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Non-Markovian waiting-time distribution for quantum jumps in open systems

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Simulation methods based on stochastic realizations of state vector evolutions are commonly used tools to solve open quantum system dynamics, both in the Markovian and non-Markovian regimes. Here, we address the question of the waiting time distribution (WTD) of quantum jumps for non-Markovian systems. We generalize Markovian quantum trajectory methods in the sense of deriving an exact analytical WTD for non-Markovian quantum dynamics and show explicitly how to construct this distribution for certain commonly used quantum optical systems.

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I. INTRODUCTION

An open quantum system interacting with its environment undergoes nonunitary evolution and typically loses its quantum properties, such as entanglement, due to decoherence [1]. Whilst the theory of Markovian dynamics in terms of semigroups and completely positive trace preserving maps is fairly well understood since the pioneering work of Lindblad, Gorini, Kossakowski, and Sudarshan [2,3], non-Markovian quantum dynamics displaying memory effects has come under active study during the recent years. The advances here include the development of simulation schemes [4–16], the limits for the existence of physically valid dynamical maps [17], the discussion about the applicability of different types of master equations [18], the very definition and quantification of quantum non-Markovianity [19–21], and the role of initial correlations between the system and its environment [22–27]. Moreover, it is also possible to control and quantify experimentally the non-Markovian features of quantum dynamics [28,29] and the influence of initial system-environment correlations [30,31]. Subsequently, this progress allows one to look for ways how non-Markovian features with memory effects can be exploited for quantum information processing [32], and for quantum control and engineering tasks [33,34].

Here, our focus is on fundamental aspects of non-Markovianity and, in particular, on the jumplike stochastic unravellings, or simulation schemes, for open system dynamics [5,9–14,35,36]. For Markovian systems, some of the most popular stochastic schemes include the Monte Carlo wave function (MCWF) [37,38] and quantum trajectory (QT) [39–41] methods. In both of these methods the time evolution of a single realization consists of periods of continuous deterministic evolution interrupted by stochastic jumps, i.e., both methods simulate a piecewise deterministic stochastic process (PDP). In the MCWF method, the time evolution of a single realization progresses in a stepwise fashion, e.g., during each time step we decide whether the realization evolves deterministically or jumps. The mean time evolution of the ensemble of realizations, over small time increments, matches with the solution of a Markovian master equation for the density matrix (for the first order in time increment). The central concept for the QT methods, in turn, is the waiting time distribution (WTD). The random jump time of the realization can be sampled from the WTD, and the state vector is directly evolved deterministically till this point. The solution to the Markovian master equation is formed from the weighted average over all possible stochastic evolutions that the realizations might take. Generally speaking, the MCWF method exploits the increments of the WTD while the QT uses the full exact form of the WTD.

A few years ago the MCWF was generalized to the non-Markovian region by the Non-Markovian quantum jump method (NMQJ) [13,14,35]. In the NMQJ, the evolution of the ensemble average over a time step δt matches with the solution given by the local in time master equation with possibly temporarily negative rates. The central ingredient of the NMQJ method is a quantum jump which can restore coherence, e.g., by returning the stochastic realization to the superposition which was destroyed earlier. Formally, the probability of the reverse jump can be calculated using the concept of positive definite jump probability density [36]. However, to the best of our knowledge, the QT methods—without using the auxiliary extensions of the state space of an open quantum system—have not yet been extended to the non-Markovian region. The main obstacle here has been the fact that the WTD for non-Markovian systems, when calculated along the Markovian line of reasoning, displays oscillations which render its physical meaning invalid and prevent the technical implementation of the simulations, whilst the mathematical calculation of the WTD still is, in some sense, correct.

With the help of the insight provided by the NMQJ method and the concept of positive definite jump probability density, we derive a general analytical form of the waiting distribution, which is both physically and mathematically correct for non-Markovian quantum dynamics. This is the main result of our paper. We thereby generalize the QT formalism into the non-Markovian regime and show explicitly how to construct the WTD for some commonly used quantum optical systems. It is worth keeping in mind here that, as already featured in the NMQJ method, the stochastic realizations depend on each other as a consequence of the memory effects. Moreover, it has

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been recently argued that non-Markovian unravelings can not be interpreted as stemming from a continuous measurement of the environment [42] despite of some attempts in that direction [43,44]. It seems to us that the functional form of the derived non-Markovian WTD indicates the former choice of answers.

The structure of the paper is the following. In Sec. II we introduce the PDP corresponding to the NMQJ method and most importantly the positive definite jump probability density. In Sec. III, we give the general form of the waiting time distribution and connect it to the PDP defined in Sec. II. In Sec. IV we present some quantum optical examples that illustrate the general construction of the WTD and the effects of non-Markovianity, in Sec. V we present some further discussion about our results, and we conclude in Sec. VI.

II. PIECEWISE DETERMINISTIC PROCESS FOR NON-MARKOVIAN SYSTEM

In this section we formulate the non-Markovian piecewise deterministic process for pure states ψ [13,14,36]. The reduced state of the system, ρ, is obtained as an ensemble average

$$\rho(t) = \mathsf{E}[|\psi\rangle\langle\psi|] = \int d\psi\, P[\psi,t]|\psi\rangle\langle\psi|, \tag{1}$$

where $d\psi = D\psi D\psi^*$ is a singular volume element of the Hilbert space of the system, and $P[\psi,t]$ is the time dependent, phase invariant probability density functional concentrated on the surface of a unit sphere ($||\psi|| = 1$). $\rho(t)$ solves also the following time convolutionless (TCL) master equation [1]

$$\begin{aligned}\dot\rho(t) &= -i\hbar^{-1}[H_S(t),\rho(t)]\\ &\quad + \sum_i \Delta_i(t)\left(C_i\rho(t)C_i^\dagger - \frac{1}{2}\{\rho(t),C_i^\dagger C_i\}\right)\\ &= -i\hbar^{-1}\,[H_S(t),\rho(t)]\\ &\quad + \sum_j \Delta_j^+(t)\left(C_j\rho(t)C_j^\dagger - \frac{1}{2}\{\rho(t),C_j^\dagger C_j\}\right)\\ &\quad - \sum_k \Delta_k^-(t)\left(C_k\rho(t)C_k^\dagger - \frac{1}{2}\{\rho(t),C_k^\dagger C_k\}\right),\end{aligned} \tag{2}$$

