Operational Markov Condition for Quantum Processes

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We derive a necessary and sufficient condition for a quantum process to be Markovian which coincides with the classical one in the relevant limit. Our condition unifies all previously known definitions for quantum Markov processes by accounting for all potentially detectable memory effects. We then derive a family of measures of non-Markovianity with clear operational interpretations, such as the size of the memory required to simulate a process or the experimental falsifiability of a Markovian hypothesis.

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In classical probability theory, a stochastic process is the collection of joint probability distributions of a system's state (described by the random variable X) at different times, $\{P(X_k, t_k; X_{k-1}, t_{k-1}; \ldots; X_1, t_1; X_0, t_0) \quad \forall\ k \in \mathbb{N}\}$; to be a valid process, these distributions must additionally satisfy the Kolmogorov consistency conditions [1]. A Markov process is one where the state X_k of the system at any time t_k depends conditionally on only the state of the system at the previous time step and not on the remaining history. That is, the conditional probability distributions satisfy

$$P(X_k, t_k|X_{k-1}, t_{k-1}; \ldots; X_0, t_0) = P(X_k, t_k|X_{k-1}, t_{k-1}) \quad (1)$$

for all k. This simple-looking condition has profound implications, leading to a massively simplified description of the stochastic process. The study of such processes forms an entire branch of mathematics, and the evolution of physical systems is frequently approximated to be Markov (when it is not exactly so). This is in part due to the fact that the properties of Markov processes make them easier to manipulate analytically and computationally [2].

Implicit in this description of a classical process is the assumption that the value of X_j at a given time can be observed without affecting the subsequent evolution. This assumption cannot be valid for quantum processes. In quantum theory, a measurement must be performed to infer the state of a system. And the measurement process, in general, *must* disturb that state. Therefore, unlike its classical counterpart, a generic quantum stochastic process cannot be described without interfering with it [3]. These complications make it challenging to define the process independently of the control operations of the experimenter. From a technical perspective, a serious consequence of this is that joint probability distributions of quantum observables at different times do not satisfy the Kolmogorov conditions [1] and do not constitute stochastic processes in the classical sense.

Nevertheless, temporal correlations between observables do play an important role in the dynamics of many open quantum systems, e.g., in the emission spectra of quantum dots [5] and in the vibrational motion of interacting molecular fluids [6]. Quantifying memory effects, and clearly defining the boundary between Markovian and non-Markovian quantum processes, represents an important challenge in describing such systems.

Attempts at solving this problem tend to take a *necessary*, but not sufficient, condition for a classical process to satisfy Eq. (1) and extend it to the quantum domain. This has led to a zoo of quantum Markov definitions, and accompanying "measures" of non-Markovianity [7,8], that do not coincide with Eq. (1) in the classical case [9]. Examples include measures based on the monotonicity of trace-distance distinguishability [10], the divisibility of dynamics [11,12], how quantum Fisher information changes [13], the detection of initial correlations [14–20], changes to quantum correlations or coherence [21,22], channel capacities and information flow [23–26], and positivity of quantum maps [27–30].

All these methods offer valid ways to witness memory effects. Unfortunately, however, they often lack a clear operational basis. Moreover, different measures of non-Markovianity agree neither on the degree of non-Markovianity of a given process nor even on whether it is Markovian [31]. Put another way, they each fail to quantify demonstrable memory effects in some cases. These inconsistencies have led some to the conclusion that there can be no unique condition for a quantum Markov process.

In this Letter, we use the process tensor framework, introduced in an accompanying article [32], to demonstrate that this conclusion is false. We first present a robust operational definition for a quantum Markov process, which unifies all previous definitions and, most importantly, reduces to Eq. (1) for classical processes. We then go on

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to derive a family of measures for non-Markovianity which quantify *all* detectable memory effects and which have a clear operational interpretation.

Quantum stochastic processes.—Conventional approaches to open quantum dynamics describe a process solely in terms a system's time-evolving density matrix ρ_t, which is related to the initial state of the system by a completely positive trace-preserving (CPTP) map $\Lambda_{t:0}$. However, as has also been argued in the classical case [33], a framework that captures non-Markovian effects cannot be a simple extension of one which characterizes memoryless processes. In order to describe the joint probability distributions of multiple measurement outcomes, and hence capture memory effects which appear only in multitime correlation functions, we must go beyond the paradigm of CPTP maps [34].

