exponential substitution of the form
with $a = 0.5$, $b = 0.1$, $c = 0.9$.

4. Case of a finite temperature

4.1. Thermal fluctuations as a classical noise

In the most situations of interest, the open system is surrounded by a medium at a finite temperature. The idea of how to treat the finite temperature case was already discussed in the literature [48, 63, 64]. Suppose that the joint OQS-bath initial density matrix is a factorized one:

$$\rho_{bs}(t = 0) = |\psi(0)\rangle_s \langle \psi(0)| \otimes \rho_b(T),$$

where the bath density matrix $\rho_b(T)$ corresponds to an equilibrium state at temperature $T$. In the spirit of our approach, we want to represent the effect of the temperature as an additional classical noise $\xi_{th}(t)$. Technically this is accomplished by decomposing the bath thermal density operator into the coherent states:

$$\hat{\rho}_b(T) = \int d[u] |u\rangle_b \langle u| \ P(u, T),$$

where $|u\rangle_b$ is the normalized form of coherent states (13), and the expansion coefficient is the thermal Glauber–Sudarsan $P$-function

$$P(u, T) \propto \exp \left( -\int d\omega \frac{|u(\omega)|^2}{n_{th}(\omega, T)} \right),$$

with the thermal Bose–Einstein occupation numbers

$$n_{th}(\omega, T) = \frac{1}{\exp (\omega/T) - 1}.\tag{97}$$

Inserting the thermal coherent states expansion (95) into the initial condition (94), we obtain:

$$\hat{\rho}_{bs}(t = 0) = \int d[u] P(u, T) D(u) \left( |\psi(0)\rangle_s \otimes |0\rangle_b \right) \left( |0\rangle_b \otimes |\psi(0)\rangle_s \right) D^{-1}(u),\tag{98}$$

where the unitary displacement operator $D(u)$,

$$D(u) = \exp \left[ \int d\omega \left( u^*(\omega) \hat{a}^\dagger(\omega) - u(\omega) \hat{a}(\omega) \right) \right],$$

comes from the coherent states, since $|u\rangle_b = D(u) |0\rangle_b$. In order to apply the dressed trajectory approach described in previous sections, we want to have a time-dependent problem with vacuum initial conditions for the bath. Therefore, we always keep $D(u)$ and $D^{-1}(u)$ on their places in equation (98), and at later times, the joint thermal state is represented as

$$\tau = \tau(\zeta) = \frac{1}{2\hbar} \left( a s + b \{ e^{i\zeta^2} - 1 \} \right), \tag{93}$$

with $a = 0.5$, $b = 0.1$, $c = 0.9$. 

Figure 3. Time dependence of the occupation of the driven two-level system in a wave-guide, introduced in section 2.7. The simulation is by the numerical scheme for delay times (section 3.8). Two virtual quanta ($n = 2$) are taken into account (green line). When a soft coarsegraining of the memory function on large delay times is performed, the revivals disappear. There is no deterioration of accuracy on large time scales. We also compare with the exact results which required us to include 8 bath quanta, and are available only up to $t_c = 180$ (black line). The vacuum noise $\xi_{vac}(t)$ was discretized on $N = 100$ modes. The averaging was done over $M = 8 \times 10^4$ trajectories. Here are the times needed to compute 500 trajectories sequentially on a single core of Intel Xeon CPU E5-2680: 15 min for $n = 1$; 8 h for $n = 2$. 

\[\text{Figure 3. Time dependence of the occupation of the driven two-level system in a wave-guide, introduced in section 2.7. The simulation is by the numerical scheme for delay times (section 3.8). Two virtual quanta ($n = 2$) are taken into account (green line). When a soft coarsegraining of the memory function on large delay times is performed, the revivals disappear. There is no deterioration of accuracy on large time scales. We also compare with the exact results which required us to include 8 bath quanta, and are available only up to $t_c = 180$ (black line). The vacuum noise $\xi_{vac}(t)$ was discretized on $N = 100$ modes. The averaging was done over $M = 8 \times 10^4$ trajectories. Here are the times needed to compute 500 trajectories sequentially on a single core of Intel Xeon CPU E5-2680: 15 min for $n = 1$; 8 h for $n = 2$.} \]
\[ \tilde{\rho}_{\text{th}}(t) = \int \text{d}[u] P(u, T) D(u) \langle \Psi(u, t) \rangle_{\text{th}} \langle \Psi(u, t) \rangle D^{-1}(u). \]  

