Heisenberg treatment of multiphoton pulses in non-Markovian waveguide-QED

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The calculation of the non-Markovian dynamics of waveguide-QED systems with coherent time-delayed feedback within the Heisenberg picture gives access to the microscopic dynamics and allows the inclusion of dissipation channels. However, typically a hierarchy of multi-time correlations arises. We propose to unravel these multi-time correlations via a projection onto a complete set of states in the Hilbert space. In particular, we consider a two-level system inside a semi-infinite waveguide subjected to quantum light pulses. Our approach makes it possible to calculate the dynamics in a numerically exact and efficient manner for multiphoton pulses of arbitrary shape with memory requirements known a priori.

I. INTRODUCTION

Quantum networks, in which quantum information is transferred between flying and stationary qubits, form the basis for a plethora of applications in quantum computation and communication [1][4]. In this context, waveguide quantum electrodynamics (WQED) systems are of particular interest as model systems for the interaction of quantum emitters with the electromagnetic field inside a one-dimensional geometry [5][9]. In large-scale quantum networks where the spatial separations are non-negligible in comparison to the wavelength of the light, the information backflow from the environment into the system has to be accounted for and renders the dynamics non-Markovian [10][13]. These delay times can play a constructive role since they allow the control of the system by means of coherent time-delayed feedback where the quantum state itself steers the dynamics and no measurement is necessary so that quantum coherence is preserved [14][23].

Non-Markovian feedback in WQED systems generates strongly entangled system-reservoir states which are intractable with perturbative and master equation methods typically used in the Markovian case [24][27]. Besides the brute force integration of the full Schrödinger equation [17][28], feasible only for very few excitations and short-time dynamics, in recent years, two main schemes have been proposed to deal with such systems: The first one, an optimized Schrödinger equation method, relies on the evaluation of the quantum stochastic Schrödinger equation within the matrix product state framework [29][31]. Here, the dynamics are cast into a time-discrete basis and justified truncations of the Hilbert space enable the efficient handling of the entanglement. This way, the numerically exact method allows for long-time simulations and fast convergence times but is intrinsically limited to unitary evolutions and the exact treatment of additional Hamiltonian-based interactions. Furthermore, as the number of necessary Schmidt values is not known without convergence analysis, the required memory cannot be determined beforehand. The second method is based on the von Neumann equation and exploits a series of cascaded quantum systems to account for the system being driven by its own past [18][32]. This insightful approach is highly expensive memory-wise as it scales with the exponentially growing dimension of the corresponding Liouvillian and, thus, is limited to the study of small systems and short times. Moreover, factorization schemes have not been implemented so far due to the tedious construction of the corresponding Liouvillian. Recently, another approach for studying coherent time-delayed feedback has been proposed that relies on the treatment of the space-discretized waveguide using quantum trajectory simulations [31][33]. Complementing these methods, we present a numerically exact Heisenberg picture method using a time-discrete basis where the memory requirements are known in advance. The approach allows for the inclusion of dissipation and many-particle dynamics as well as approximation methods without the cost of losing exactness in the coherent quantum feedback dynamics.

When treating non-Markovian WQED systems in the Heisenberg picture, the time non-locality usually introduces a hierarchy of multi-time correlations [11]. For the efficient calculation of the dynamics of arbitrary WQED systems excited via quantum pulses and subjected to coherent time-delayed feedback, we propose to unravel the emerging multi-time correlations via the insertion of a Hilbert space unity between the operators with different time arguments. This corresponds to a projection onto a complete set of states in the Hilbert space. In this way, we decompose the multi-time correlations and obtain a closed system of differential equations for single-time correlations.

The paper is structured as follows: After this introduction in Sec. I, we introduce the proposed Heisenberg picture method using the example of a two-level system (TLS) coupled to a semi-infinite waveguide and benchmark the dynamics that can be obtained this way in Sec. II. In Sec. III, we use our approach to study the impact of multiphoton pulses of variable shape as well as the effect of a phenomenological pure dephasing as an exemplary additional dissipation channel. Finally, we conclude in Sec. IV.

II. METHOD

We introduce our approach for the calculation of the exact feedback dynamics in WQED systems within the Heisenberg picture using the fundamental example of a TLS coupled to a semi-infinite one-dimensional waveguide as depicted in Fig. 1a [34][36]. The closed end of the waveguide at the dis-
tance $d$ from the TLS functions as a mirror. It provides feedback at the delay time $\tau = 2d/c$ where $c$ is the speed of light in the waveguide. The quantized treatment of the light field allows modeling the excitation of the TLS through the waveguide via a quantum pulse of temporal shape $f(t)$. In dipole as well as rotating wave approximation, the Hamiltonian describing the system after a transformation into the rotating frame defined by its non-interacting part takes the form \[ H' = \hbar \int \mathrm{d}w g(w) \left( e^{i(\omega - \omega_0)t} r^\dagger \sigma_+ + \text{H.c.} \right). \] (1)