We consider a scenario where the role of the observer in a stochastic process is made explicit: A series of control operations $\mathcal{A}_j^{(r)}$ act on the system at times t_j (here, r labels one of a set of operations that could have been realized, with some probability, at that time). These can correspond to measurements, unitary transformations, interactions with an ancilla, or anything in between and are represented mathematically by completely positive (*CP*) maps. As implied above, their action need not be deterministic (for example, in the case of different measurement outcomes), but the average control operation applied at a given point corresponds to a deterministic CPTP map $\mathcal{A}_j = \sum_r \mathcal{A}_j^{(r)}$. The choice of CPTP map and its decomposition into operations $\mathcal{A}_j^{(r)}$ is often referred to as an *instrument*, and the latter can equivalently be thought of as a decomposition of $\mathcal{A}_j$ into Kraus operators. The entire sequence of control operations at times $\{t_0, t_1, \ldots, t_{k-1}\}$ may, furthermore, be correlated, and we denote it by $\mathbf{A}_{k-1:0}$ (which is an element of the tensor product of spaces of control operations at each step). When the operations are uncorrelated, this can simply be thought of as the sequence $\mathbf{A}_{k-1:0} = \{\mathcal{A}_{k-1}^{(r_{k-1})}; \ldots; \mathcal{A}_1^{(r_1)}, \mathcal{A}_0^{(r_0)}\}$.

In an accompanying article [32], we describe how a process can be fully characterized by a linear and *CP* mapping $\mathcal{T}_{k:0}$, called the process tensor, which takes a sequence of operations to the density operator at a later time: $\rho_k = \mathcal{T}_{k:0}[\mathbf{A}_{k-1:0}]$. $\mathcal{T}_{k:0}$ encodes all uncontrollable properties of the process, including any interactions of the system with its environment, as well as their (possibly correlated) average initial state. When the control operations are nondeterministic, ρ_k is subnormalized, with a trace that gives the joint probability of applying those operations. Any given process tensor is guaranteed to be consistent with unitary dynamics of the system with a suitable environment. If the process tensor, defined on any set of time steps in an interval, and the control operations all act in a fixed basis, then the description reduces to that of a classical stochastic process as described in the introduction. Interestingly, quantum stochastic processes have been defined in a mathematically related way several times in the past [39–41], without being widely adopted by the open quantum systems community.

Our description, in terms of the process tensor, fully contains the conventional one; doing nothing to the system, represented by the identity map $\mathcal{I}$, is a perfectly valid control operation, and, for a system initially uncorrelated with its environment, $\mathcal{T}_{k:0}[\mathcal{I}^{\otimes k}] = \Lambda_{k:0}[\rho_0]$. The main achievement of the process tensor framework is to separate "the process," as dictated by nature, from an experimenter's control operations. In other words, the process tensor describes everything that is independent of the choices of the experimenter. Using this framework, we are now in a position to present our main result.

Criterion for a quantum Markov process.—To clearly and operationally formulate a quantum Markov condition, we introduce the idea of a *causal break*, where the system's state is actively reset, dividing its evolution into two causally disconnected segments. We then test for conditional dependence of the future dynamics on the past control operations. If the future process depends on the past controls, then we must conclude that the process carries memory and it is non-Markovian.

To formalize this notion, we begin by explicitly denoting the state of the system at time step l as a function of previous control operations: $\rho_l = \rho_l(\mathbf{A}_{l-1:0})$. Now, suppose at time step $k < l$ we make a measurement (of our choice) on the system and observe outcome r, which occurs with probability $p_k^{(r)}$; the corresponding positive operator is denoted $\Pi_k^{(r)}$. We then reprepare the system into a known state $P_k^{(s)}$, chosen randomly from some set $\{P_k^{(s)}\}$. The measurement and the repreparation at k break the causal link between the past $j \leq k$ and the future $l > k$ of the system; more generally, any operation whose output is independent of its input constitutes a causal break. If we let the system evolve to time step l, its state will depend on the choice and the outcome of the measurement at k, the preparation P_k, and the control operations from 0 to $k-1$. Therefore, we have a conditional subnormalized state $\tilde{\rho}_l = p_r \rho_l(P_k^{(s)}|\Pi_k^{(r)}; \mathbf{A}_{k-2:0})$, where the conditioning argument is the choice of past measurement $\Pi_k^{(r)}$ and controls $\{\mathbf{A}_{k-1:0}\}$. The probability p_r, which also, in general, depends on $\{\mathbf{A}_{k-1:0}\}$, is not relevant to whether the process is Markovian or not; we are interested only in whether the normalized state $\rho_l = \rho_l(P_k^{(s)}|\Pi_k^{(r)}; \mathbf{A}_{k-1:0})$ depends on its conditioning argument. This operationally well-defined conditional state is fully consistent with conditional classical probability distributions. However, it is very different from the quantum conditional states defined in Ref. [42].