(100)

Here the joint wavefunction \( \langle \Psi(u, t) \rangle_{\text{th}} \) has the vacuum–bath initial conditions
\[ \langle \Psi(u, t = 0) \rangle_{\text{th}} = \langle \psi(0) \rangle_s \otimes |0\rangle_b. \]  

(101)

In the interaction picture with respect to the bath, the time evolution for \( \langle \Psi(u, t) \rangle_{\text{th}} \) is given by
\[ \partial_t \langle \Psi(u, t) \rangle_{\text{th}} = -i \tilde{H}(u, t) \langle \Psi(u, t) \rangle_{\text{th}}, \]  

(102)

where the Hamiltonian \( \tilde{H}(u, t) \) is a shifted variant of the interaction picture one (6):
\[ \tilde{H}(u, t) = D(u) \tilde{H}(t) D^{-1}(u) = \tilde{H}_s + \hat{s} \hat{b} + \xi_{\text{th}}(t) + \xi_{\text{th}}(t)^\dagger. \]  

(103)

Here we have introduced the classical thermal noise
\[ \xi_{\text{th}}(t) = \int_0^{\infty} \text{d} \omega e^{\omega t} \xi^\omega(\omega) e^{-i \omega t}, \]  

(104)

and according to (96), the complex spectral noise \( u(\omega) \) has the Gaussian statistics
\[ u(\omega) u^\dagger(\omega') = \delta(\omega - \omega') n_{\text{th}}(\omega, T). \]  

(105)

When computing the reduced density matrix of OQS, we take the trace over the bath degrees of freedom in (100). The factors \( D(u) \) and \( D^{-1}(u) \) cancel each other under this trace operation, so that we have:
\[ \tilde{\rho}_s(t) = \int \text{d}[u] P(u, T) \text{Tr}_b \langle \Psi(u, t) \rangle_{\text{th}} \langle \Psi(u, t) \rangle. \]  

(106)

This equation can be interpreted stochastically: we draw the samples of \( u(\omega) \) from the probability distribution \( P(u, T) \). Then, for each \( u(\omega) \), we compute the evolution under the driving field \( \xi_{\text{th}}(t) \), equations (102)–(103). The resulting reduced OQS density matrix is averaged over \( u(\omega) \).

### 4.2. Numerical scheme for finite temperature

Essentially, we apply the dressed trajectory approach to the time-dependent problem (101)–(103) for a fixed \( u(\omega) \), and then average over \( u(\omega) \). This leads to the following numerical scheme. At the chosen discretization \( \omega_1, \ldots, \omega_N \) of the bath frequency range, the thermal Bose–Einstein occupation numbers \( n_{\text{th}}(\omega_i, T) \) are computed. Introducing the complex random numbers \( v_i \) with the Gaussian statistics
\[ v_i = v_i^\dagger = v_i v_i^\dagger = v_i^\dagger v_i = 0, \quad v_i v_i^\dagger = \delta_{i,k}, \]  

(107)

the discretized thermal noise is calculated for each realization of \( v_i \) as
\[ \xi_{\text{th}}(t) = \sqrt{N \Delta \omega} \sum_{i=1}^N \epsilon(\omega_i) \sqrt{n_{\text{th}}(\omega_i, T)} v_i e^{-i \omega_i t}. \]  

(108)

Then, if one wants to use the numerical method for wavefunctions of section 2.6, one should follow the steps of this method with the only difference that now
\[ \tilde{H}_\text{drew}(t) = \tilde{H}_s + \hat{s} \hat{b} + \xi_{\text{th}}(t) + \xi_{\text{th}}(t)^\dagger + \hat{b} + \tilde{H}_b, \]  