Here, the operator $\sigma_-$ (or $\sigma_+$) is the lowering (raising) operator of the TLS with transition frequency $\omega_0$, $\sigma_+ = \sigma_+^\dagger$. Under the assumption that only a single excitation in the TLS is possible, the commutator of these operators is $[\sigma_-^\dagger, \sigma_+] = 1 - 2\sigma_+ \sigma_-$. The annihilation (creation) of a photon with frequency $\omega$ in the reservoir is described by the bosonic operator $r^{(1)}_\omega$. The interaction between the TLS and the reservoir is quantified by the coupling strength $g(\omega)$ which is, in general, frequency dependent. In particular, the feedback mechanism in our system imposes a boundary condition and results in a sinusoidal frequency dependence of the coupling strength, $g(\omega) = g_0 \sin(\omega \tau/2) \left[ \frac{37}{8} \right]^{34,36}$.

**A. Heisenberg treatment**

Modeling the system dynamics within the Heisenberg picture, we use the Hamiltonian in Eq. (1) to derive differential equations for the time-dependent operators $\sigma_-(t)$ and $r^{(1)}_\omega(t)$ via the Heisenberg equation of motion. The explicit reservoir dynamics can be eliminated by integrating out the reservoir operator $r_\omega(t)$,

$$r_\omega(t) = r_\omega(0) - ig(\omega) \int_0^t \mathrm{d}t' e^{i(\omega - \omega_0)t'} \sigma_-(t').$$ (2)

Thus, the occupation of the reservoir modes is governed by the initial occupation of the reservoir which encodes the pulse driving the emitter as well as by the interaction of the reservoir with the TLS.

The initial occupation of the reservoir is transformed into the time domain via

$$r_i = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}\omega r_\omega(0) e^{-i(\omega - \omega_0)t},$$ (3)

which can be interpreted as an input operator in the context of the input-output theory \left[ \frac{38}{8} \right]. While the operator $r_\omega(0)$ annihilates a photon of frequency $\omega$, the operator $r_i$ as its Fourier transform annihilates a photon at time $t$. This way, for the TLS operator $\sigma_-$ the delay differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \sigma_-(t) = -\Gamma \sigma_- - \sqrt{\Gamma} \left( 1 - 2\sigma_+(t)\sigma_-(t) \right) r_i$$

$$+ \Gamma e^{i\omega t} \left[ \sigma_-(t - \tau) - 2\sigma_+(t)\sigma_-(t - \tau) \right] \Theta(t - \tau)$$ (4)

with the decay rate $\Gamma = \frac{\pi g_0^2}{\hbar}$ and the delayed input operator

$$r_i(t) = r_{i+\frac{\tau}{2}} e^{i\omega \frac{\tau}{2}} - r_{i+\frac{\tau}{2}} e^{-i\omega \frac{\tau}{2}}$$

can be determined. Eq. (4) implies that a photon emitted from the TLS towards the mirror is reflected and interacts with the TLS again after the delay time $\tau$. Thus, for times $t \geq \tau$, feedback effects come into play since the feedback signal interferes with the emission from the TLS where the impact of the feedback depends on the feedback phase $\omega \tau$.

The observable of interest is the occupation of the excited state of the TLS, $\sigma_-^\dagger(t)\sigma_-(t)$, which we will refer to as the TLS occupation in what follows with the corresponding expectation value $\langle \psi | \sigma_-^\dagger(t)\sigma_-(t) | \psi \rangle$. The initial state $|\psi\rangle$ is the combined state of the TLS and the reservoir. For demonstration purposes, we assume a separable pure initial state of the form $|\psi\rangle = |j\rangle \otimes |n\rangle \equiv |j,n\rangle$ which denotes the TLS either in the ground ($j = g$) or the excited state ($j = e$) and $n$ photons in the reservoir, $n \in \mathbb{N}$. Note, however, that our method is not limited to this class of states but is also applicable in the case of entangled and mixed states. The $n$-photon state $|j,n\rangle$ can be obtained from the vacuum state of the reservoir via \left[ \frac{39}{8}, \frac{40}{8} \right].

$$|j,n\rangle = \frac{1}{\sqrt{n!}} \left( a_j^\dagger \right)^n |j,0\rangle, \quad a_j^\dagger = \int \mathrm{d}t f(t) r_i^\dagger.$$ (5)

Here, $a_j^\dagger$ is the creation operator of a photon in the temporal mode defined by a wave packet with normalized pulse shape $f(t)$ satisfying

$$\int \mathrm{d}t |f(t)|^2 = 1$$ (6)
so that the creation of a single excitation via \( \sigma^*_g \) in Eq. (5) is ensured. When calculating the expectation value of the TLS occupation, we have to solve the differential equation

\[
\frac{d}{dt} \langle j, n | \sigma_+ (t) \sigma_- (t) | j, n \rangle = -2 \Gamma \langle j, n | \sigma_+ (t) \sigma_- (t) | j, n \rangle
\]

