Assessing Non-Markovian Quantum Dynamics

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(Received 3 December 2007; revised manuscript received 13 April 2008; published 6 October 2008)

We investigate what a snapshot of a quantum evolution—a quantum channel reflecting open system dynamics—reveals about the underlying continuous time evolution. Remarkably, from such a snapshot, and without imposing additional assumptions, it can be decided whether or not a channel is consistent with a time (in)dependent Markovian evolution, for which we provide computable necessary and sufficient criteria. Based on these, a computable measure of "Markovianity" is introduced. We discuss how the consistency with Markovian dynamics can be checked in quantum process tomography. The results also clarify the geometry of the set of quantum channels with respect to being solutions of time (in)dependent master equations.

DOI: 10.1103/PhysRevLett.101.150402 PACS numbers: 03.65.Yz, 03.65.Ta, 03.67.Hk, 03.67.Mn

Much of the power of information theory, classical and quantum, comes from the separation of information from its physical carriers. This level of abstraction favors a black box approach describing physical processes by their input-output relations in discrete time steps. For quantum systems the most general black box is described by a trace preserving and completely positive map—a quantum channel. This might describe the application of a gate in a quantum processor, a quantum storage device, a communication channel, or any open systems dynamics where one merely has partial access to the relevant degrees of freedom. In any case it can be considered a snapshot of a physical evolution after a certain time.

In the present Letter we investigate what such a snapshot reveals about the intermediate continuous time evolution, in particular, regarding the Markovian and hence memoryless or non-Markovian character of the process. This will link the black box approach to the dynamical theory of open quantum systems. Remarkably, fixing a single point in time enables us to gain nontrivial information about the path along which the system has or has not evolved, even without making additional assumptions about the physics of the environment and its coupling to the system. On the one hand, this analysis thus provides a model-independent means of investigating non-Markovian features. On the other hand, it tells us which type of evolution is required for the continuous realization of theoretically given quantum channels.

Recent experimental progress in the field of quantum information science has shown more and more precise determination of input-output relations via *quantum process tomography*. This has by now been achieved in various systems including NMR [1], ion traps [2], linear optics implementations [3], and solid state qubits [4]. Some of them rely on the *a priori* assumption that the process in fact is Markovian. Non-Markovian effects moved to the center of interest in the study of open quantum systems [5,6] as well as in the context of quantum error correction [7].

Before we start, some remarks concerning the central notions "Markovian" and "time-dependent Markovian" are in order. We will call a quantum channel Markovian if it is an element of any one-parameter continuous completely positive semigroup, i.e., a solution of a master equation with generator in Lindblad form. If the generator depends on time, we use the term time-dependent Markovian instead. In both cases the continuous evolution is memoryless in that at any point in time the future evolution only depends on the present state and not on the history of the system. Our findings are: (i) The sets of (time-dependent) Markovian channels are strictly included within the set of all quantum channels and exhibit a nonconvex geometry. (ii) For arbitrary finite dimensions, there is an efficient algorithm for deciding whether or not a quantum channel is Markovian. (iii) A computable measure is introduced which quantifies the Markovian part of a channel. (iv) For qubits, a simple criterion for time-dependent Markovianity is given together with a detailed analysis of the geometry of the sets of quantum channels. (v) Examples of non-Markovian processes are discussed. (vi) An application for renormalization group (RG) transformations on quantum spin chains is outlined.

Preliminaries.—Throughout we will consider quantum channels on finite dimensional systems, i.e., linear maps $T: \mathcal{M}_d \to \mathcal{M}_d$ on $d \times d$ (density) matrices, $\rho \mapsto T(\rho)$ referred to as *dynamical maps*, reflecting the snapshot in time [8]. When occasionally changing from the Schrödinger to the Heisenberg picture we will denote the respective map by T^*. It will be convenient to consider $\mathcal{M}_d$ as a Hilbert space $\mathfrak{H}$ equipped with the scalar product $\langle A, B\rangle_{\mathfrak{H}} = \mathrm{tr}[A^\dagger B]$. On this space the map T is represented by a matrix $\hat{T}_{\alpha,\beta} = \mathrm{tr}[F_\alpha^\dagger T(F_\beta)] = \langle F_\alpha|T|F_\beta\rangle_{\mathfrak{H}}$, where $\{F_\alpha\}_{\alpha=1,\ldots,d^2}$ is any orthonormal basis in $\mathfrak{H}$. Unless otherwise stated, we will use matrix units $\{|i\rangle\langle j|\}_{i,j=1,\ldots,d}$ as basis elements. Note that a concatenation of two maps T_1, T_2 simply corresponds to a product of the respective matrices $\hat{T}_2\hat{T}_1$ and that a density matrix ρ in this language becomes a vector with entries $\langle i,j|\hat{\rho}\rangle = \langle i|\rho|j\rangle$. A useful operation is the involution $\langle i,j|\hat{T}^\Gamma|k,l\rangle = \langle i,k|\hat{T}|j,l\rangle$ [9,10]. It connects the matrix representation $\hat{T}$ of the map to its Choi matrix $\hat{T}^\Gamma = d(T\otimes \mathrm{id})(\omega)$ where ω is a maximally entangled state $\omega = |\omega\rangle\langle\omega|$, $|\omega\rangle = \sum_{i=1}^d |i,i\rangle/\sqrt{d}$. Complete positivity is then equivalent to $\hat{T}^\Gamma \geq 0$. *Quantum channels* are completely positive and trace preserving maps.