where $\Delta_i(t)$ is time dependent decay rate. After the second equality sign, we have split the decay rates into two components $\Delta_j^\pm(t) = [|\Delta_j(t)| \pm \Delta_j(t)]/2$ to account better for the overall sign of the decay rate [14]. However, note that $\Delta_j^\pm(t)$ are non-negative for all times t. From now on we assume that $\hbar = 1$. Operators C_j are called jump operators and we make a simplifying assumption that they are time invariant. Un-normalized states are labeled with $\tilde\psi$ and normalized with ψ. We formulate the process for pure initial states only, since mixedness adds no novelty here.

Between two subsequent jumps at times T and $t = T + \tau$ ($\tau > 0$), pure states evolve deterministically according to an effective non-Hermitian Hamiltonian

$$H_{\rm eff}(t) = H_S(t) - \frac{i}{2}\sum_j \Delta_j(t)C_j^\dagger C_j, \tag{3}$$

such that state $\psi(t)$ is expressed as

$$\psi(t) = \psi(T+\tau) = \frac{\tilde\psi_T(\tau)}{||\tilde\psi_T(\tau)||}, \tag{4}$$

where $\tilde\psi_T(\tau)$ satisfies the Schrödinger equation $\dot{\tilde\psi}_T(\tau) = -iH_{\rm eff}(T+\tau)\tilde\psi_T(\tau)$ with the initial condition $\tilde\psi_T(0) = \psi(T)$.

The discontinuous part of the process consists of jumps between different pure states. Given that the process is in pure state ψ, the conditional jump probability density from a source state ψ to a target state ϕ using a channel k during a time interval $[T,T+\delta t]$ is [36]

$$\begin{aligned}p_k[\phi|\psi,T] &= \delta t\Delta_k^+(T)||C_k\psi(T)||^2\delta\left[\phi(T) - \frac{C_k\psi(T)}{||C_k\psi(T)||}\right]\\ &\quad + \delta t\Delta_k^-(T)\frac{P\,[\phi,T]}{P\,[\psi,T]}||C_k\phi(T)||^2\\ &\quad \times\delta\left(\psi(T) - \frac{C_k\phi(T)}{||C_k\phi(T)||}\right).\end{aligned} \tag{5}$$

Above, δ functional satisfies $\int d\phi\,\delta(\psi-\phi)F[\phi] = F[\psi]$, where F is an arbitrary smooth functional. The δ functionals in Eq. (5) give a temporal channelwise stochastic connection between different regions of projective Hilbert space (the global phase of the states is irrelevant). The connection of the positive part (i.e., part proportional to Δ_k^+) is of one-to-one type: $\psi \to \frac{C_k\psi}{||C_k\psi||}$, which corresponds to Markovian quantum jumps. Interestingly, connection of the negative part is one-to-many type: Each source state ψ may jump to one of the states $\{\phi\}$ that satisfy $\psi = \frac{C_k\phi}{||C_k\phi||}$ provided that the corresponding jump probability is nonzero. It follows that the connection provided by the negative part requires the knowledge of the different states in the pure state decomposition of ρ, since the range of the one-to-many mapping is not obtainable from the structure of Eq. (2). To summarize, a negative channel induces a one-to-many mapping for the pure states, and, therefore, in general, one decay channel connects several different regions of the projective Hilbert space stochastically.

Next we sketch the stepwise progression of the PDP; more details may be found in Refs. [35,36]. During an interval $I = [T+\tau,T+\tau+\delta t]$, a realization of the process in state ψ may either jump or evolve deterministically. The total jump rate away from state ψ during the interval I is the total jump probability to any other state via any channel divided by the length of the interval

$$\Gamma[\psi,T+\tau] = \frac{1}{\delta t}\int d\phi\sum_k p_k[\phi|\psi,T+\tau]. \tag{6}$$

Therefore, with probability $1 - \Gamma[\psi,T+\tau]\delta t$, the realization does not jump away from state ψ but evolves deterministically. Deterministic evolution is governed by the Schrödinger equation and Eq. (3). With probability $\Gamma[\psi,T+\tau]\delta t$, the realization jumps; the target state of the jump is chosen from the probability distribution $\frac{p_k[\phi|\psi,T+\tau]}{\Gamma[\psi,T+\tau]\delta t}$. After the stochastic evolution of the ensemble over a small time step, the average over the ensemble provides us Eq. (2) for the first order in δt.

III. WAITING TIME DISTRIBUTION FOR NON-MARKOVIAN SYSTEM

In this section we derive the general form of the waiting time distribution, which is valid also for non-Markovian systems, starting from the positive definite jump probability density. We also provide a formula for estimating the WTD from a sample of realizations.

A. Analytical WTD

By definition, the waiting time distribution $F(\tau|\psi,T)$ is a conditional probability distribution function which gives the probability for the next jump to occur during a time interval $[T,T+\tau]$ conditioned on that at time T the state of the realization is known to be ψ [1].