- \( \sqrt{\Gamma} f(t) \langle j, n - 1 | \sigma_- (t) | j, n \rangle + \text{H.c.} \]

\[
+ \Gamma e^{-i\omega t} \langle j, n | \sigma_+ (t - \tau) \sigma_- (t) | j, n \rangle + \text{H.c.} \Theta(t - \tau)
\]  

with \( f(t) = f(t - \frac{\tau}{2} e^{i\omega t}) - f(t + \frac{\tau}{2} e^{-i\omega t}) \). In Eq. (7), the expectation value of the TLS occupation couples to the single-time matrix element of the TLS operator \( \langle j, n - 1 | \sigma_- (t) | j, n \rangle \) which, in turn, obeys

\[
\frac{d}{dt} \langle j, n - 1 | \sigma_- (t) | j, n \rangle = -\Gamma \langle j, n - 1 | \sigma_- (t) | j, n \rangle
\]

- \( \sqrt{\Gamma} f(t) \langle j, n - 1 | \sigma_+ (t) \sigma_- (t) | j, n - 1 \rangle \]

\[
+ \Gamma e^{-i\omega t} \langle j, n - 1 | \sigma_+ (t - \tau) \sigma_- (t) | j, n \rangle - 2 \langle j, n - 1 | \sigma_+ (t) \sigma_- (t - \tau) | j, n \rangle \Theta(t - \tau).\]  

Before the feedback mechanism sets in, that is, for \( t < \tau \) as built-in by \( \Theta(t - \tau) \), we obtain time-local and, thus, essentially Markovian dynamics. In this case, the dynamics for \( n \) photons in the reservoir initially can be calculated by recursively inserting the results for \( n - 1 \) photons \([41, 42]\). The equations for the contributing matrix elements are given explicitly in Appendix A. For a TLS initially in the ground state and a three-photon pulse in the reservoir, they are exemplarily sketched in Fig. 1b where the abbreviation \([A]_{m, n}^{i, j}\) encodes the matrix element \( \langle i, m | A(t) | j, n \rangle \).

For later times, that is, for \( t \geq \tau \), when the feedback mechanism influences the dynamics, however, the time-delayed terms in Eqs. (7) and (8) become relevant, and the single-time correlations couple to two-time correlations. In general, these two-time correlations couple to three-time correlations and so on. To deal with this hierarchical structure, we unravel the multi-time correlations via the insertion of a unity operator, that is, a projector onto a complete set of states in the Hilbert space, between the operators with different time arguments. In the time basis, this unity operator takes the form

\[
1 = |g⟩⟨g| + |e⟩⟨e|⊗
\]

\[
\{ |0⟩⟨0| + \int dt' |t'⟩⟨t'| + \frac{1}{2} \int dt' \int dt'' |t', t''⟩⟨t', t''| + \ldots \}.
\]  

(9)

The reservoir state \( |t'⟩ \) denotes a single photon in the reservoir created at time \( t' \), \( |t''⟩ = r^*_g |0⟩ \). Here, as in the following, we generally consider all times \( t' \in \mathbb{R} \). The state \( |t', t''⟩ \) refers to two photons in the reservoir, one created at time \( t' \), the other at time \( t'' \), \( |t', t''⟩ = r^*_g r^*_g |0⟩ \), etcetera. The photons are indistinguishable so that \( |t', t''⟩ = |t'', t'⟩ \) and the factor 1/2 (in general 1/\( n! \)) for \( n \) photons in the reservoir is required to ensure normalization. Inserting Eq. (9) between operators at different times in Eq. (8), we avoid the explicit calculation of multi-time correlations with time-ordering in the Heisenberg picture. This way, we shift the problem to the calculation of the matrix elements of single-time Heisenberg operators. Furthermore, we can insert the unity operator between the TLS operators \( \sigma_x \) at the same time to only have to deal with matrix elements of the TLS operator \( \sigma_+ \).

It depends on the number of excitations in the system which elements of the unity operator in Eq. (9) effectively contribute to the dynamics. For simplicity, in what follows, we focus on the case where the TLS is initially in the ground state so that all excitations are in the reservoir. However, the results can be extended to the case of an initially excited TLS straightforwardly. We start with the decomposition of the expectation value of the TLS occupation, that is, of the single-time matrix element

\[
\langle g, n | \sigma_+ (t) \sigma_- (t) | g, n \rangle = \langle g, n | \sigma_+ (t) \sigma_- (t) | g, n \rangle.
\]  

(10)

Here, we find that only matrix elements of the form \( |\psi_{n-1}⟩ |σ_-(t)⟩ |g, n⟩ \) contribute to the dynamics where \( |\psi_{n-1}⟩ \) is a shorthand notation for a state comprising \( n - 1 \) excitations. The state \( |\psi_{n-1}⟩ \) can describe either an excitation in the TLS or \( n - 2 \) excitations in the reservoir or zero excitations in the TLS and \( n - 1 \) excitations in the reservoir. As a consequence, only projectors onto such states \( |\psi_{n-1}⟩ \) have to be taken into account in the unity operator. Subsequently, we use this result to decompose all matrix elements so that we only have to deal with single-time correlations of the TLS operator \( \sigma_+ \).

