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Phenomenological memory-kernel master equations and time-dependent Markovian processes

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Do phenomenological master equations with a memory kernel always describe a non-Markovian quantum dynamics characterized by reverse flow of information? Is the integration over the past states of the system an unmistakable signature of non-Markovianity? We show by a counterexample that this is not always the case. We consider two commonly used phenomenological integro-differential master equations describing the dynamics of a spin 1/2 in a thermal bath. By using a recently introduced measure to quantify non-Markovianity [Breuer *et al.*, Phys. Rev. Lett. **103**, 210401 (2009)] we demonstrate that as far as the equations retain their physical sense, the key feature of non-Markovian behavior does not appear in the considered memory kernel master equations. Namely, there is no reverse flow of information from the environment to the open system. Therefore, the assumption that the integration over a memory kernel always leads to a non-Markovian dynamics turns out to be vulnerable to phenomenological approximations. Instead, the considered phenomenological equations are able to describe time-dependent and unidirectional information flow from the system to the reservoir associated with time-dependent Markovian processes.

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I. INTRODUCTION

The study of non-Markovian open quantum systems has attracted extraordinary attention and efforts in recent years [1]. Many analytical methods and numerical techniques have been developed to treat non-Markovian processes [2–11]. In addition to their importance in addressing fundamental questions [12], this recent attention is mainly due to the applications non-Markovian systems find in many branches of physics. Non-Markovian processes appear in quantum optics [1,13,14], solid state physics [15], quantum chemistry [16], quantum information processing [17], and even in the description of biological systems [18].

Recently, several more rigorous definitions and quantifications of non-Markovian behavior in open quantum systems have been proposed [19–23]. In fact, in the past the concept of non-Markovian dynamics has been quite loosely defined. The term non-Markovian process could, for example, stand for "not describable by a master equation with Lindblad structure," or "leading to nonexponential decay," or "characterized by a time-dependent generator," or "involving an integral over the past states of the system."

Quite often it has been argued that the treatment of non-Markovian dynamics necessarily requires solving an integro-differential equation for the reduced density matrix of the system. However, it has been shown that master equations which are local in time can also represent the memory effects of a non-Markovian process (see, e.g., Ref. [1] and references therein), without the need to take into account a time integration over the past history of the system. Here we take a step forward: Not only do we accept that memory kernel master equations are a nonunique tool to treat non-Markovian dynamics, but we also demonstrate that the presence of a memory kernel alone does not guarantee the non-Markovian character of the process associated with the reverse flow of information from the system to the environment. This surprising result is obtained by applying a recently proposed measure of non-Markovianity [20,21] to two quite commonly used nonlocal master equations: the generalized memory kernel master equation discussed by one of us [7] and the post-Markovian Shabani-Lidar master equation [10], both used to study the time evolution of a spin 1/2 particle in a thermal bath. Our results are connected to the issue of phenomenological versus microscopically derived master equations in quantum optics, which do not always produce coinciding results in all of the relevant parameter regimes [24]. Here we show that there can also be qualitative differences in addition to the quantitative ones when the two approaches are used.

Before proceeding with our treatment we would like to emphasize that we do not intend to discourage the use of memory kernel master equations, which indeed in many cases constitute a fundamental tool to study non-Markovian systems (see, for example, Ref. [6]). Instead, we rather want to point out that the mathematical features of phenomenological kernel equations do not guarantee that the feedback effects from the environment and the physical characteristics of non-Markovian dynamics are taken into account.

We begin by briefly describing the measure for non-Markovianity introduced by three of us in Refs. [20,21]. Then we present the master equations under investigation and their solutions for the density matrix of the reduced system. Finally, we use these solutions to evaluate the degree of non-Markovianity for the two quantum processes, concluding with a discussion and some remarks.

II. MEASURE FOR NON-MARKOVIANITY

The construction of the measure for the degree of non-Markovianity in open systems is based on the definition of Markovian processes as those that continuously reduce the distinguishability of quantum states [20]. One can interpret this loss of distinguishability as a flow of information from the open

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system to its environment. By contrast, in a non-Markovian process there exists a pair of states for which the distinguishability grows for certain times. This growth of the distinguishability of states can be interpreted as a reverse flow of information from the environment to the open system, which is defined to be the essential feature of non-Markovianity [20,21].