The workhorse in the dynamical theory of open quantum systems are semigroups $\{e^{tL}\}$ depending continuously on one parameter $t \geq 0$ (time) and giving rise to completely positive evolution for all time intervals. Two equivalent standard forms for the respective generators have been derived in Ref. [11]:

$$L(\rho) = i[\rho, H] + \sum_{\alpha,\beta} G_{\alpha,\beta}\Big(F_\alpha \rho F_\beta^\dagger - \frac{1}{2}\{F_\beta^\dagger F_\alpha, \rho\}_+\Big), \quad (1)$$

so $L(\rho) = \phi(\rho) - \kappa\rho - \rho\kappa^\dagger$, where $G \geq 0$, $H = H^\dagger$, ϕ is completely positive and $\phi^*(\mathbb{1}) = \kappa + \kappa^\dagger$. A channel will be called *time (in)dependent Markovian* if it is the solution of any master equation $\dot{\rho} = L(\rho)$ with time (in) dependent Liouvillian in *Lindblad form* (1), i.e., $T = \exp(\int_0^1 dt L_t)$ time ordered.

Deciding Markovianity.—Given a quantum channel T when is it Markovian, i.e., of the form $T = e^L$? *a priori*, this might be a trivial question: as the channel fixes only one point within a continuous evolution, there might always be a "Markovian path" through that point. As the attentive reader might already guess, this turns out to not be the case. One attempt to decide whether T is Markovian could be to start from a Markovian ansatz and then calculate $\inf_L ||T - e^L||$, e.g., by numerical minimization. The major drawback of such an approach is the nonconvex geometry of the set of Markovian channels [12] which inevitably leads to the occurrence of local minima. The following approach circumvents this problem and guarantees to find the correct answer efficiently by first taking the log of T and then deciding whether this is a valid Lindblad generator.

The latter can easily be decided: a map L: $\mathcal{M}_d \to \mathcal{M}_d$ can be written in Lindblad form iff (a) it is Hermitian, (b) $L^*(\mathbb{1}) = 0$ corresponding to the trace preserving property and (c) L is *conditionally completely positive* (ccp) [13], i.e.,

$$\omega_\perp \hat{L}^\Gamma \omega_\perp \geq 0, \quad (2)$$

where $\omega_\perp = \mathbb{1} - \omega$ is the projector onto the orthogonal complement of the maximally entangled state (see Appendix).

Before applying (2) to $\log\hat{T}$ we need to discuss some spectral properties of quantum channels. For simplicity we will restrict ourselves to the generic case where $\hat{T}$ has nondefective and nondegenerate Jordan normal form. Hermiticity of a channel implies that its eigenvalues are either real or come in complex conjugate pairs. The *Jordan normal form*—achievable via a similarity transform—is then

$$\hat{T} = \sum_r \lambda_r P_r + \sum_c \lambda_c P_c + \bar{\lambda}_c \mathbb{F}\bar{P}_c\mathbb{F}, \quad (3)$$

where r labels the real and c the complex eigenvalues, respectively. The P's are orthogonal (but typically not self-adjoint) spectral projectors and $\mathbb{F}$ is the flip-operator ($\mathbb{F}|a\rangle\otimes|b\rangle = |b\rangle\otimes|a\rangle$). Projectors corresponding to complex conjugate eigenvalues are related via $P \leftrightarrow \mathbb{F}\bar{P}\mathbb{F}$ due to Hermiticity of the channel which can in turn be expressed as $\mathbb{F}\hat{T}\mathbb{F} = \bar{\hat{T}}$.