As in the case without feedback, the results with feedback for \( n \) photons in the reservoir initially can be obtained recursively by using the results for \( n - 1 \) photons in the reservoir. However, to account for the implemented feedback mechanism, further matrix elements have to be evaluated as sketched in Fig. 1c for up to three photons in the reservoir. Correspondingly, we outline the approach, starting with a single photon and progressing to two and three photons in the pulse. Higher excitation numbers can be treated analogously. The explicit equations for the relevant matrix elements are deferred to Appendix B.

In the single-excitation limit, only the projector onto the state \( |g, 0⟩ \) describing the TLS in the ground state and zero photons in the reservoir contributes when inserting the unity operator into the TLS occupation. Consequently, we can decompose the TLS occupation according to

\[
\langle g, 1 | \sigma_+ (t) \sigma_- (t) | g, 1 \rangle = \langle g, 1 | \sigma_+ (t) | g, 0⟩ \langle g, 0 | \sigma_- (t) | g, 1 \rangle
\]  

(11)

(Fig. 1c, red, solid box). The computational resources required for the calculation of the dynamics in the single-excitation case grow linearly with the number of time steps \( T, O(T) \).

With two excitations in the system, the elements in the unity operator describing a single excitation in the system contribute. This excitation can be either in the TLS or in the reservoir so that

\[
\langle g, 2 | \sigma_+ (t) \sigma_- (t) | g, 2 \rangle = \langle g, 2 | \sigma_+ (t) | e, 0⟩ \langle e, 0 | \sigma_- (t) | g, 2 \rangle
\]

\[
+ \int dt' \langle g, 2 | \sigma_+ (t) | g, t'⟩ \langle g, t' | \sigma_- (t) | g, 2 \rangle
\]  

(12)
FIG. 2. (Color online) Benchmark for the dynamics of the TLS occupation in the initial state |g, n⟩ with a rectangular pulse of duration $\Gamma t_D = 2$ (yellow shaded area) containing n photons, $n \in \{1, 2, 3\}$. (a) Benchmark for the decomposition of the TLS occupation without feedback where the expectation value is either directly calculated (solid lines) or decomposed via the insertion of a unity operator (dashed lines). (b) Benchmark of the feedback dynamics for feedback at $\Gamma t = 2$ with feedback phase $\omega_0 = 2\pi m$, $m \in \mathbb{N}$, calculated using the matrix product state framework (solid lines) or within the Heisenberg picture (dashed lines).

If there are three excitations in the system, all states describing two excitations in the system in the unity operator contribute to the dynamics and we can decompose the TLS occupation according to

$$\langle g, 3 | \sigma_+ (t) \sigma_- (t) | g, 3 \rangle = \int dt' \int dt'' \langle g, 3 | \sigma_+ (t) | e, t' \rangle \langle e, t' | \sigma_- (t') | g, 3 \rangle$$

+ $\frac{1}{2} \int dt' \int dt''\int dt''' \langle g, 3 | \sigma_+ (t) | g, t', t'' \rangle \langle g, t', t'' | \sigma_- (t') | g, 3 \rangle$ \hspace{1cm} (13)

(Fig. 1c, turquoise, dotted box). A feature that becomes important if at least three excitations in the system are considered, is the indistinguishability of the photons in the states the unity operator projects onto. For three excitations in the system, the calculation of the dynamics requires computational resources growing with the number of time steps $T$ to the power of six, $O(T^6)$, as indicated in Fig. 1c by the turquoise dotted underlined times.

B. Benchmark

To verify the validity of our approach, we benchmark the dynamics without as well as with feedback. We use the dynamics we obtain before the feedback sets in, $t < \tau$, from the direct calculation of the expectation value of the TLS occupation as given in Appendix A to ensure the validity of the decomposition of the TLS occupation via the insertion of a unity operator. In this regime, the dynamics are essentially Markovian. The dynamics for a TLS excited by a rectangular pulse of duration $\Gamma t_D = 2$ (yellow shaded area) containing up to three photons are presented in Fig. 2a. We see that the results without (solid lines) and with the decomposition of the expectation value via the insertion of a unity operator (dashed lines) coincide perfectly indicating the correctness of the decomposition.

In the next step, we proceed to the non-Markovian regime, that is, we include times $t \geq \tau$ where the feedback mechanism influences the dynamics. In Fig. 2b, the dynamics for a TLS subjected to feedback at delay time $\Gamma \tau = 2$ with feedback phase $\omega_0 = 2\pi m$, $m \in \mathbb{N}$, are presented. The TLS is again excited by a rectangular pulse of duration $\Gamma t_D = 2$ (yellow shaded area) containing up to three photons. We use the matrix product state framework (solid lines) to benchmark the results we obtain with our Heisenberg-operator method (dashed lines) \cite{29, 30, 42}. The agreement of the results obtained with both methods confirms the validity of our approach in the non-Markovian regime.

III. RESULTS

The method we introduced above allows the efficient simulation of multiphoton-pulse dynamics for non-Markovian WQED setups. We illustrate the capabilities of the approach by studying the excitation of an atom-photon bound state for different pulse shapes and system parameters and, furthermore, show that within the Heisenberg formalism a phenomenological pure dephasing rate can be included as an additional dissipation channel.