Because of the causal break, the system itself cannot carry any information beyond step k about $\Pi_k^{(r)}$ or its earlier

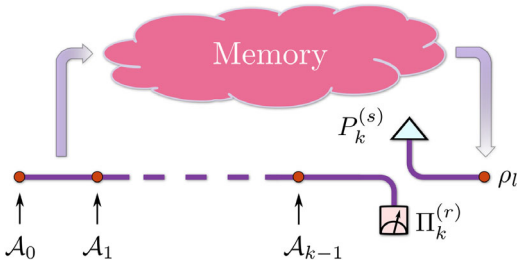

FIG. 1. Determining whether a quantum process is Markovian. Generalized operations $\mathbf{A}_{k:0}$ are made on the system during a quantum process, where the subscripts represent the time. At time step k, we make a causal break by measuring the system with $\Pi_k^{(r)}$ and repreparing it in randomly chosen state $P_k^{(s)}$. The process is said to be Markovian if and only if $\rho_l(P_k|\Pi_k^{(r)};\mathbf{A}_{k-1:0}) = \rho_l(P_k^{(s)})$ at all time steps l, k, for all inputs $P_k^{(s)}$, measurements $\{\Pi_k^{(r)}\}$, and control operations $\{\mathbf{A}_{k-1:0}\}$.

history. The only way ρ_l could depend on the controls is if the information from the past is carried across the causal break via some external environment (see Supplemental Material [43] for some examples). We have depicted this in Fig. 1, with the memory as a cloud that transmits information from the past to the future across the causal break. This immediately results in the following operational criterion for a Markov process.

Definition.—A quantum process is Markovian when the state of the system ρ_l, after a causal break at time step k (with $l > k$), depends only on the input state $P_k^{(s)}: \rho_l(P_k^{(s)}|\Pi_k^{(r)};\mathbf{A}_{k-1:0}) = \rho_l(P_k^{(s)}), \forall \{P_k^{(s)}, \Pi_k^{(r)}, \mathbf{A}_{k-1:0}\}$ and $\forall\ l, k \in [0, K]$.

Note that this definition is directly analogous to the *causal Markov condition* for a discrete-time classical stochastic evolution that allows for interventions [4]: While the definition in Eq. (1) refers only to the system state at different times, more modern descriptions of (classical) stochastic processes in terms of their causal structure allow for interventions between time steps. Recently, and independently of this work, a generalization of this kind of "Markovian causal modeling" has been developed for quantum Markov processes [45].

From the definition, we have the following theorem.

Theorem.—A quantum process is non-Markovian iff there exist at least two different choices of controls $\{\Pi_k^{(r)}; \mathbf{A}_{k-1;0}\}$ and $\{\Pi_k^{\prime(r')}; \mathbf{A}'_{k-1;0}\}$, such that after a causal break at time step k, the conditional states of the system at time step l are different:

$$\rho_l(P_k^{(s)}|\Pi_k^{(r)};\mathbf{A}_{k-1;0}) \neq \rho_l(P_k^{(s)}|\Pi_k^{\prime(r')};\mathbf{A}'_{k-1;0}). \quad (2)$$

Conversely, if ρ_l is constant for all linearly independent controls, then the process is Markovian.

The proof, which relies on the linearity of the process tensor, is given in Sec. A of Supplemental Material [43]. Identifying two controls that lead to different conditional states may, in pathological cases, require testing Eq. (2) for all possible (exponentially many) linearly independent control operations, though the discovery of any pair of control sequences that lead to an inequality in Eq. (2) is a witness for non-Markovianity; this is directly analogous to the problem of testing for correlations in a many-body state. The implication of the theorem is that it is possible to determine whether a process is Markovian in a finite number of experiments.

Our theorem also has the appealing consequence that quantum Markov processes give rise to classical ones.

Corollary.—Fixing a choice of instruments always leads to a classical probability distribution satisfying Eq. (1) iff the quantum process is Markovian according the definition provided above.