An appropriate measure for the distinguishability between two quantum states given by density matrices ρ_1 and ρ_2 is the trace distance [25]

$$D(\rho_1,\rho_2) = \tfrac{1}{2}\mathrm{Tr}|\rho_1 - \rho_2|, \tag{1}$$

where $|A| = \sqrt{A^\dagger A}$. The trace distance represents a metric on the space of physical states. It has the important property that all quantum operations, that is, all completely positive and trace preserving (CPT) maps, are contractions for this metric. Given a pair of initial states $\rho_{1,2}(0)$ the rate of change of the trace distance under the time evolution is defined by

$$\sigma\big(t,\rho_{1,2}(0)\big) = \frac{d}{dt}D\big(\rho_1(t),\rho_2(t)\big). \tag{2}$$

A given process is said to be Markovian if for all pairs of initial states the rate of change of the trace distance is smaller than zero for all times [i.e., $\sigma\big(t,\rho_{1,2}(t)\big) \leqslant 0$]. Thus, a process is defined to be non-Markovian if there exists a pair of initial states $\rho_{1,2}(0)$ and a certain time t at which the trace distance increases [$\sigma\big(t,\rho_{1,2}(t)\big) > 0$]. As shown in Ref. [20,21] one can construct on the basis of this definition a measure for non-Markovianity which represents a functional $\mathcal{N}(\Phi)$ of the corresponding quantum dynamical map Φ. This measure is defined as the maximum over all pairs of initial states of the total increase of the distinguishability during the whole time evolution:

$$\mathcal{N}(\Phi) = \max_{\rho_{1,2}(0)} \int_{\sigma>0} \sigma\big(t,\rho_{1,2}(0)\big)dt. \tag{3}$$

In the following we are going to prove that for the dynamics of a simplified spin-boson model generated by the generalized memory kernel master equation [7] and by the Shabani-Lidar post-Markovian master equation [10] the rate of change of the distinguishability of any pair of states is always negative, implying that the measure of non-Markovianity is equal to zero. Thus, despite the presence of the time integral over the past history, the two master equations do not describe any feedback of information from the environment to the system and are thus memoryless in this sense. However, it is important to note that the treated master equations can describe time-dependent unidirectional flow of information from the system to the environment.

III. MEMORY KERNEL AND POST-MARKOVIAN MASTER EQUATIONS

We first present a paradigmatic example of a phenomenological memory kernel master equation, describing the dynamics of a spin 1/2 particle interacting with a bosonic reservoir at temperature T under the rotating-wave approximation,

$$\frac{d\rho(t)}{dt} = \int_0^t k(t')\mathcal{L}\rho(t-t')dt'. \tag{4}$$

Here, $\rho(t)$ represents the reduced density matrix of the spin, $k(t)$ is a memory kernel function containing information about the properties of the reservoir, and $\mathcal{L}$ is a Markovian superoperator. This superoperator is given by

$$\begin{aligned}\mathcal{L}\rho = {}& \frac{\gamma_0(N+1)}{2}(2\sigma_-\rho\sigma_+ - \sigma_+\sigma_-\rho - \rho\sigma_+\sigma_-)\\ &+ \frac{\gamma_0 N}{2}(2\sigma_+\rho\sigma_- - \sigma_-\sigma_+\rho - \rho\sigma_-\sigma_+),\end{aligned} \tag{5}$$

with γ_0 being the phenomenological dissipation constant, N the mean number of excitations of the reservoir, and $\sigma_\pm$ the usual raising and lowering operators of the spin. We consider a widely used form for the memory kernel function, namely an exponential function

$$k(t) = \gamma e^{-\gamma t}. \tag{6}$$

The memory kernel master equation (4) can be solved by using the method of the damping basis [26]. In Ref. [8] the solution for the components of the Bloch vectors was derived, from which one easily obtains the solution for the spin density matrix $\rho(t)$ corresponding to a generic initial state. By using the basis $\{|0\rangle,|1\rangle\}$ of the eigenstates of σ_z the elements of $\rho(t)$ can be written as