A. Bound state excitation

We subject the TLS inside the semi-infinite waveguide as shown in Fig. 1a to two-photon pulses of various shapes $f(t)$ and evaluate the steady-state excitation of the emitter $\langle \sigma_+ \sigma_- \rangle_{\text{st.st.,}} \equiv \lim_{t \to \infty} \langle g, 2 | \sigma_+ (t) \sigma_- (t) | g, 2 \rangle$ as a function of the pulse parameters as well as of the feedback delay time $\tau$. Our method is ideally suited for such a parameter study since it allows the exact and efficient calculation of the dynamics as well as the straightforward inclusion of arbitrary pulse shapes. A non-zero occupation of the emitter in the long-time limit despite the radiative decay is possible if an atom-photon bound state is excited. In this case, the emission from the TLS and the feedback signal interfere, and the excitation is partially trapped between emitter and mirror \cite{22, 30, 33, 44}. A prerequisite for the excitation of this bound state in the contin-
FIG. 3. (Color online) Excitation of an atom-photon bound state via a two-photon pulse. (a) Expectation value of the TLS occupation as a function of time (blue line) for a TLS with feedback at $\Gamma \tau = 2$ excited via a two-photon pulse of shape $f(t)$ (red line). From left to right: Rectangular pulse with $\Gamma_D = 2$, Gaussian pulse with $\Gamma \sigma = 1$, exponentially decaying pulse with $\Gamma \tau = 1$. (b) Steady-state excitation of the TLS as a function of the width of the pulse and the feedback delay time, $\tau$. From left to right: Rectangular pulse with duration $\Gamma_D$, Gaussian pulse with width $\sigma$, exponentially decaying pulse with decay rate $\Gamma_{\text{pulse}}$.

The vacuum of propagating modes is a feedback phase $\omega_0 \tau = 2\pi m$, $m \in \mathbb{N}$, which we assume is realized in our system via a suitable emitter-mirror distance. Only multiphoton pulses, that is, pulses containing two or more photons, can excite the atom-photon bound state while an emitter subjected to a single-photon pulse necessarily decays to the ground state in the long-time limit [35]. It is the intrinsic nonlinearity of the TLS that allows the excitation of the bound state via stimulated emission which, however, only comes into play if the emitter is excited with at least two photons. Another possibility to address the atom-photon bound state is by letting an initially excited emitter decay in vacuum [36]. While for this scheme, the steady-state excitation decreases monotonously with the delay time $\tau$, the behavior is more complex in the case of multiphoton pulses.

In Fig. 3 the excitation of an atom-photon bound state is studied for three different pulse shapes: We consider a rectangular pulse with $f(t) = A \Theta(t-t_0) \Theta(t_0+\tau D-t)$ where $A$ is a constant ensuring that the normalization condition $\int dt |f(t)|^2 = 1$ is fulfilled, $t_0$ is the starting point, and $\tau D$ is the duration of the pulse. Furthermore, a Gaussian pulse is applied with $f(t) = A \exp \left[ -|t-\mu|^2/(2\sigma^2) \right]$ where $A$ again is a normalization constant, $\mu$ is the offset of the pulse, and $\sigma$ determines its width. Finally, we subject the system to an exponentially decaying pulse characterized by $f(t) = A \Theta(t-t_0) \exp \left[ -\Gamma_{\text{pulse}}(t-t_0) \right]$ with normalization constant $A$, starting point $t_0$, and decay constant $\Gamma_{\text{pulse}}$. In Fig. 3a, the dynamics of the expectation value of the TLS occupation (blue line) are shown for a TLS subjected to feedback at $\Gamma \tau = 2$ which is excited via a two-photon pulse of shape $f(t)$ (red line) where the considered pulses are a rectangular pulse with $\Gamma_D = 2$, a Gaussian pulse with $\Gamma \sigma = 1$, and an exponentially decaying pulse with $\Gamma_{\text{pulse}}/\Gamma = 1$ (from left to right). For all considered pulse shapes, the TLS is excited and, after a transient time, stabilizes at a non-trivial steady-state excitation which indicates the excitation of an atom-photon bound state. In Fig. 3b, the steady-state excitation of the TLS as a function of time under the influence of pure dephasing at different rates $\gamma$ for feedback at $\Gamma \tau = 1.2$ for a system in the initial state $|\psi\rangle$.

(a) Initially excited emitter decaying in vacuum ($|\psi\rangle = |e,0\rangle$) with feedback phase $\omega_0 \tau = 2\pi m$, $m \in \mathbb{N}$. (b) Emitter initially in the ground state excited via a rectangular two-photon pulse of duration $\Gamma_D = 1$ ($|\psi\rangle = |g,2\rangle$) with feedback phase $\omega_0 \tau = 2\pi m$. (c) Emitter initially in the ground state excited via a rectangular single-photon pulse of duration $\Gamma_D = 1$ ($|\psi\rangle = |g,1\rangle$) with feedback phase $\omega_0 \tau = 2\pi m$. (d) Initially excited emitter decaying in vacuum ($|\psi\rangle = |e,0\rangle$) with feedback phase $\omega_0 \tau = (2m + 1)\pi$. (b) Initially excited emitter decaying in vacuum ($|\psi\rangle = |e,0\rangle$) with feedback phase $\omega_0 \tau = (2m + 1)\pi$.