The probability for a jump to occur during a short time interval $I=[T+\tau,T+\tau+\delta t]$ away from state ψ is then $\delta F(\tau|\psi,T)\equiv F(\tau+\delta t|\psi,T)-F(\tau|\psi,T)$, which is equal to the probability of having no jumps before $T+\tau$ and a jump during the following δt, i.e., $\delta F(\tau|\psi,T)=[1-F(\tau|\psi,T)]\Gamma[\psi,T+\tau]\delta t$. Dividing both sides by δt and taking the limit $\delta t\to 0$, we obtain the following differential equation that every valid WTD must satisfy [1]:

$$\frac{d}{d\tau}F(\tau|\psi,T)=[1-F(\tau|\psi,T)]\Gamma[\psi,T+\tau]. \tag{7}$$

This can be solved formally with an initial condition $F(0|\psi,T)=0$, such that

$$F(\tau|\psi,T)=1-\exp\left\{-\int_T^{T+\tau}ds\Gamma[\psi,s]\right\}. \tag{8}$$

Then, by using Eqs. (5), (6), and (8) we can obtain the following form for the generic WTD corresponding to Eq. (2):

$$\begin{aligned}F(\tau|\psi,T)=1-\exp\Bigg\{&-\int_T^{T+\tau}ds\int d\phi\\ &\times\sum_k\Bigg(\Delta_k^+(s)||C_k\psi(s)||^2\delta\left[\phi(s)-\frac{C_k\psi(s)}{||C_k\psi(s)||}\right]\\ &+\Delta_k^-(s)\frac{P[\phi,s]}{P[\psi,s]}||C_k\phi(s)||^2\\ &\times\delta\left[\psi(s)-\frac{C_k\phi(s)}{||C_k\phi(s)||}\right]\Bigg)\Bigg\}.\end{aligned} \tag{9}$$

Terms proportional to Δ_k^+ depend only on the state of the particular realization, its deterministic time evolution, and the quantities obtainable from Eq. (2). Terms proportional to Δ_k^- are more complicated, since they depend on the probability functionals and on the deterministic time evolution of other states to which the realization might jump via a channelwise one-to-many mapping.

Random waiting time $\tau^\star$ is sampled from the waiting time distribution by comparing a random number η to the WTD: $\tau^\star(\eta)=\min\{\tau|F(\tau|\psi,T)>\eta\}$ [1]. Probabilities $P[\psi,s]$ appear on the right hand side of Eq. (9), and they are modified each time a jump occurs in the ensemble.

When all decay rates $\Delta_i(t)$ for all times t are non-negative in Eq. (2), the total jump rate away from pure state ψ is $\Gamma[\psi,t]=\sum_k\Delta_k(t)||C_k\psi(t)||^2$. Inserting this into Eq. (9) and taking into account the deterministic evolution of ψ, we obtain the following familiar Markovian limit for the WTD [1,39,40,45]:

$$F(\tau|\psi,T)=\frac{||\tilde{\psi}_T(0)||^2-||\tilde{\psi}_T(\tau)||^2}{||\tilde{\psi}_T(0)||^2}. \tag{10}$$

Details of the derivation of the Markovian limit can be found in the Appendix A.

B. Estimation of WTD

We assume that the reduced state of a non-Markovian open quantum system can be expressed at all times as a linear combination of a finite number of, in general, nonorthogonal pure state projectors. Then we can write Eq. (1) as

$$\rho(t)=\sum_\alpha P_\alpha(t)|\psi^\alpha\rangle\langle\psi^\alpha|. \tag{11}$$

Assume that we have a sample of N_S realizations from the PDP in Sec. II over a time interval $[t_0,t_s]$ divided into N_t time steps. The samples are collected to an $N_t\times N_S$ matrix $\mathbf{M}$ where the element $\mathbf{M}_{i,j}=\beta$ means that a realization j is in state ψ^β at time $t_i=(i-1)\delta t+t_0$. The set of column indices I_i^β of row i of $\mathbf{M}$ give the indices of the realizations which are in state β at time t_i. Hence each set I_i^β has N_S elements, where the kth element is 1 if realization k is in state β at time t_i; otherwise the kth element is 0. $|I_i^\beta|=\sum_{k=1}^{N_S}(I_i^\beta)_k$ is the total number of realizations in state β at time i.

If we know that the realization r is in state α at time t_i, then the discrete sample estimate for the probability to jump away from state α during the discrete time interval $[t_i,t_j]$ is

$$W_r(t_k|t_i,\alpha)=1-\sum_{l=i+1}^{k}\frac{|I_{l-1}^\alpha\cap I_l^\alpha|}{|I_i^\alpha|}. \tag{12}$$

Naturally we have that $W_r(t_i|t_i,\alpha)=0$. The meaning of this equation is that the intersection of two sets consists of the indices of those realizations that were in a state α at the previous time and are still there at the present time. The number of such realizations is divided by the number of the realizations in α at time t_i (beginning of the time interval).

IV. CONSTRUCTION OF WTD FOR QUANTUM OPTICAL SYSTEMS

In this section we construct the waiting time distribution explicitly for a few simple quantum optical systems interacting with a leaky cavity mode. In Fig. 1 we have presented schematically the different systems that we shall study.

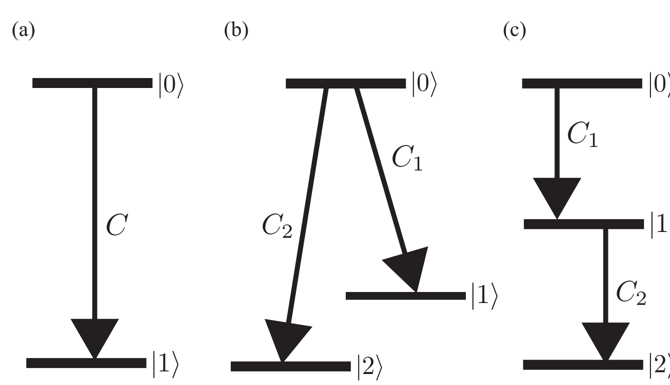

FIG. 1. Schematic figures of the different systems. (a) Two level system, (b) Λ system, and (c) ladder system.

A. Two level system

The orthonormal basis for the Hilbert space of the system is $\{|0\rangle,|1\rangle\}$, where $|1\rangle$ is the ground state and $|0\rangle$ is the excited state of a two level atom (TLA) [see Fig. 1(a)]. The initial state is $\psi^0(t_0) = c_0(t_0)|0\rangle + c_1(t_0)|1\rangle$, which is the only state with nontrivial deterministic evolution. The state of the system is decomposed for all times t as $\rho(t) = P_0(t)|\psi^0\rangle\langle\psi^0| + P_1(t)|\psi^1\rangle\langle\psi^1|$, where ψ^1 is the ground state. The detailed description of the system is given in Appendix (B1).