$$\begin{aligned}\rho_{11}(t) &= u(t)\rho_{11}(0) + v(t)\rho_{00}(0),\\ \rho_{00}(t) &= [1-u(t)]\rho_{11}(0) + [1-v(t)]\rho_{00}(0),\\ \rho_{10}(t) &= z(t)\rho_{10}(0),\end{aligned} \tag{7}$$

where $u(t)$, $v(t)$, and $z(t)$ depend on the damping matrix $\Lambda = \mathrm{diag}\{\lambda_1,\lambda_2,\lambda_3\}$ and the translation vector $\overrightarrow{T} = (T_1,T_2,T_3)$ as $u(t) = (1+T_3+\lambda_3)/2$, $v(t) = (1+T_3-\lambda_3)/2$, and $z(t) = \lambda_1$. The damping matrix elements and the translation vector components can in turn be expressed as [7]

$$\begin{aligned}\lambda_1 = \lambda_2 &= \xi_M(R/2,t),\\ \lambda_3 &= \xi_M(R,t),\\ T_1 = T_2 &= 0,\\ T_3 &= \frac{\xi_M(R,t)-1}{2N+1},\end{aligned} \tag{8}$$

where the function $\xi_M(R,t)$ is given by

$$\begin{aligned}\xi_M(R,t) = e^{-\gamma t/2}\Bigg\{&\frac{1}{\sqrt{1-4R}}\sinh\left[\frac{\gamma t}{2}\sqrt{1-4R}\right]\\ &+ \cosh\left[\frac{\gamma t}{2}\sqrt{1-4R}\right]\Bigg\},\end{aligned} \tag{9}$$

with $R = \gamma_0(2N+1)/\gamma$.

An interesting master equation which interpolates between the generalized measurement interpretation of the Kraus operators and the continuous measurement interpretation of the Markovian dynamics is the Shabani-Lidar post-Markovian master equation. The general form of this master equation is [10]

$$\frac{d\rho}{dt} = \mathcal{L}\int_0^t k(t')\exp(\mathcal{L}t')\rho(t-t')dt', \tag{10}$$

where once more $\rho(t)$ is the density matrix of the reduced system, $k(t)$ is the Shabani-Lidar memory kernel, and $\mathcal{L}$ is the Markovian superoperator. In the following $\mathcal{L}$ is taken to be of the form of Eq. (5), and the kernel function is again an exponential function given by Eq. (6). The solution for the density matrix elements of the spin can be written again in the general form of Eq. (7), where $u(t)$, $v(t)$, and $z(t)$ depend in the same way as before on the damping matrix elements and the translation vector components [7]. They in turn have the same analytic expressions of Eqs. (8) with the exception that $\xi_M(R,t)$ has to be replaced by the quantity $\xi_P(R,t)$, which is given by

$$\xi_P(R,t) = \exp\left(-\frac{R+1}{2}\gamma t\right) \times \left\{\frac{1}{\sqrt{1-r(R)}}\sinh\left[\sqrt{1-r(R)}\frac{(R+1)\gamma t}{2}\right] + \cosh\left[\sqrt{1-r(R)}\frac{(R+1)\gamma t}{2}\right]\right\}, \tag{11}$$

with $r(R) = 4R/(R+1)^2$ and $R = \gamma_0(2N+1)/\gamma$.

In Ref. [7] the conditions for the positivity and complete positivity of the dynamical maps associated with the master equations (4) and (10) were studied. There it was found that $4R \leqslant 1$ is a necessary and sufficient condition for the positivity of the dynamical map associated with the memory kernel master equation, while complete positivity is satisfied only for moderate and high temperatures of the reservoir. On the other hand, the dynamical map corresponding to the post-Markovian master equation (10) is always completely positive. These results are in agreement with Ref. [8], where it was noticed that the memory kernel master equation can be derived from the post-Markovian one in the limit in which the phenomenological dissipation constant γ_0 is much smaller than the reservoir correlation decay rate γ, suggesting that the post-Markovian master equation is somehow more fundamental than the former one. Therefore, while for the post-Markovian Shabani-Lidar master equation we can freely investigate the non-Markovianity for the whole range of parameters, in the case of the memory kernel master equation we are restricted to the conditions $4R \leqslant 1$ and $N \gg 1$.