B. Additional dissipation channel

In realistic WQED systems, a complete isolation of the system of interest from its environment is not possible and typically leads to energy dissipation and loss of quantum coherence. Thus, the dynamics are effectively rendered non-unitary. If the setup is, for example, realized in a solid-state environment where semiconductor quantum dot functions as the emitters, the interaction with the surrounding bulk material has to be taken into consideration [46,52].

As a first proof of principle, we include a phenomenologically pure dephasing at rate $\gamma$ and study its impact on the TLS occupation. Pure dephasing affects coherences while it does not have an immediate influence on populations. Therefore, to model pure dephasing, we treat the coherence operator $\sigma_-$ and the TLS occupation operator $E \equiv \sigma_+ \sigma_-$ separately and introduce pure dephasing in the differential equations for the matrix elements of the coherence operator as an additional Markovian decay channel, see Appendix C. In this model, for
example, the matrix element \( \langle g, 0 | \sigma_-(t) | g, 1 \rangle \) which is relevant in the case of a single-photon pulse in the reservoir initially, obeys the differential equation

\[
\frac{d}{dt} \langle g, 0 | \sigma_-(t) | g, 1 \rangle = - (\Gamma + \gamma) \langle g, 0 | \sigma_-(t) | g, 1 \rangle - \sqrt{\Gamma} f_r(t) + \sqrt{\gamma} e^{i\omega_0 \tau} \langle g, 0 | \sigma_-(t-\tau) | g, 1 \rangle \Theta(t-\tau).
\] (14)

The results for the dynamics of the expectation value of the TLS occupation for different pure dephasing rates \( \gamma \) are shown in Fig. 4. In the setup, feedback at the delay time \( \Gamma \tau = 1.2 \) is implemented and different scenarios are considered. For an initially excited emitter decaying in vacuum, as illustrated in Fig. 4a, pure dephasing does not influence the TLS occupation before the feedback mechanism sets in. Since it only dephases the coherence, its effect emerges for \( t > \tau \) and renders the long-time stabilization of the excitation impossible. In the considered setup, a feedback phase of \( \omega_0 \tau = 2\pi m, m \in \mathbb{N} \), is assumed as a prerequisite for the stabilization. For a dephasing rate \( \gamma \neq 0 \), however, we find a decay of the TLS occupation where it holds that the higher the dephasing rate, the faster the decay.

In the next step, we assume the TLS to be initially in the ground state and excited via a two-photon pulse. The dynamics that can be observed in the case of a rectangular pulse with duration \( \Gamma \tau = 1.2 \) are shown in Fig. 4b. In this case, the dephasing already influences the dynamics before the first feedback round trip is completed and reduces the effectiveness of the excitation of the emitter. The higher the dephasing rate compared to the pulse width, the less effective the excitation becomes. In addition, the atom-photon bound state becomes inaccessible with pure dephasing and the emitter inevitably decays to the ground state. In Fig. 4c, an emitter subjected to a single-photon pulse is considered. Here, a dephasing at higher rates than considered for Figs. 4a and b results in an even more apparent reduction of the excitation effectiveness. Furthermore, we see that the dephasing is not necessarily detrimental at all times. Since it counteracts constructive as well as destructive interference, dephasing can result in an occupation that temporarily exceeds the occupation observed in the case without dephasing.

After concentrating on the case of a feedback phase \( \omega_0 \tau = 2\pi m \) so far, we now look at the impact of pure dephasing for an initially excited TLS degrading in vacuum with feedback at phase \( \omega_0 \tau = (2m + 1)\pi \) as illustrated in Fig. 4d. At this feedback phase, without dephasing, the decay of the TLS occupation is maximally accelerated. With dephasing, we observe that the effect of the feedback is diminished and the dynamics are approaching the exponential Wigner-Weisskopf decay we observe in the absence of feedback.

IV. CONCLUSION AND OUTLOOK

We presented an approach for efficiently calculating the non-Markovian dynamics in WQED systems with feedback in the Heisenberg picture. The hierarchical structure of multi-time correlations which typically arises when treating such systems in the Heisenberg picture can be unraveled via the insertion of a unity operator between the operators with different time arguments. This way, the complexity of the problem is shifted to the calculation of matrix elements of single-time Heisenberg operators. We introduced the method using the example of a TLS inside a semi-infinite waveguide which can be excited via multiphoton pulses. For this setup, we demonstrated that our method is a versatile tool that allows the consideration of arbitrary pulse shapes as well as the inclusion of additional dissipation channels.