The non-Hermitian Hamiltonian generating the deterministic pieces of the time evolution is obtained from Eq. (3) (see details in the Appendix (B1)). The total rate away from the deterministic state $\psi^0(t)$ is

$$\Gamma[\psi^0,t] = \begin{cases} \Delta(t)||C\psi^0(t)||^2, & \Delta(t) \geqslant 0, \\ 0, & \Delta(t) < 0, \end{cases} \tag{13}$$

and the total rate away from the state ψ^1 is

$$\Gamma[\psi^1,t] = \begin{cases} 0, & \Delta(t) \geqslant 0, \\ |\Delta(t)|\frac{P_0(t)}{P_1(t)}||C\psi^0(t)||^2, & \Delta(t) < 0. \end{cases} \tag{14}$$

Inserting the rates (13) and (14) as well as the analytical solutions of Appendix (B1) for the probabilities $P_0(t)$ and $P_1(t)$ into Eq. (7), we may solve a formal expression for the WTD. The solution depends on the particular path that one realization might take. For example, the WTD is different for a jump $\psi^0 \to \psi^1$ somewhere in the interval $[T,T+\tau]$ if the realization has made zero or two transitions before time T. We illustrate this in Fig. 2, where we have plotted the decay rate $\Delta(t)$, three sample realizations, and the WTDs for each realization solved from Eq. (7) and also from Eq. (12). The initial state is $\psi^0(0) = |0\rangle$ and we use parameter values $\gamma_0 = 5\lambda$ and $\delta = 8\lambda$ (see Appendix (B1)) and a sample size of 10^5. Points of discontinuity in the waiting time distribution in panel (e) of Fig. 2 correspond to jumps, and since the state of the realization changes, the waiting time distribution also changes. We see that during periods of negative decay rate, the derivative of WTD is zero for realizations that are in state ψ^0, since the jump rate is zero.

This system is the simplest one since it has only one decay channel, and the pure state decomposition of Eq. (11) consists of two states. Jump paths between the different states in the pure state decomposition show that both the positive and the negative channels act as a one-to-one map in the projective Hilbert space of the system.

It is interesting to consider the WTD for a realization, which jumps at some time during the first positive decay rate region and then makes a reverse jump during the first negative region. For the first positive region $[t_0,t_1)$, we obtain

$$F(\tau|\psi^0,t_0) = \frac{\left\|\tilde{\psi}^0_{t_0}(0)\right\|^2 - \left\|\tilde{\psi}^0_{t_0}(\tau)\right\|^2}{\left\|\tilde{\psi}^0_{t_0}(0)\right\|^2}, \tag{15}$$

and for the first negative region $[t_1,t_2)$

$$F(\tau|\psi^1,t_1) = \frac{\left\|\tilde{\psi}^0_{t_0}(t_1+\tau-t_0)\right\|^2 - ||\tilde{\psi}^0_{t_0}(t_1-t_0)\|^2}{1-\left\|\tilde{\psi}^0_{t_0}(t_1-t_0)\right\|^2}. \tag{16}$$

When comparing the WTD of Eq. (15) for the positive jumps to the WTD of Eq. (16) for the negative jumps, we see that they are complementary: in the numerator the norm decrease of the state $\tilde{\psi}^0$ in the positive region is switched to a norm increase in the negative region, and the denominator in the negative region is the complement of the denominator in the positive region.

Equations (15) and (16) provide a simple way of doing a simulation for the TLA. For example, during the kth negative region we could calculate the random waiting time using Eq. (16) with substitution $t_1 \to t_k$, for each realization that is in the ground state. During the kth negative period, realizations that are not in the ground state do not have a possibility to jump. During the kth positive period, we would use Eq. (15) with $t_0 \to t_{k-1}$ for jumps away from the state ψ^0.

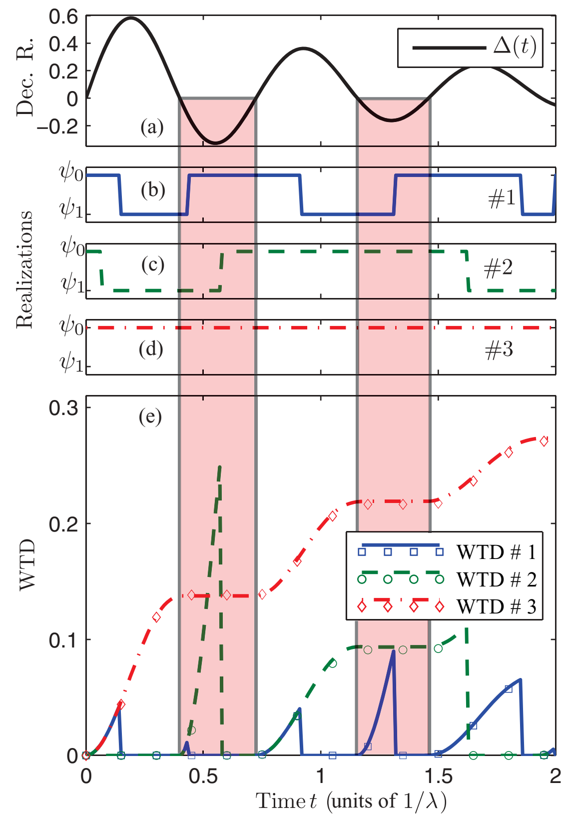

FIG. 2. (Color online) Initial state is $|\psi^0(0)\rangle = |0\rangle$, parameters are $\gamma_0 = 5\lambda$ and $\delta = 8\lambda$, and sample size was 10^5. In panel (a) we have the decay rate, and in (b)–(d) we have three different realizations. In panel (e) we have WTDs for the realizations. Line styles and color coding match with the sample realizations. Lines are for exact numerical solutions and markers for sample estimates.