(109)

and the average in (51) is both over the realizations of \( z_j \) and of \( v_i \). If one wants to use the numerical method for the delay-time amplitudes from section 3.8, one again follows the steps of that method, with the substitution
\[ \tilde{H}_\text{stoch}(t) = \tilde{H}_s + \hat{s} \hat{b} + \xi_{\text{th}}(t) + \xi_{\text{th}}(t)^\dagger + \hat{b} + \tilde{H}_b, \]  

(110)

and the average in (92) is both over the realizations of \( z_j \) and of \( v_i \).

### 4.3. Example calculation

Let us again consider the case of spin–boson model described in section 2.7, but now with the qubit initially unoccupied \( \langle \sigma_z \rangle_{\text{fs}}(t = 0) = 0 \) and without driving \( \langle f(t) \rangle_{\text{fs}} \equiv 0 \), and the bath is at finite temperature. In figure 4 we present the results of calculation of the scheme for delay times of section 3.8 for a set of temperatures for the bath. We see that the occupation reaches the limit of a free spin at a finite temperature, which is justified due to a small coupling constant \( \hbar \).

### 5. Current through an open system and bath observables

#### 5.1. Dressed quantum trajectories for multiple baths

In many realistic situations (especially in physical chemistry applications) there are several different dissipation channels. This situation can be taken into account by generalizing our model (2)–(4) to multiple harmonic baths. Specifically, let us assume that there are several baths with Hamiltonians...
and each of them is coupled through its own pair of OQS and bath operators, $\hat{s}_k$ and $\hat{b}_k$ correspondingly. The resulting joint Hamiltonian is

$$H_{sk} = \int_0^{+\infty} d\omega \left( \hat{a}_k^\dagger(\omega) \hat{a}_k(\omega) + [\hat{a}_k(\omega), \hat{a}_k^\dagger(\omega')] = \delta(\omega - \omega') \delta_{kk'} \right),$$

and each of them is coupled through its own pair of OQS and bath operators, $\hat{s}_k$ and $\hat{b}_k$ correspondingly. The resulting joint Hamiltonian is

$$H = H_t + \sum_{k=1}^L \{ \hat{s}_k \hat{b}_k^\dagger + \hat{s}_k^\dagger \hat{b}_k + H_{sk} \}.$$

Additionally, we suppose that each bath is at its own temperature $T_k$. This model can be straightforwardly treated by the techniques described in previous sections. It is enough to introduce the tensor product of coherent states

$$\langle \zeta_1 \ldots \zeta_L | \otimes \xi_1 \ldots \xi_L |,$$

and then reiterate all the steps of the sections 2–4. As a result, we will obtain the dressed trajectory Hamiltonian

$$\tilde{H}_{\text{dress}}(t) = \tilde{H} + \sum_{k=1}^L \{ \tilde{s}_k (\xi_{\text{track}}(t) + \xi_{\text{th}}^\dagger(k) + \phi_{\text{th}}^\dagger(k) + \tilde{b}_k^\dagger + \tilde{b}_k) + \tilde{s}_k^\dagger \xi_{\text{th}}(t) (t) + (\tilde{s}_k^\dagger - \tilde{\phi}_{\text{th}}(t)) \hat{b}_k + \tilde{H}_{sk} \}.$$ (115)

Here the retarded fields

$$\phi_k(t) = -i \int_{t'}^t dt' M_k(t - t') \tilde{s}_k(t')$$

are defined in terms of the bath memory functions

$$M_k(t - t') = \{ \tilde{b}_k(t), \tilde{b}_k^\dagger(t') \} = \int_0^{+\infty} d\omega |\xi_{\text{th}}(\omega)|^2 \exp(-i\omega(t - t'))$$

and the per-trajectory average $\tilde{s}_k(t)$ of the corresponding coupling operator $\tilde{s}_k$,

$$\tilde{s}_k(t) = \langle b \langle \Psi_{\text{dress}}(z_1(t) \ldots z_L(t), t) | \otimes b \langle \Psi_{\text{dress}}(z_1(t) \ldots z_L(t), t) | \otimes \rangle b \langle \Psi_{\text{dress}}(z_1(t) \ldots z_L(t), t) | \otimes \rangle \rangle_{\text{th}} \rangle_{\text{th}}.$$ (118)