We focussed particularly on the atom-photon bound state that exists in the system, and studied the complex interplay of the feedback delay time and the pulse shape which determine the excitation efficiency of the bound state. Furthermore, we showed that the bound state is inaccessible in the presence of Markovian pure dephasing.

In future research, we plan to use the proposed method to study the impact of interactions in the many-body context in more detail.

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APPENDIX A: DYNAMICS WITHOUT FEEDBACK

Before the feedback sets in, that is, for times \( t < \tau \), the dynamics are essentially Markovian and no multi-time correlations arise. The expectation value of the TLS occupation for \( n \) photons in the reservoir initially, \( \langle g, n | \sigma_+(t)\sigma_-(t) | g, n \rangle \), can be calculated from Eq. (14) of the main text recursively using the results for up to \( n-1 \) photons in the reservoir. In this case, the dynamics are governed by

\[
\frac{d}{dt} \langle g, n | \sigma_+(t)\sigma_-(t) | g, n \rangle = - 2\Gamma \langle g, n | \sigma_+(t)\sigma_-(t) | g, n \rangle - \sqrt{n\Gamma} [f_r(t) \langle g, n-1 | \sigma_-(t) | g, n \rangle + H.c.],
\] (A1)

\[
\frac{d}{dt} \langle g, n-1 | \sigma_-(t) | g, n \rangle = - \Gamma \langle g, n-1 | \sigma_-(t) | g, n \rangle - \sqrt{n\Gamma} f_r(t) [1 - 2 \langle g, n-1 | \sigma_+(t)\sigma_-(t) | g, n-1 \rangle].
\] (A2)

APPENDIX B: DYNAMICS UNDER THE INFLUENCE OF FEEDBACK

For larger times \( t \geq \tau \) where the feedback mechanism influences the dynamics, we insert the unity operator given in Eq. (9) of the main text so that we only have to deal with single-time matrix elements of the TLS operator \( \sigma_- \). Here, we present the calculations for one and two photons in the reservoir initially. The extension to three and more photons then works analogously.
Single-photon pulse

For an initial state \(|g, 1\rangle\), only the projector onto the state \(|g, 0\rangle\) describing the TLS in the ground state and no photons in the reservoir contributes when decomposing the expectation value into matrix elements of the TLS operator \(\sigma_−\) and it holds that

\[
(g, 1|\sigma_+(t)\sigma_-(t)|g, 1) = (g, 1|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|g, 1\rangle. \tag{B1}
\]

Thus, the only relevant matrix element is \(|g, 0|\sigma_-(t)|g, 1\rangle\) which can be determined via the differential equation

\[
\frac{d}{dt} (g, 0|\sigma_-(t)|g, 1) = -\Gamma (g, 0|\sigma_-(t)|g, 1) - \sqrt{f(t)} + \Sigma^\text{inh}(t) (g, 0|\sigma_-(t)|g, 1) \Theta(t - \tau). \tag{B2}
\]

Two-photon pulse

In the case of an initial state \(|g, 2\rangle\), the projector onto states describing one excitation in the system, either in the TLS or in the reservoir, contributes to the dynamics and we can decompose the expectation value of the TLS occupation according to

\[
(g, 2|\sigma_+(t)\sigma_-(t)|g, 2) = (g, 2|\sigma_+(t)|e, 0\rangle \langle e, 0|\sigma_-(t)|g, 2\rangle + \int dt' (g, 2|\sigma_+(t)|g, t') \langle g, t'|\sigma_-(t)|g, 2\rangle \tag{B3}
\]

The matrix elements of the TLS operator \(\sigma_−\) describing the transition from two to one excitation in the system that have to be evaluated evolve as

\[
\frac{d}{dt} \langle e, 0|\sigma_-(t)|g, 2\rangle = -\Gamma \langle e, 0|\sigma_-(t)|g, 2\rangle + 2\sqrt{2\Gamma} f(t) \langle e, 0|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|g, 1\rangle + \Sigma^\text{inh}(t) \langle e, 0|\sigma_-(t)|g, 2\rangle
\]

\[
-2 \left[ \langle e, 0|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|e, 0\rangle \langle e, 0|\sigma_-(t)|g, 2\rangle + \int dt_1 \langle e, 0|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|g, t_1\rangle \langle g, t_1|\sigma_-(t)|g, 2\rangle \right] \times \Theta(t - \tau) \tag{B4}
\]

and

\[
\frac{d}{dt} \langle g, t'|\sigma_-(t)|g, 2\rangle = -\Gamma \langle g, t'|\sigma_-(t)|g, 2\rangle - \sqrt{2\Gamma} f(t) \langle g, t'|g, 1\rangle - 2 \langle g, t'|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|g, 1\rangle
\]

\[
+ \Sigma^\text{inh}(t) \left\{ \langle g, t'|\sigma_-(t)|g, 2\rangle - 2 \left[ \langle g, t'|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|e, 0\rangle \langle e, 0|\sigma_-(t)|g, 2\rangle
\]

\[
+ \int dt_1 \langle g, t'|\sigma_+(t)|g, 0\rangle \langle g, 0|\sigma_-(t)|g, t_1\rangle \langle g, t_1|\sigma_-(t)|g, 2\rangle \right] \right\} \Theta(t - \tau) \tag{B5}
\]