B. Λ system

Let us indicate the basis for the Hilbert space of the system with $\{|0\rangle,|1\rangle,|2\rangle\}$, where $|1\rangle$ and $|2\rangle$ are the ground states and $|0\rangle$ is the common excited state. A schematic representation of this system is in Fig. 1(b). Initial state is $\psi^0(t_0) = c_0(t_0)|0\rangle + c_1(t_0)|1\rangle + c_2(t_0)|2\rangle$, which is the only state with nontrivial deterministic evolution (see Appendix (B2) for more details).

Deterministic evolution is generated by $H_{\rm eff}(t)$ [see Eq. (3) and Appendix (B2)]. The state of the system $\rho(t)$ can be decomposed for all times t as $\rho(t) = \sum_{k=0}^{2} P_k(t)|\psi^k\rangle\langle\psi^k|$. States $\psi^k \equiv |k\rangle$, with $k = 1,2$, are the ground states of the system. The probabilities appearing in the decomposition are explicitly calculated in the Appendix (B2).

Since we have two decay rates, we have four possible combinations of the decay rate signs. For each pure state of the decomposition, we only present the decay rate sign combinations which lead to a nonzero jump rate away from the state under consideration. Other sign combinations would produce zero rate. The jump rate away from the state ψ^0 is

$$\Gamma[\psi^0,t] = \begin{cases} \sum_i \Delta_i(t)||C_i\psi^0(t)||^2, & \Delta_1,\Delta_2 \geqslant 0, \\ \Delta_i(t)||C_i\psi^0(t)||^2, & \Delta_i \geqslant 0 \wedge \Delta_j < 0. \end{cases} \quad (17)$$

The jump rate away from the ground state ψ^k is

$$\Gamma[\psi^k,t] = |\Delta_k(t)|\frac{P_0(t)}{P_k(t)}||C_k\psi^0(t)||^2, \quad (18)$$

when $\Delta_k(t) < 0$. This is the case irrespective of the sign of the other decay rate.

Both channels, irrespective of the sign of the decay rate, are one-to-one maps. However, when both channels are positive, ψ^0 may be mapped to ψ^1 or ψ^2 when considering the effect of both channels. All rates are proportional to $\|C_k\psi^0(t)\|^2 = |c_0(t)|^2$.

Some realizations are plotted together with their WTD in Fig. 3. The initial state is $\psi^0(0) = |0\rangle$, and we use parameter values $\gamma_0^{(1,2)} = 5\lambda$, $\delta^{(1)} = 4\lambda$, and $\delta^{(2)} = 8\lambda$ (see Appendix (B2)) and a sample size of 10^5. We obtain an interesting expression for the WTD for a reverse jump $\psi^1 \to \psi^0$, if we let $\Delta_1(t) < 0$ during time intervals $[s_1^1,s_2^1]$, $[s_3^1,s_4^1]$, etc. If a jump to the state ψ^1 occurred at time $T \in [t_0,s_1^1]$, then the probability for a jump away from ψ^1 somewhere in the interval $[t_0,T+\tau]$, where $T+\tau \in [s_{2n-1}^1,s_{2n}^1]$, is

$$F(\tau|\psi^1,T) = 1 - \frac{P_1(s_2^1)}{P_1(s_1^1)}\frac{P_1(s_4^1)}{P_1(s_3^1)}\cdots\frac{P_1(T+\tau)}{P_1(s_{2n-1}^1)}. \quad (19)$$

Since $\Delta_1(t) < 0$ when $t \in [s_{2n-1}^1,s_{2n}^1]$, the probabilities $P_1(s_{2n}^1) < P_1(s_{2n-1}^1)$. Therefore, each fraction is smaller than unity and $F(\tau|\psi^1,T)$ is a monotonically increasing function.

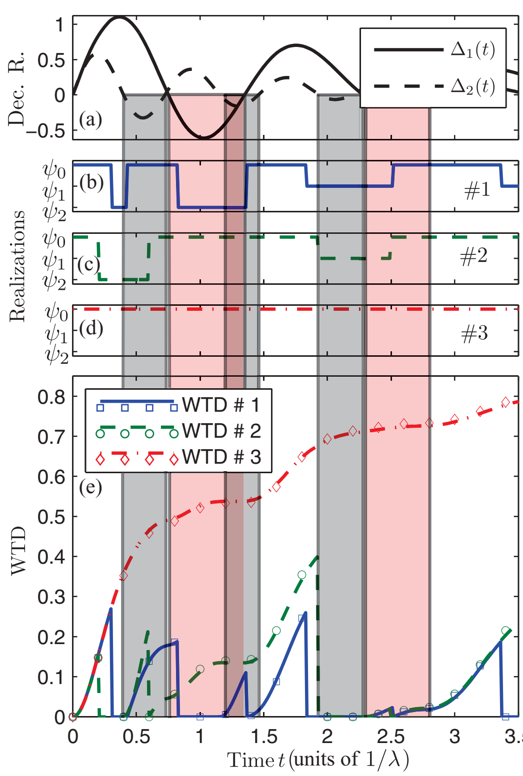

FIG. 3. (Color online) Initial state is $|\psi^0(0)\rangle = |0\rangle$, parameters are $\gamma_0^{(1,2)} = 5\lambda$, $\delta^{(1)} = 4\lambda$, and $\delta^{(2)} = 8\lambda$, and sample size was 10^5. In panel (a) we have the decay rate, and in (b)–(d) we have three different realizations. In panel (e) we have WTDs for the realizations. Line styles and color coding match with the sample realizations. Lines are for exact numerical solutions and markers for sample estimates.