Having constructed the solution of the two master equations we can now determine the rate of change of the distinguishability given by Eq. (2), which leads to

$$\sigma(t,\rho_{1,2}(0)) = \frac{a(t)\frac{d}{dt}a(t) + |b(t)|\frac{d}{dt}|b(t)|}{\sqrt{a^2(t)+|b(t)|^2}}, \tag{12}$$

where $a(t) = \rho_{11}^1(t) - \rho_{11}^2(t)$ and $b(t) = \rho_{10}^1(t) - \rho_{10}^2(t)$ represent the differences of the populations and the coherences of the density matrices $\rho_1(t)$ and $\rho_2(t)$. It is easy to see that these function are equal to $a(t) = \lambda_3(\rho_{11}^1(0) - \rho_{11}^2(0)) = \lambda_3 a_0$ and $b(t) = \lambda_1(\rho_{10}^1(0) - \rho_{10}^2(0)) = \lambda_1 b_0$, with $\lambda_3 = \xi_{M(P)}(R,t)$ and $\lambda_1 = \xi_{M(P)}(R/2,t)$ for the memory kernel and the post-Markovian master equation, respectively. The derivative of the trace distance can thus be written as

$$\sigma(t) = \frac{a_0^2\xi(R,t)\frac{d}{dt}\xi(R,t) + |b_0|^2\xi(R/2,t)\frac{d}{dt}\xi(R/2,t)}{\sqrt{a_0^2\xi(R,t)^2 + |b_0|^2\xi(R/2,t)^2}}, \tag{13}$$

with $\xi(R,t) = \xi_{M(P)}(R,t)$ in the two cases. At this point we need to study the properties of these two functions.

Let us consider first the memory kernel master equation: Under the condition $4R \leqslant 1$, $\xi_M(R,t)$ is a positive, monotonically decreasing function, which means that $\frac{d}{dt}\xi_M(R,t) < 0$ and $\frac{d}{dt}\xi_M(R/2,t) < 0$. Since a_0^2 and $|b_0|^2$ are obviously positive for any pairs of states we thus have $\sigma(t) \leqslant 0$. We conclude that the rate of change of the distinguishability of any pair of initial states always decreases and, hence, the flow of information from the system to the environment is never inverted during the dynamics and non-Markovian effects do not appear. Analogously, also in the case of the post-Markovian master equation, $\xi_P(R,t)$ is a positive, monotonically decreasing function such that $\sigma(t) \leqslant 0$. This implies that also the post-Markovian master equation does not describe any feedback of information from the environment to the open system. In contrast to purely Markovian evolution fulfilling the semigroup property, the dynamics generated by the memory-kernel and the post-Markovian master equations can be classified as time-dependent Markovian processes since they do not fulfill the semigroup property while the information flow is nevertheless unidirectional from the system to the reservoir. This is demonstrated by the time dependence of the decay rates in the corresponding time-local description given in the following.

Indeed, both master equations studied here can be written in the time-convolutionless form

$$\frac{d\rho(t)}{dt} = \frac{\gamma_1(t)}{2}(2\sigma_-\rho\sigma_+ - \sigma_+\sigma_-\rho - \rho\sigma_+\sigma_-) + \frac{\gamma_2(t)}{2}(2\sigma_+\rho\sigma_- - \sigma_-\sigma_+\rho - \rho\sigma_-\sigma_+) + \frac{\gamma_3(t)}{2}(2\sigma_z\rho\sigma_z - \sigma_z\sigma_z\rho - \rho\sigma_z\sigma_z), \tag{14}$$

where

$$\begin{aligned}\gamma_1(t) &= -\frac{N+1}{2N+1}\frac{\frac{d}{dt}\xi(R,t)}{\xi(R,t)},\\ \gamma_2(t) &= -\frac{N}{2N+1}\frac{\frac{d}{dt}\xi(R,t)}{\xi(R,t)},\\ \gamma_3(t) &= \frac{1}{2}\left(\frac{\frac{d}{dt}\xi(R,t)}{2\xi(R,t)} - \frac{\frac{d}{dt}\xi(R/2,t)}{\xi(R/2,t)}\right),\end{aligned} \tag{15}$$

and $\xi(R,t) = \xi_{M(P)}(R,t)$ in the two cases. Thus we see that the integro-differential master equations given by Eqs. (4)–(6) and by Eq. (10) can be transformed into a form which is local in time and does not involve any time integration over a memory kernel.