Proof.—Fixing a choice of instruments means allowing only one of a set of operations $\mathcal{A}_j^{(r)}$ to act at each time step, such that $\sum_r \mathcal{A}_j^{(r)}$ is a CPTP map (the instrument may be different at different time steps). As such, the trace of the state at time k is the probability distribution $P(r_{k-1}, t_{k-1}; \ldots; r_1, t_1; r_0, t_0) = \mathrm{tr}\rho_k(\mathcal{A}_{k-1}^{(r_{k-1})}, \ldots, \mathcal{A}_1^{(r_1)}, \mathcal{A}_0^{(r_0)})$, where the r_j can be treated as classical random variables. For a Markov process, we have that $\rho_j(\mathcal{A}_{j-1}^{(r_{j-1})}, P_{j-2}^{(s)}|\Pi_{j-2}^{(r_{j-2})}, \mathbf{A}_{j-3:0}) = \rho_j(\mathcal{A}_{j-1}^{(r_{j-1})}, P_{j-2}^{(s)}|\Pi_{j-2}^{(r_{j-2})}) = \rho_j(\mathcal{A}_{j-1}^{(r_{j-1})}|P_{j-2}^{(s)}, \Pi_{j-2}^{(s')})$ for any deterministic choice of preparation $P_{j-2}^{(s)}$. By writing $\mathcal{A}_{j-2}^{(r_{j-2})} = \sum_{ss'} c_{ss'}^{(r_{j-2})} P_{j-2}^{(s)} \otimes \Pi_{j-2}^{(s')}$ [46], it follows that $P(r_{j-1}, t_{j-1}|\ldots; r_1, t_1; r_0, t_0) = P(r_{j-1}, t_{j-1}|r_{j-2}, t_{j-2})\ \forall\ k > j > 0$. From our theorem, if the process is non-Markovian, then there is at least some pair of control operations for which the inequality in Eq. (2) is true. By choosing an instrument which acts with these operations, one realizes a classical process with $P(r_{j-1}, t_{j-1}|r_{j-2}, t_{j-2}, \ldots; r_0, t_0) \neq P(r_{j-1}, t_{j-1}|r_{j-2}, t_{j-2})$ for some values of $\{r_j\}$. ∎

This remedies an important issue with existing definitions of quantum Markov processes, namely, that they fail to classify classical stochastic processes correctly [7]. Instead, as discussed above, conventional approaches are based on necessary, but not sufficient, conditions for a classical process to be Markov. The above corollary demonstrates that our definition corresponds to a necessary and sufficient condition. Of course, those necessary conditions are still satisfied by Markov processes in our framework. In particular, we have the following lemma.

Lemma.—Markov processes are K divisible; i.e., they can be written as a sequence of CPTP maps between the K time steps on which they are defined.

Proof.—If the condition introduced in our definition is satisfied, then ρ_k depends only on the previous choice of input $P_{k-1}^{(s)}$ for any k. By choosing from a complete set of linearly independent inputs $\{P_j^{(\nu_j)}\}$, quantum process

tomography can be performed independently for each pair of adjacent time steps. Since the dynamics between any two time steps is free from the past (there is no conditioning on prior operations), the resulting set of CPTP maps completely describes the dynamics. These maps can then be composed to calculate the dynamics between any two time steps. In other words, the dynamics between time steps $l > k > j$ is described by maps $\Lambda_{k:j}$, $\Lambda_{l:k}$, and $\Lambda_{l:j}$, with the last map being the composition of the former two: $\Lambda_{l:j} = \Lambda_{l:k} \circ \Lambda_{k:j}$. ∎

This means our result verifies the well-known hypothesis that Markovian dynamics is divisible. However, the converse of this statement does not hold, contrary to what is often postulated [7]. That is, $\Lambda_{l:j} = \Lambda_{l:k} \circ \Lambda_{k:j}\ \forall\ l > k > j \in [0, K]$ does not imply that the process is Markovian according to our main theorem. In principle, there could be multitime correlations between time steps that affect future dynamics *conditioned* on past operations. In this light, the theorem we present here can be seen as both a unification and a generalization of previous theories of quantum non-Markovianity, since all of these require non-Markovian processes to be indivisible. This direct consequence of the above lemma is encapsulated in the following remark.

Remark.—Any process labeled non-Markovian according to the definitions given in Refs. [10–30] will be non-Markovian according to our main theorem. The converse does not hold.

In fact, because it contains information about the density operator as a function of time, the process tensor formalism could be used to explicitly calculate any of the measures of non-Markovianity introduced in the above references. In Sec. B of Supplemental Material [43], we give several examples of non-Markovian effects which are not detected by conventional approaches but which are detected in our framework. The first manifests the discussion below the above lemma, demonstrating that divisible (even *CP*-divisible) dynamics can have memory. We also show how the trace-distance definition of Markov processes can fail to characterize non-Markovianity and that a quantum process can be non-Markovian even when there are no system-environment quantum correlations.