Now T is Markovian iff there is a branch of the logarithm $\log\hat{T}$, defined via the logarithm of the eigenvalues in Eq. (3), which fulfills the above mentioned conditions (a)–(c). Note that (b) is always satisfied if we start from a trace preserving map. Moreover, Hermiticity holds iff there is no negative real eigenvalue and branches for each complex pair of eigenvalues are chosen consistently so that the eigenvalues remain complex conjugates of each other. If $\hat{T}$ has negative eigenvalues, the dynamics will not be Markovian. The set of Hermitian logarithms is then characterized by a set of integers $m_c \in \mathbb{Z}$,

$$\hat{L}_m = \log\hat{T} = \hat{L}_0 + 2\pi i \sum_c m_c(P_c - \mathbb{F}\bar{P}_c\mathbb{F}), \quad (4)$$

where $\hat{L}_0$ denotes the principal branch. The infinity of discrete branches looks a bit awkward at first glance, but the problem can now be cast into a familiar form. Defining the matrices $A_0 = \omega_\perp \hat{L}_0^\Gamma \omega_\perp$, $A_c = 2\pi i \omega_\perp (P_c - \mathbb{F}\bar{P}_c\mathbb{F})^\Gamma \omega_\perp$ and applying Eq. (2) to $\hat{L}_m$ yields that T is Markovian iff

$$A_0 + \sum_c m_c A_c \geq 0 \quad (5)$$

for any set of integers $\{m_c\}$. These matrices A_0, A_c will be Hermitian if $\hat{T}$ has only positive real eigenvalues. Note that the real solutions $m_c \in \mathbb{R}$ of Eq. (5) form a convex set $\mathcal{S} \subseteq \mathbb{R}^C$ (C being the number of complex pairs of eigenvalues). The present problem is then to decide whether $\mathcal{S}$ contains an integer point. Fortunately, this has an efficient solution in terms of a semidefinite integer program. That is, there is an algorithm [14] which either finds a solution or guarantees that none exists within a run time of order ld^2 where l is the number of digits to which the input is specified [15].

In practice it turns out that checking the vicinity of the principle branch ($m_c \in \{-1, 0, 1\}$) is typically sufficient. For qubit channels the problem simplifies further since it becomes (at most) one-dimensional as $C \leq 1$. Hence, one has merely to maximize the smallest eigenvalue (a concave function) of Eq. (5) with respect to real m and then check positivity for the two neighboring integers. This criterion will detect whether the dynamics were consistent with being Markovian.

Measuring Markovianity.—When applying the above criterion to random quantum channels one finds that only a small (but remarkably nonzero) fraction of them are Markovian, see Fig. 1. We will now show how one can otherwise quantify the deviation from Markovianity. Desirable properties of a measure of Markovianity M are (i) some form of normalization, e.g., $M \in [0, 1]$ with $M(T) = 1$ iff T is Markovian, (ii) computability, (iii) continuity, (iv) basis independence, i.e., $M(U^\dagger T U) = M(T)$ for all unitary channels U and (v) an operational or physical interpretation.

One possibility would again be to start from a distance measure $\inf_L \|T - e^L\|$ which, however, looses much of its appeal by the apparent difficulties in computing it. We therefore propose a different approach based on the criterion in Eq. (5). To this end let us regard L_m as Liouvillian of a master equation. If the channel is not Markovian this will not give rise to completely positive, i.e., physical, evolution for all times. However, adding an additional dissipative term might yield a physical Markovian evolution. If we choose isotropic noise of the form $\rho \mapsto e^{-\mu}\rho + (1 - e^{-\mu})\mathbb{1}/d$, $\mu \geq 0$ with corresponding generator $\hat{\mathcal{L}}_\mu = -\mu\omega_\perp$ then $L_m + \mathcal{L}_\mu$ becomes a valid Lindblad generator for some m iff μ exceeds

$$\mu_{\min} = \inf\left\{\mu \geq 0 : \exists m \in \mathbb{Z}^C : A_0 + \sum_c m_c A_c + \frac{\mu}{d}\mathbb{1} \geq 0\right\}.$$