The decay rate $\gamma_3(t)$ in Eq. (15) is always negative. It follows that the dynamical map Φ corresponding to the master equation is nondivisible [21]. On the other hand, we have just found that the process is Markovian. Thus we have an explicit example of a nondivisible quantum process with zero measure for non-Markovianity, $\mathcal{N}(\Phi) = 0$. The existence of such processes was already conjectured in Ref. [21]. Physically this means that the influence of the decay channel with a negative rate is overcompensated by the effect of the other channels with positive rates, such that the distinguishability of quantum states is still monotonically decreasing. We include these nondivisible processes which have unidirectional information flow into the class of time-dependent Markovian processes. This class also includes processes whose decay rates are time-dependent, positive quantities [21]. We emphasize that the time-dependent unidirectional (time-dependent Markovian) processes and the reversed information flow (non-Markovian) processes have important fundamental differences, as described recently, for example, in Refs. [3,20,21].

Going back to the memory kernel master equation (4), we also notice that the nonappearance of memory effects depends on the restrictions of the range of parameters imposed by the requirement of positivity. In fact, when positivity breaks down for $4R > 1$, the hyperbolic sine and cosine of Eq. (9) are replaced by trigonometric sine and cosine. The function $\xi_M(R,t)$ then shows damped oscillations, its derivative has no definite sign, and, consequently, there can be intervals of time in which the rate of change of the trace distance $\sigma(t)$ becomes positive, implying that non-Markovian effects appear. We mention that a violation of the positivity of the dynamical map in phenomenological master equations was previously studied by Barnett and Stenholm in Ref. [27]. There it was shown that the introduction of an exponential memory kernel function in the dynamics of a damped harmonic oscillator can lead to blatantly nonphysical behavior.

IV. DISCUSSION AND CONCLUSIONS

We have applied a recently developed measure for the degree of non-Markovianity of quantum processes to the dynamical solutions of a simplified spin-boson model given by two widely used integro-differential master equations. It has been demonstrated that, as long as the requirement of the positivity of the associated dynamical maps is fulfilled, no non-Markovian behavior occurs; that is, the measure of non-Markovianity is equal to zero. This means that the phenomenological memory kernel master equations considered here are not able to describe a genuine non-Markovian behavior involving a backflow of information from the environment to the open system.

Recently, the exact memory kernel master equation for a two-state system coupled to a zero-temperature reservoir has been constructed [28], showing that in this case the structure of the master equation given by Eqs. (4) and (5) is incompatible with a nonperturbative treatment of the underlying microscopic system-reservoir model. The perturbation expansion of the exact memory kernel reveals that in higher orders a new decay channel appears in the superoperator (5) which is not present in the standard Born approximation. Thus, while the exact memory kernel master equation describes correctly all non-Markovian features of the model, approximation schemes and phenomenological models can lead to strong restrictions in the treatment of non-Markovianity.

Generally, one might be tempted to think that the introduction of a memory kernel necessarily leads to a dynamics with non-Markovianity and memory effects. However, our results demonstrate that one needs to be cautious when characterizing the physical properties of open systems only through the mathematical structure of their equations of motion. The presence of an integral over the past history in a phenomenological or approximate master equation does not necessarily guarantee a proper description of memory effects, namely, the feedback of information from the environment to the open system. Even though memory kernel master equations certainly provide a very useful tool for the description of non-Markovian quantum processes, our results lead to the following questions: Which of the commonly used phenomenological or approximate memory kernel master equations are able to reproduce the key features of non-Markovianity? Can one formulate general conditions for the structure of the memory kernels which guarantee the presence of these features in the dynamics?

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