According to the section 2.5, the dressed trajectory is defined as a self-consistently evolving pair of $(z_1(t), \ldots, z_L(t))$ and $|\Psi_{\text{dress}}(z_1(t), \ldots, z_L(t), t)\rangle_{\text{th}}$:

$$\partial_t |\Psi_{\text{dress}}(z_1(t), \ldots, z_L(t), t)\rangle_{\text{th}} = -i \tilde{H}_{\text{dress}}(t) |\Psi_{\text{dress}}(z_1(t), \ldots, z_L(t), t)\rangle_{\text{th}}.$$ (119)

The complex noise of vacuum fluctuations of the $k$th bath is

$$\xi_{\text{track}}(t) = \int_0^{+\infty} d\omega \hat{c}_k^\dagger(\omega) z_k(\omega) e^{i\omega},$$ (120)
where the complex white noises $z_k(\omega)$ are independent for different $k$:

$$
\overline{z_k(\omega) z_q^*(\omega')} = \delta(\omega - \omega') \delta_{kk'}.
$$

The complex noise of thermal fluctuations

$$
\xi_{\text{thk}}(t) = \int_0^{+\infty} d\omega \nu_k(\omega) \sqrt{n_{\text{th}}(\omega, T_k)} v_k(\omega) e^{-i\omega t}
$$

depends on the temperature $T_k$ of the $k$th bath and on additional white noises $v_k(\omega)$:

$$
\nu_k(\omega) v_k^*(\omega') = \delta(\omega - \omega') \delta_{kk'}.
$$

The expected value $\langle \hat{a} \rangle$ of an OQS observable $\hat{a}$ is computed as

$$
\langle \hat{a} \rangle = \frac{\langle \Psi_{\text{dres}}(z_1(t), \ldots, z_L(t), t) | 0 \rangle_b \hat{a} | 0 \rangle \Psi_{\text{dres}}(z_1(t), \ldots, z_L(t), t) \rangle_h}{\| |_b \langle 0 | \Psi_{\text{dres}}(z_1(t), \ldots, z_L(t), t) \rangle_h \|^2} \xi_{\text{thk}}(t). \tag{124}
$$

By performing a direct discretization of the bath frequency range $[0, \omega_{\max}]$, we obtain the extension of the numerical scheme for wavefunctions (section 2.6) to the multiple bath case. At the same time, the generalization of the numerical scheme for delay-time amplitudes of section 3.8 is performed by employing

$$
\hat{H}_{\text{stoch}}(t) = \hat{H}_t + \sum_{k=1}^L \delta_k (\xi_{\text{thk}}(t) + \xi_{\text{vac}}^k(t) + \xi_{\text{thk}}^k(t)) + \sum_{k=1}^L \xi_{\text{thk}}^k(t).
$$

Here, in the discretized delay-time equations (91), (87), (88), the upper subscripts in $\phi_P^{(k_1 \ldots k_L)}$ now enumerate the memory channels of all the baths. The prefactor $(\delta^k - \delta^k(t))$ in (91) and in the last lines of equations (87) and (88) should be changed to $(\delta^k - \delta^k(t))$, where $k$ is the bath to which the channel $l$ belongs in $\phi_P^{(k_1 \ldots k_L)}$.