Hence $\mu_{\min}$ is the minimum amount of isotropic noise required to make the channel Markovian. Note that $\mu_{\min}$ can again be calculated by semidefinite integer programming and that it is basis independent in the sense of (iv). In order to meet the normalization condition and to add an intuitive geometric interpretation to the physical one we use $M(T) = \exp[\mu_{\min}(1 - d^2)] \in [0, 1]$ as a *measure for Markovianity.* If A_0 is not Hermitian we assign $M(T) = 0$. This turns out to be precisely the factor by which the additional dissipation shrinks the output space of the channel in order to make it Markovian. In order to see this, note that the volume of the output space (one might think in terms of the Bloch sphere for $d = 2$) is quantified by the determinant of the channel [10]. Moreover, $\det(e^{L_m + \mathcal{L}_{\mu_{\min}}}) = e^{\mathrm{tr}\hat{L}_m} e^{\mathrm{tr}\hat{\mathcal{L}}_{\mu_{\min}}} = \det(T) M(T)$, since $\mathrm{tr}[\hat{L}_m]$ is independent of m. In this sense $M(T)$ quantifies the Markovian part of the channel [16].

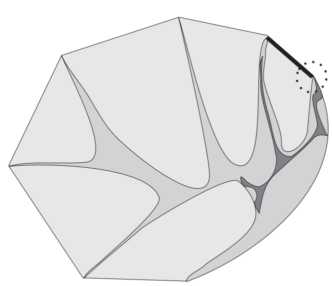

FIG. 1. Schematic depiction of the (12-dimensional) convex set of qubit channels. The (dark gray) subset of Markovian channels is nonconvex and contains 2% of the channels. The larger nonconvex set of time-dependent Markovian channels (17%) contains all extremal channels. All sets, including the measure zero set of indivisible channels (black line), can be found in the neighborhood of the identity (dotted circle).

Discussion.—Figure 2(a) shows the Markovianity of a convex combination $T = pT_1 + (1 - p)T_2$ of a unitary channel T_1 corresponding to $\pi/4$-Rabi oscillation (with Hamiltonian σ_x) and a dephasing process $T_2 = e^L$ with $L(\rho) = \sigma_z \rho \sigma_z - \rho$. This confirms the *nonconvex geometry* in Fig. 1 and shows that non-Markovian effects can arise from an environment which is in a mixture of states each of which leads to a Markovian evolution. Interestingly, there also exist non-Markovian processes that could have arisen from a Markovian process when judged from a snapshot in time: The *spin-star network* in Ref. [5] has the property that for all times $A_0 = \omega_\perp \hat{L}_0^\Gamma \omega_\perp \geq 0$, and hence the channel is consistent with Markovianity. This is perfectly physical, as in each time step there could have been a different memoryless evolution. Figure 2(b) in turn depicts the deviation from Markovianity for the *damped Jaynes-Cummings model*, where the non-Markovian character of the dynamics is clearly displayed [17]. Further examples where this competing effect of time scales can be observed are non-Markovian models arising from spins coupled to *structured baths* with an energy gap as studied, e.g., in Ref. [5].

Time-dependent Markovian channels.—For deciding whether a channel is a solution of a time-dependent master

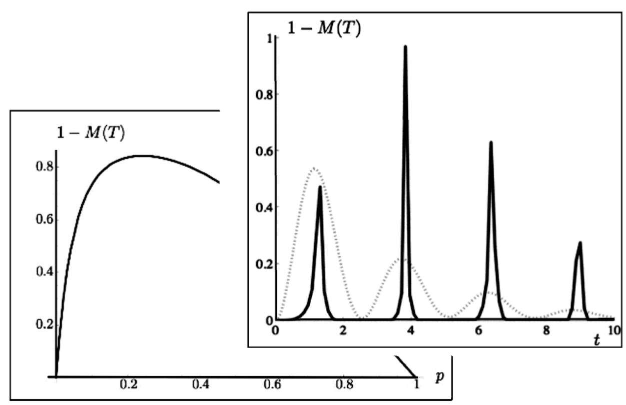

FIG. 2. Deviation from Markovianity. (a) For a mixture of a $\pi/4 - \sigma_x$ rotation ($p = 1$) and a dephasing channel ($p = 0$). (b) For the damped Jaynes-Cummings model (as a function of time), in which a single spin or qubit is coupled to a single cavity mode undergoing lossy dynamics. The field mode serves as an intermediate system preserving correlations that are relevant for the systems's dynamics. The figure shows the interplay between the time scale of truly irreversible cavity losses and apparent decay on the time scale of oscillations, leaving intervals which are consistent with a Markovian process ($\omega = 0.2$, $\gamma = 0.35$, $\alpha_{x,z} = 1/2$, $\alpha_y = 1$). Also shown (dotted line) is the evolution of $\langle 0|\rho|0\rangle$ for initial condition $\langle 1|\rho|1\rangle = 1$.