C. Ladder system

We label the orthonormal basis for the Hilbert space of the system with $\{|0\rangle,|1\rangle,|2\rangle\}$, where $|0\rangle$ is the excited state, $|1\rangle$ is the middle state, and $|2\rangle$ is the ground state. A schematic representation of this system is in Fig. 1(c). The initial state is of the form $\psi^0(t_0) = c_0(t_0)|0\rangle + c_1(t_0)|1\rangle + c_2(t_0)|2\rangle$. The deterministic evolution is generated by $H_{\rm eff}(t)$ [see Appendix (B3) and Eq. (3)]. For all times t the state of the system $\rho(t)$ may be decomposed as $\rho(t) = \sum_{k=0}^2 P_k(t)|\psi^k\rangle\langle\psi^k|$, where $\psi^k = |k\rangle$, with $k = 1,2$, are the middle and the ground states, respectively. Analytical expressions for the probabilities $P_i(t)$ are in Appendix (B3). For this system, the only state invariant in respect to $H_{\rm eff}$ is ψ^2 (see Appendix (B3)).

As in Sec. IV B we write down only those combinations of the decay rates that give a nonzero jump rate. For the initial state $\psi^0(t)$, we have

$$\Gamma[\psi^0,t] = \begin{cases} \sum_k \Delta_k(t)||C_k\psi^0(t)||^2, & \Delta_1,\Delta_2 \geqslant 0, \\ \Delta_i(t)||C_i\psi^0(t)||^2, & \Delta_i \geqslant 0 \wedge \Delta_j < 0, \end{cases} \quad (20)$$

and for the middle state $\psi^1(t)$, we have

$$\Gamma[\psi^1,t] = \begin{cases} \Delta_2(t), & \Delta_1,\Delta_2 \geqslant 0, \\ \Delta_2(t) & \\ +|\Delta_1(t)|\frac{P_0(t)}{P_1(t)}\|C_1\psi^0(t)\|^2, & \Delta_2 \geqslant 0 \wedge \Delta_1 < 0, \\ |\Delta_1(t)|\frac{P_0(t)}{P_1(t)}\|C_1\psi^0(t)\|^2, & \Delta_1,\Delta_2 < 0, \end{cases} \quad (21)$$

and for the ground state ψ^2, we have

$$\Gamma[\psi^2,t] = |\Delta_2(t)|\left(\frac{P_0(t)}{P_2(t)}\|C_2\psi^0(t)\|^2 + \frac{P_1(t)}{P_2(t)}\right), \quad (22)$$

when $\Delta_2(t) < 0$ irrespective of the sign of $\Delta_1(t)$.

Channel 1 maps ψ^0 to ψ^1 and channel 2 maps ψ^0 to ψ^2 and ψ^1 to ψ^2. When decay rates are negative, channel 1 maps ψ^1 to ψ^0. However, channel 2 maps ψ^2 to ψ^1 or ψ^0 when negative. Therefore, when a jump to channel 2 occurs when it is negative, we still have a probability distribution over the two different target states from which, we have to choose the actual target state for the jump.

In Fig. 4 we have plotted decay rates and three realizations with their respective WTDs. There, the initial state we use is $\psi^0(0) = |0\rangle$, the parameters are $\gamma_0^{(1,2)} = 5\lambda$, $\delta^{(1)} = 8\lambda$, and $\delta^{(2)} = 4\lambda$ (see Appendix (B3)), and we used a sample size of 10^6.

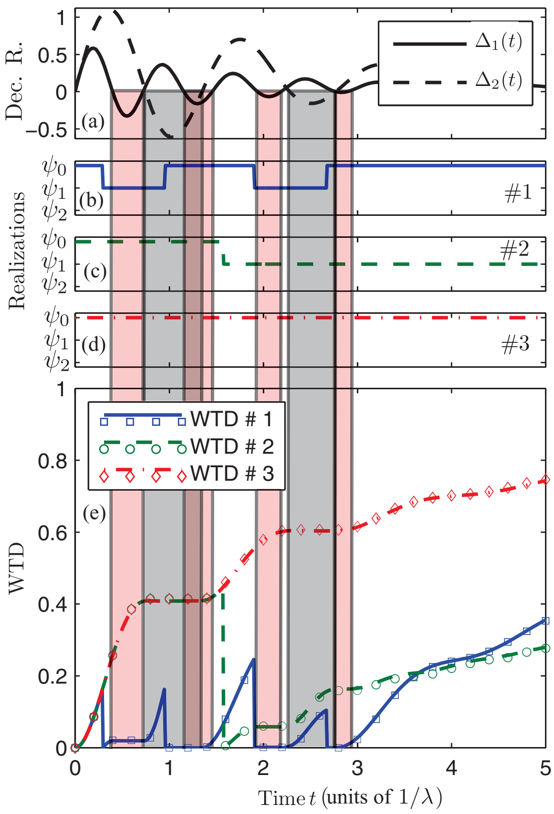

FIG. 4. (Color online) Initial state is $|\psi^0(0)\rangle = |0\rangle$, parameters are $\gamma_0^{(1,2)} = 5\lambda$, $\delta^{(1)} = 8\lambda$, and $\delta^{(2)} = 4\lambda$, and sample size was 10^6. In panel (a) we have the decay rate, and in (b)–(d) we have three different realizations. In panel (e) we have WTDs for the realizations. Line styles and color coding match with the sample realizations. Lines are for exact numerical solutions and markers for sample estimates.

It has been shown in Ref. [35] that for some parameter values the approximations made while obtaining the master equation for this level scheme fail, which is manifested by the breakdown of positivity. This is due to the fact that the population of the ground state ψ^2 is drained completely while the decay rate $\Delta_2(t)$ is still negative. This causes Eq. (22) to diverge. Let us assume that $\Delta_2(t) < 0$ during intervals the $[t_1^2, t_2^2]$, $[t_3^2, t_4^2]$, etc. and that at time $T \in [t_0, t_1^2)$ the realization jumps to state ψ^2. Assuming that $T + \tau \in [t_{2n-1}^2, t_{2n}^2]$, then the analytical form for WTD reads

$$F(\tau|\psi^2, T) = 1 - \frac{P_2(t_2^2)}{P_2(t_1^2)} \frac{P_2(t_4^2)}{P_2(t_3^2)} \cdots \frac{P_2(T+\tau)}{P_2(t_{2n-1}^2)}. \quad (23)$$

From Eq. (23) we see that if $\lim_{t' \to T+\tau} P_2(t') = 0$, the waiting time distribution reaches unity in a finite time but it is still well defined. Dynamical consequences of this are that a simulation method utilizing a full WTD would not break down. Instead, population of the state ψ^2 would go to zero, and the total population is distributed between the pure states ψ^0 and ψ^1.