### 5.2. Example calculation

As an example, let us consider the spin-boson model from section 2.7, without driving ($f(t) \equiv 0$), but coupled to two identical waveguides (55), with $\tilde{s}_1 = \tilde{s}_2 = \tilde{\sigma}$, and at two different temperatures, $T_1 = 2$ and $T_2 = 0.1$. Therefore, the first bath is hot, and the second one is cold. The spin is initially in its ground state. Suppose that the coupling is switched on at time $t = 0$. We have performed the calculations by the numerical scheme for wavefunctions of section 2.6. In figures 5 and 6 we present the time dependence of the current distribution in the hot and cold bath respectively. For the $l$th bath, the current $J_l(t)$ of energy flow from site $j$ to site $j + 1$ is calculated according to the formula

$$
J_l(t) = -\frac{1}{i\hbar} (\tilde{a}_l^\dagger (j + 1) \tilde{a}_l(j) - \tilde{a}_l^\dagger (j) \tilde{a}_l(j + 1)), \tag{126}
$$

where $\tilde{a}_l^\dagger (j)$ and $\tilde{a}_l(j)$ are the creation and annihilation operators for the $j$th site of the $l$th chain. At large times, the current distribution becomes flat. As is required by conservation laws, asymptotically we have

$$
J_2(j) = -J_1(j) = (1.67 \pm 0.01) \times 10^{-2}.
$$

The bath observables where computed using the property of Husimi function that antinormally ordered observables of the bath are averaged as

![Figure 5. Distribution of the current in the hot bath. Negative value means the flow towards the OQS. As the coupling is switched on, the heat energy starts to flow into the OQS (which is coupled to the lattice site 1), and this flow gradually involves increasingly larger parts of the bath. Simulation was done by a finite-temperature two-bath extension of the numerical scheme for wavefunction (section 2.6). Approximation of two virtual quanta ($\eta = 2$) is done.](Image 238x633 to 424x767)

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Now let us take into account the convection interpretation (29) of the Husimi function master equation, and that there are displacements \( D(u) \) due to the classical thermal fluctuations, equation (100). Then, when doing the dressed trajectory simulation, we evaluate the averages according to the formula

\[
\bar{a}(\omega_1) \ldots \bar{a}^\dagger(\omega_m) = \int d[z] z^\pm(\omega_1) e^{-i\omega_1 t} \ldots z(\omega_m) e^{+i\omega_m t} Q(z, t).
\]  

(127)

where \( z(\omega, t) \) are the solutions of the convection equation (29).

6. Conclusion

In this work we propose a novel formulation for the dynamics of open quantum systems in the non-Markovian environment. In the conventional approaches, the quantum field of the bath can develop large occupations of quanta, with correlations of high dimensions. This presents a formidable obstacle both to the description of the non-Markovian physics and to the development of long-time simulation methods. Here we demonstrate that the full quantum field can be divided into two components, of a different physical nature, and each with its own favorable properties. The virtual component is an intrinsically quantum object, but tends to be asymptotically bounded at large times, so that it can be efficiently simulated within a truncated basis. The second component of the quantum field, the observable part, can grow without the bounds with time, but the hierarchy of its correlations has a classical stochastic structure, so that its dynamics can be efficiently simulated by the Monte Carlo methods.

The proposed formulation also helps us to solve another problem of real-time quantum dynamics: that the number of the involved bath modes grows with time. This problem also occurs in two other equivalent forms: (i) that when the bath Hilbert space is truncated, there is always a revival in simulations; (ii) the bath memory function has the long-range tails, and their truncation distorts the large-time behavior of the observables. In the proposed formulation it turns out that the virtual cloud gradually forgets about the retarded behavior of OQS. Important role in this irreversible memory loss mechanism is played by the singularities in the bath spectral density \( J(\omega) \), where \( J(\omega) \) or some of its derivatives change sharply. The virtual cloud remembers the OQS behavior only in the progressively small vicinity of these singular frequencies. We have arranged the numerical scheme which respects this mechanism: it keeps what is remembered, and discards what is forgotten. This way we have solved the problem of the memory tails.