APPENDIX C: IMPLEMENTATION OF PURE DEPHASING

Pure dephasing dephases coherences while populations are not directly affected. To be able to account for this fact, not all matrix elements are decomposed into single-time matrix elements of the operator \(\sigma_−\) but are distinguished into the coherence operator \(\sigma_−\) and the TLS occupation operator \(E \equiv \sigma_+\sigma_−\). This way, for the calculation of the dynamics for a TLS initially in the ground state and a single-photon pulse in the reservoir, we have to solve

\[
\frac{d}{dt} \langle g, 1|E(t)|g, 1\rangle = -2\Gamma \langle g, 1|E(t)|g, 1\rangle
\]

\[
- \sqrt{\Gamma [\delta(t) \langle g, 0|\sigma_-(t)|g, 1\rangle]}
\]

\[
+ \Gamma \left[ \epsilon^{-\text{inh}}(t) \langle g, 1|\sigma_+(t)\sigma_-(t)|g, 1\rangle + \text{H.c.} \right] \Theta(t - \tau). \tag{C1}
\]
The insertion of a unity between the operators with different time arguments yields

\[
\frac{d}{dt} \langle g, 1 | E(t) | g, 1 \rangle = -2\Gamma \langle g, 1 | E(t) | g, 1 \rangle - \sqrt{2f_\tau(t)} \langle g, 0 | \sigma_-(t) | g, 1 \rangle + \text{H.c.}
\]

\[
+ \Gamma \left[ e^{-i\omega t} \langle g, 1 | \sigma_+(t - \tau) | g, 0 \rangle \langle g, 0 | \sigma_-(t) | g, 1 \rangle + \text{H.c.} \right] \times \Theta(t - \tau).
\]  

(C2)

The expectation value couples to the matrix element \( \langle g, 0 | \sigma_-(t) | g, 1 \rangle \) for which we add a phenomenological pure dephasing at rate \( \gamma \) so that it obeys

\[
\frac{d}{dt} \langle g, 0 | \sigma_-(t) | g, 1 \rangle = -(\Gamma + \gamma) \langle g, 0 | \sigma_-(t) | g, 1 \rangle - \sqrt{2f_\tau(t)} \langle g, 0 | \sigma_-(t) | g, 1 \rangle
\]

\[
+ \Gamma e^{i\omega t} \langle g, 0 | \sigma_+(t - \tau) | g, 1 \rangle \Theta(t - \tau).
\]  

(C3)

Analogously, for a two-photon pulse in the reservoir, we have to evaluate the expectation value

\[
\frac{d}{dt} \langle g, 2 | E(t) | g, 2 \rangle = -2\Gamma \langle g, 2 | E(t) | g, 2 \rangle - \sqrt{2f_\tau(t)} \langle g, 1 | \sigma_-(t) | g, 2 \rangle + \text{H.c.}
\]

\[
+ \Gamma \left[ e^{-i\omega t} \langle g, 2 | \sigma_+(t - \tau) | e, 0 \rangle \langle e, 0 | \sigma_-(t) | g, 2 \rangle + \int d\tau' \langle g, 2 | \sigma_+(t - \tau) | g, \tau' \rangle \langle g, \tau' | \sigma_-(t) | g, 2 \rangle \right] + \text{H.c.}
\]

\times \Theta(t - \tau).
\]  

(C4)

After the introduction of a phenomenological pure dephasing at rate \( \gamma \), the matrix element \( \langle g, 1 | \sigma_-(t) | g, 2 \rangle \) which couples to the dynamics obeys the differential equation

\[
\frac{d}{dt} \langle g, 1 | \sigma_-(t) | g, 2 \rangle = -(\Gamma + \gamma) \langle g, 1 | \sigma_-(t) | g, 2 \rangle
\]

\[
- \sqrt{2f_\tau(t)} \left[ 1 - 2 \langle g, 1 | E(t) | g, 1 \rangle \right]
\]

\[
+ \Gamma e^{i\omega t} \left[ \langle g, 1 | \sigma_-(t - \tau) | g, 2 \rangle - 2 \langle g, 1 | E(t) | e, 0 \rangle \langle e, 0 | \sigma_-(t) | g, 2 \rangle
\]

\[
- 2 \int d\tau' \langle g, 1 | E(t) | g, \tau' \rangle \langle g, \tau' | \sigma_-(t - \tau) | g, 2 \rangle \right]
\]

\times \Theta(t - \tau).
\]  

(C5)

The remaining elements that contribute to the dynamics can be treated analogously until, eventually, the system of differential equations closes.

The calculation of the dynamics for other initial states such as \( |e, 0\rangle \) describing the TLS initially in the excited state and the reservoir in the vacuum state works analogously. For the differentiation into matrix elements of the operators \( \sigma_- \) and \( E \) the number of matrix elements that have to be determined and saved increases. The asymptotic runtime, however, remains unchanged.

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