V. DISCUSSION

The positive definite jump probability density of Eq. (5) shows that there is a correlation between the different regions of the projective Hilbert space. Therefore, a general form of the WTD in Eq. (9) is complicated since it takes the correlation into account cumulatively. On the other hand, it confirms that the realizations of the PDP considered in this paper do not form a trajectory, i.e., a continuous measurement interpretation can not be necessarily made. This happens because it is not possible to express the WTD for a given realization in terms of that particular realization only. This is the argument used already by Gambetta and Wiseman in the context of non-Markovian quantum state diffusion [8], but it can be also applied here. For further discussion on this highly nontrivial topic, we refer the reader to Refs. [42,44,46].

In the case that there is a state ψ^k in the pure state decomposition of $\rho(t)$ that acts only as a source state for jumps for some period $[T, T+\tau]$, then the WTD is quite simple over this period. During this period, the probability of the state ψ^k in the pure state decomposition changes only by jumps away from that state. Hence, we have the following identity $P_k(T+\tau) = P_k(T) - F(\tau|\psi^k, T)P_k(T)$ from which we can solve

$$F(\tau|\psi^k, T) = \frac{P_k(T+\tau) - P_k(T)}{P_k(T)}, \quad (24)$$

where $P_k(T) \neq 0$ is assumed. In the examples that we considered in this work, this happens in the TLA always; in the Λ system always for ground states and for the state ψ^0, when the decay rates have the same signs; and in the ladder system for the ground state always, for the middle state when the decay rates have the opposite signs, and for the state ψ^0 when the decay rates rates have equal signs.

For a short time interval δt we can approximate the full WTD as

$$F(\delta t|\psi, T) \approx \Gamma[\psi(T), T]\delta t = \int d\phi \sum_k p_k[\phi|\psi]. \quad (25)$$

Thus, for a short time interval the total jump rate is resolvable in (channel, target state) pairs: each channel maps a source state to a target state (a one-to-one relation for the Markovian jumps and a one-to-many for the non-Markovian jumps). During this short interval, the occurrence of a jump excludes the possibility of another jump at the same interval to another channel. In WTD-based methods these individual contributions are cumulatively gathered together. The process may be reset after any time interval Δt, after which a new random number must be drawn. In the limit $\Delta t \to \delta t$, a stepwise method emerges.

VI. CONCLUSIONS

We have derived a general waiting time distribution of quantum jumps for open quantum systems following non-Markovian dynamics. In this sense, our results generalize the QT methods into the non-Markovian regime. The distribution is a well defined conditional probability distribution function which takes into account in a proper manner the bidirectional probability flow between different regions of the projective Hilbert space of the system. The WTD includes probabilities which are present in the pure state decomposition of the reduced system state, i.e., the realizations of the process depend on each other—a feature stemming from the memory effects and present already in the NMQJ method. Our results seem to confirm the view that the realizations of the PDP, that the WTD governs, do not form a trajectory; therefore the PDP can not be interpreted in terms of a continuous measurement of the environment. We have constructed the WTD explicitly for some quantum optical systems and also discussed the cases when the calculation of the WTD can be simplified.

Our work complements the theory of Monte Carlo methods for non-Markovian systems, and the WTD concept familiar from the Markovian regime is now also well defined for non-Markovian systems. We hope that this work stimulates further research into non-Markovian dynamics and especially inspires new directions in the development of simulation tools for open quantum systems.

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APPENDIX A: MARKOVIAN LIMIT

In the Markovian limit, decay rates $\Delta_i(t) \geqslant 0$, for all times t. Then, the jump rate away from state ψ at time $T+s$ is

$$\Gamma[\psi,T+s] = \sum_i \Delta_i(T+s)||C_i\psi(T+s)||^2 = \sum_i \Delta_i(T+s)\frac{||C_i\tilde{\psi}_T(s)||^2}{||\tilde{\psi}_T(s)||^2}, \quad \text{(A1)}$$

where we have used the notation of Eq. (4). On the other hand,

$$\frac{d}{ds}\|\tilde{\psi}_T(s)\|^2 = -\sum_i \Delta_i(T+s)\|C_i\tilde{\psi}_T(s)\|^2, \quad \text{(A2)}$$

where we have used the Schrödinger equation and Eq. (3). Therefore, the total jump rate is

$$\Gamma[\psi,T+s] = -\frac{\frac{d}{ds}\|\tilde{\psi}_T(s)\|^2}{\|\tilde{\psi}_T(s)\|^2} = -\frac{d}{ds}\ln\|\tilde{\psi}_T(s)\|^2. \quad \text{(A3)}$$

Now, using Eq. (8) we obtain

$$\begin{aligned} F(\tau|\psi,T) &= 1 - \exp\left\{\int_0^\tau ds\ \ln\|\tilde{\psi}_T(s)\|\right\} \\ &= 1 - \exp\left\{\ln\left(\frac{\|\tilde{\psi}_T(\tau)\|^2}{\|\tilde{\psi}_T(0)\|^2}\right)\right\} \\ &= \frac{\|\tilde{\psi}_T(0)\|^2 - \|\tilde{\psi}_T(\tau)\|^2}{\|\tilde{\psi}_T(0)\|}. \end{aligned} \quad \text{(A4)}$$

APPENDIX B: SYSTEM DEFINITIONS

We are considering two- and three-level atoms interacting with a leaky cavity mode. The spectral density of the cavity is

$$J(\omega) = \frac{1}{2\pi}\frac{\gamma_0\lambda^2}{(\omega-\omega_c)^2+\lambda^2}, \quad \text{(B1)}$$

where γ_0 is the coupling constant, λ is the width of the Lorentzian, and ω_c is the cavity resonance frequency. Another important parameter is the detuning of the atom from the cavity resonance: $\delta = \omega_a - \omega_c$, where ω_a is one of the transition frequencies of the atom.