Here it is important to observe that the approximation of truncating the virtual cloud at a finite number of quanta \( n \) is non-perturbative. Rather, it is similar to the so-called \( n \)-crossing approximation (\( n \)CA) in the diagrammatic methods [78], which is known to have superior convergence properties on large times, but hard to implement numerically.
Physical importance of the proposed approach is that it provides a natural solution to the problem of decomposition of the bath state $B$ into the entangled memory part $M$ (the quanta which continue to interact with OQS) and the detector part $D$ (the irreversibly forgotten quanta). This may be useful for the analysis of the various non-Markovian phenomena such as the information and energy backflow; and for the discussion of the various information and entanglement measures in the presence of non-Markovianity. This is also important for the analysis and simulation of transport phenomena, when there is a current through OQS. Without efficient elimination of the detector part $D$ (irreversibly outgoing quanta), the transport problem quickly becomes intractable.

We have demonstrated that the finite temperature bath can be treated in our approach as easily as in the zero temperature case. It is also straightforward to consider the case of the multiple (non-commuting) baths. Here we considered only the case of the RWA-coupling. Our approach is equally applicable to the case of non-RWA coupling (by considering the special case when the OQS coupling operator $\hat s$ is Hermitian).

In this work we have considered only the case of a small OQS-bath coupling, when one or two virtual quanta are enough for the convergence on large times. Our approach can also be applied to the case of stronger coupling. However, the size of virtual cloud is expected to contain a larger number of virtual quanta [48] (but we conjecture it to be still bounded on large times). To handle this case efficiently, a more efficient discretization of the delay-time equations is needed. There is a number of options available, including the use of SVD compression for the tensor operations [50].

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Appendix. Regularization of the channel memory function

The channel decomposition of the waveguide memory function (59) is obtained by employing the identity for the Bessel function

$$J_1(z) = \frac{1}{2} H^{(1)}_1(z) + \frac{1}{2} H^{(2)}_1(z).$$

We obtain:

$$M(\tau) = e^{-i(\alpha_0 - 2\hbar\tau)M_1(\tau)} + e^{-i(\alpha_0 + 2\hbar\tau)M_2(\tau)},$$

where

$$M_1(\tau) = e^{-i2\hbar\tau} \frac{H^{(1)}_1(2\hbar\tau)}{2\hbar\tau},$$

$$M_2(\tau) = e^{+i2\hbar\tau} \frac{H^{(2)}_1(2\hbar\tau)}{2\hbar\tau}.$$

The channel memory functions (131) and (132) have a singularity at zero delay times since

$$\frac{1}{z} H^{(1)}_1(z) \sim -\frac{2i}{\pi} \frac{1}{z^2} + \frac{i}{\pi} \ln(z)$$ (133)

and

$$\frac{1}{z} H^{(2)}_1(z) \sim +\frac{2i}{\pi} \frac{1}{z^2} - \frac{i}{\pi} \ln(z).$$ (134)

However, since the channel memory functions $M_1(\tau)$ and $M_2(\tau)$ are complex conjugated to each other, they are defined up to an arbitrary real function $R(2\hbar\tau)$, equations (60) and (61). The choice of $R(2\hbar\tau)$ is done from the requirement that $M_1(\tau)$ and its first $p$ derivatives are finite at $\tau = 0$. Here $p$ is not smaller than the order of the required polynomial interpolation scheme (see section 3.7). In particular, in this work we have made the choice

$$R(z) = \frac{1}{\pi} \left( \frac{2}{z} - \ln(z) - \ln(2) + \gamma \right) \sum_{k=0}^{\infty} \alpha_k z^{2k} e^{-\hbar z^2}.$$ (135)

Here

$$\alpha_0 = 1, \quad \alpha_1 = \frac{252}{32}, \quad \alpha_2 = \frac{35718}{1152}, \quad \alpha_3 = \frac{17998824}{221184}, \quad \alpha_4 = \frac{7085222460}{44236800}, \ldots$$ (136)

where the series in $\alpha_k$ is truncated after certain $k$; $\gamma$ is the Euler–Mascheroni constant $\gamma = 0.5772156\ldots$.  

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