equation, we resort to generic qubit channels [18] and content ourselves with presenting results whose technical proofs are published elsewhere [10]. A necessary and sufficient criterion is most easily expressed in the basis of Pauli matrices $\{F_\alpha\} = \{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}/\sqrt{2}$. Let $g = \mathrm{diag}(1, -1, -1, -1)$ and s_i be the ordered square roots of the eigenvalues of $\hat{T}g\hat{T}g$. Then T is time-dependent Markovian iff $\det(T) > 0$ and $s_1^2 s_4^2 \geq \prod_i s_i$ [19]. This set contains all extremal qubit channels (Fig. 1), but only 17% of all channels [20]. A paradigmatic example outside this set is $T(\rho) = (\mathrm{tr}[\rho]\mathbb{1} + \rho^T)/3$, which is the best physical approximation to matrix transposition (or time reversal, or—in optics—phase conjugation when rotated by σ_y). This channels fails the criterion since $\det(T) = -1/27$ [10]. In fact, it belongs to the peculiar set of *indivisible channels* that can not be decomposed into a concatenation of two channels unless one of them is unitary.

Summary.—We have introduced a framework to assess whether a given dynamical map describing a physical process could have arisen from Markovian dynamics. To test this property we have provided necessary and sufficient conditions. In fact, these results can readily be applied to fields unrelated at first sight, such as to RG transformations for translationally invariant states on quantum spin chains [21,22]. We also introduced a natural measure of Markovianity, quantifying the Markovian content of a process. As such, we have provided the means to judge the forgetfulness of a process from a snapshot in time.

M. W. thanks G. Giedke and I. de Vega for valuable discussions and the Elitenetzwerk Bayern, the EU (QAP, COMPAS, Scala), the EPSRC, Microsoft Research, and the EURYI for support.

Appendix: Deciding Lindblad form.—Building upon Ref. [13], we can decide whether or not a map L can be written in Lindblad form (1). It is obvious from (1) that L has to be Hermitian ($(L(X))^\dagger = L(X^\dagger)$ for all X), and that $L^*(\mathbb{1}) = 0$. The necessity of Eq. (2) is seen by exploiting Eq. (1): $\hat{L}^\Gamma = [(\phi \otimes \mathrm{id})(\omega) - (\kappa \otimes \mathbb{1})\omega - \omega(\kappa \otimes \mathbb{1})^\dagger]d$. On the right hand side the first term is positive and the other terms vanish when projected onto $\omega_\perp = (\mathbb{1} - \omega)$. Conversely any Hermitian matrix fulfilling (2) is of the form $\hat{L}^\Gamma = P - |\psi\rangle\langle\omega| - |\omega\rangle\langle\psi|$, with $P \geq 0$ and $\psi \in \mathbb{C}^d$. To arrive at Eq. (1) we interpret P as Choi matrix of a completely positive map ϕ and set $(\kappa \otimes \mathbb{1})|\omega\rangle = |\psi\rangle$.

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[15] For small dimensions d, this leads to a practical and efficient algorithm for testing for Markovianity of a quantum channel. Note that the computational hardness in the system's dimension d is not due to any specific algorithm provided here, but in fact due to the nature of the problem as such. For practical purposes, yet, one is typically faced with channels of a given dimension d, and not with a family of channels of increasing d.

[16] This measure is continuous up to a set of measure zero: The logarithm becomes discontinuous at zero so that $M(T)$ can become discontinuous at singular channels. In the degenerate case a second set of discontinuities appears (again of measure zero): if a Markovian channel with pairwise negative eigenvalues is perturbed such that the eigenvalues remain real but the degeneracy is removed.

[17] In the damped Jaynes-Cummings model [Fig. 2(b)], the Hamiltonian is $H = (\alpha_x\sigma_x + \alpha_y\sigma_y + \alpha_z\sigma_z) \otimes \mathbb{1} + \mathbb{1} \otimes a^\dagger a + \Omega(\sigma_+ \otimes a + \mathrm{H.c.})$, with a being the annihilation operator of the field mode, undergoing Markovian damping with a Lindblad generator $D(\rho) = \gamma(a\rho a^\dagger - a^\dagger a\rho/2 - \rho a^\dagger a/2)$, and $\sigma_+ = (\sigma_x + i\sigma_y)/2$ (see, e.g., Ref. [6]). The non-Markovian dynamics is the reduced dynamics of the spin.

[18] They have diagonal normal form; see F. Verstraete, J. Dehaene, and B. DeMoor, Phys. Rev. A **64**, 062302 (2001).

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