The time convolutionless master equations for the example systems in Sec. IV are all special cases from the following general form

$$\begin{aligned} \dot{\rho}(t) = &-i\left[\sum_k s_k(t)C_k^\dagger C_k,\rho(t)\right] \\ &+ \sum_k \Delta_k(t)\left(C_k\rho(t)C_k^\dagger - \frac{1}{2}\{\rho(t),C_k^\dagger C_k\}\right), \end{aligned} \quad \text{(B2)}$$

where $s_k(t)$ is the time dependent Lamb shift, $\Delta_k(t)$ are the time dependent decay rates, and C_k are the time independent jump operators. For simplicity, we have assumed in the actual calculations that $s_k(t) = 0$. We use the 4th order time-convolutionless result for the decay rate [1] corresponding to a spectral density of Eq. (B1):

$$\begin{aligned} \Delta(t) = &\frac{\gamma_0\lambda^2}{\lambda^2+\delta^2}\left[1 - e^{-\lambda t}\left(\cos(\delta t) - \frac{\delta}{\lambda}\sin(\delta t)\right)\right] \\ &+ \frac{\gamma_0^2\lambda^5 e^{-\lambda t}}{2(\lambda^2+\delta^2)^3}\left\{\left[1 - 3\left(\frac{\delta}{\lambda}\right)^2\right][e^{\lambda t} - e^{-\lambda t}\cos(2\delta t)]\right. \\ &- 2\left[1 - \left(\frac{\delta}{\lambda}\right)^4\right]\lambda t\cos(\delta t) + 4\left[1 + \left(\frac{\delta}{\lambda}\right)^2\right]\delta t\sin(\delta t) \\ &\left. + \frac{\delta}{\lambda}\left[3 - \left(\frac{\delta}{\lambda}\right)^2\right]e^{-\lambda t}\sin(2\delta t)\right\}. \end{aligned} \quad \text{(B3)}$$

1. Two level system

Master equation:

$$\begin{aligned} \dot{\rho}(t) = &-is(t)[|0\rangle\langle 0|,\rho(t)] + \Delta(t)|1\rangle\langle 0|\rho(t)|0\rangle\langle 1| \\ &- \tfrac{1}{2}\Delta(t)\{\rho(t),|0\rangle\langle 0|\}. \end{aligned} \quad \text{(B4)}$$

Jump operator:

$$C = |1\rangle\langle 0|. \quad \text{(B5)}$$

Solution for the probabilities in the pure state decomposition of Sec. IV A:

$$P_0(t) = \left\|\tilde{\psi}_{t_0}^0(t-t_0)\right\|^2, \quad \text{(B6)}$$

$$P_1(t) = 1 - \left\|\tilde{\psi}_{t_0}^0(t-t_0)\right\|^2. \quad \text{(B7)}$$

2. Λ system

Master equation:

$$\begin{aligned} \dot{\rho}(t) = &-is_1(t)[|0\rangle\langle 0|,\rho(t)] - is_2(t)[|0\rangle\langle 0|,\rho(t)] \\ &+ \Delta_1(t)\big[|1\rangle\langle 0|\rho(t)|0\rangle\langle 1| - \tfrac{1}{2}\{\rho(t),|0\rangle\langle 0|\}\big] \\ &+ \Delta_2(t)\big[|2\rangle\langle 0|\rho(t)|0\rangle\langle 2| - \tfrac{1}{2}\{\rho(t),|0\rangle\langle 0|\}\big]. \end{aligned} \quad \text{(B8)}$$

Jump operators:

$$C_1 = |1\rangle\langle 0|, \quad \text{(B9)}$$

$$C_2 = |2\rangle\langle 0|. \quad \text{(B10)}$$

Solution for the probabilities in the pure state decomposition of Sec. IV B:

$$P_0(t) = ||\tilde{\psi}^0_{t_0}(t-t_0)||^2,$$
$$P_j(t) = \int_{t_0}^{t} ds\, \Delta_j(s)|\tilde{c}_0(s)|^2, \tag{B11}$$

for $j \in \{1,2\}$.

3. Ladder system

Master equation:

$$\dot{\rho}(t) = -is_1(t)[|0\rangle\langle 0|,\rho(t)] - is_2(t)[|1\rangle\langle 1|,\rho(t)] + \Delta_1(t)\big[|1\rangle\langle 0|\rho(t)|0\rangle\langle 1| - \tfrac{1}{2}\{\rho(t),|0\rangle\langle 0|\}\big] + \Delta_2(t)\big[|2\rangle\langle 1|\rho(t)|1\rangle\langle 2| - \tfrac{1}{2}\{\rho(t),|1\rangle\langle 1|\}\big]. \tag{B12}$$

Jump operators:

$$C_1 = |1\rangle\langle 0|, \tag{B13}$$
$$C_2 = |2\rangle\langle 1|. \tag{B14}$$

Solution for the probabilities in pure state decomposition of Sec. IV C:

$$P_0(t) = \left|\left|\tilde{\psi}^0_{t_0}(t-t_0)\right|\right|^2, \tag{B15}$$

$$P_1(t) = e^{-D_2(t)}\int_{t_0}^{t} ds\, \Delta_1(s)e^{-D_1(s)+D_2(s)}||C_1\psi^0(t_0)||^2, \tag{B16}$$

$$P_2(t) = (1-e^{-D_2(t)})||C_2\psi^0(t_0)||^2 + \int_{t_0}^{t} ds\, \Delta_2(s)P_2(s), \tag{B17}$$

where $D_i(t) = \int_{t_0}^{t} ds\, \Delta_i(s)$.

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