It is worth noting that all open quantum evolutions generated by a time-independent system-environment Hamiltonian are non-Markovian according to our main theorem, when considering more than two time steps. A similar point was also made in Ref. [47], albeit in the context of dynamical decoupling. The strictness of the operational Markov definition, however, does not render the notion of non-Markovianity meaningless; on the contrary, it allows us to construct meaningful measures of non-Markovianity.

Quantifying non-Markovianity.—One of the key features of the process tensor formalism is the isomorphism between a process $\mathcal{T}_{k:0}$ and a many-body generalized Choi state $\Upsilon_{k:0}$. The correlations between subsystems in $\Upsilon_{k:0}$ encode the temporal correlations in the corresponding process. As we prove in our lemma above, a Markov process is divisible; i.e., it can be described by a sequence of independent CPTP maps. The corresponding Choi state will have correlations only between subsystems corresponding to neighboring preparations and subsequent measurements; it can be written as the tensor product $\Upsilon^{\text{Markov}}_{k:0} = \Lambda_{k:k-1} \otimes \Lambda_{k-1:k-2} \otimes \cdots \otimes \Lambda_{1:0} \otimes \rho_0$, where $\Lambda_{j+1:j}$ is the Choi state of the CPTP map between time steps j and $j+1$ and ρ_0 is the average initial state of the process.

This observation allows us to define a degree of non-Markovianity.

Proposition.—Any *CP*-contractive quasidistance $\mathcal{D}$ between the generalized Choi state of a non-Markovian process and the closest Choi state of a Markov process measures the degree of non-Markovianity:

$$\mathcal{N} \coloneqq \min_{\Upsilon^{\text{Markov}}_{k:0}} \mathcal{D}[\Upsilon_{k:0} \| \Upsilon^{\text{Markov}}_{k:0}]. \tag{3}$$

Here, *CP* contractive means that $\mathcal{D}[\Phi(X)\|\Phi(Y)] \leq \mathcal{D}[X\|Y]$ for any *CP* map Φ on the space of generalized Choi states, and a quasidistance satisfies all the properties of a distance except that it may not be symmetric in its arguments. Other quasidistance measures may also be used, with different operational interpretations, but those which are not *CP* contractive do not lead to consistent measures for non-Markovianity [48]. If we choose relative entropy [49] as the metric, then the closest Markov process is straightforwardly found by discarding the correlations. This measure of non-Markovianity has an operational interpretation: $\text{Prob}_{\text{confusion}} = \exp\{-n\mathcal{N}\}$ measures the probability of confusing the given non-Markovian process for a promised Markovian process after n measurements of the Choi state. In other words, $\Upsilon^{\text{Markov}}_{k:0}$ represents a Markovian hypothesis for an experiment that is really described by $\Upsilon_{k:0}$. If $\mathcal{N}$ is large, then an experimenter will very quickly realize that the hypothesis is false and the model needs updating.

Furthermore, other meaningful definitions of non-Markovianity can be derived from the properties of the Choi state. For example, the bond dimension of the matrix product representation of $\Upsilon_{k:0}$ indicates the size of the system required to store the memory between time steps; it is unity (no memory) only in the case of a Markov process. This clearly has importance for the efficiency of numerical simulations of complex quantum systems.

Discussion.—We have used the process tensor framework to introduce an unambiguous condition for quantum Markov dynamics. This condition is constructed in an entirely operational manner, and it meaningfully corresponds to the classical one in relevant settings. We have then used this condition to derive a family of measures for non-Markovianity, including one with a natural interpretation in terms of hypothesis testing with a Markovian

model. Our measure will therefore enable experimenters to incrementally construct better models for a given system, by accounting for nontrivial non-Markovian memory. By means of the Trotter formula, we can also extend the measure for non-Markovianity to continuous processes.

There are well-known methods to develop master equations for Markov processes. We can meaningfully quantify the error associated with using such methods for non-Markovian processes if we can bound their fidelity using Eq. (3). This should be possible in many cases, since large environments tend not to retain long-term memory. We anticipate that most processes of physical interest will be almost Markovian and the corresponding process tensor should be highly sparse with a block-diagonal structure. In fact, equipped with a suitable measure on the space of Choi states, our proposition allows for quantitative statements about typical non-Markovianity to be made, though we leave this for future work.

Because it captures all operationally accessible memory effects (and no more), the framework we have introduced in this Letter enables the unambiguous comparison of non-Markovianity between different systems. In particular, the fact that it puts quantum and classical processes on the same footing will allow for a meaningful quantification of the advantages (or not) that quantum mechanics brings when using memory as a resource.

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