Leggett-Garg inequalities for multitime processes

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We study some aspects of the Leggett-Garg inequalities by using the operator-state formalism for multitime processes. A new type of temporal quantum state, which we call process states, is introduced to investigate the Leggett-Garg inequalities and their violations. We find the sufficient conditions on process states for the Leggett-Garg inequalities to hold, in line with the no-signaling in time conditions. Based on these new conditions on process states, we find a new way of characterizing the environmental influences on the violation of Leggett-Garg inequalities through the structure of process states.

I. INTRODUCTION

The Bell or Clauser-Horne-Shimony-Holt (CHSH) inequalities \cite{1,2} are known to be able to test the local realism of a physical theory. The violation of these inequalities in quantum theory shows that quantum theory is not locally realistic, which means there exist nonlocal quantum correlations that are inconsistent with a local hidden-variable theory. The CHSH inequalities in the simplest form involve the probabilities of pairs of four bivalent variables. According to Fine’s theorem \cite{3}, the CHSH inequalities are the necessary and sufficient conditions for these pair probabilities to be the marginals of a joint probability of all the four probabilities, and therefore these inequalities are the necessary and sufficient conditions for the local realism. In this sense, the violation of the CHSH inequalities is a clear-cut witness for the violation of local realism, or equivalently, the existence of quantum correlations.

The temporal analogs of the CHSH equalities are the Leggett-Garg (LG) inequalities \cite{4}, which test the macroscopic realism or macrorealism. The macrorealism requires the physical properties not to be influenced by measurements, just like the macroscopic classical objects. The LG inequalities involve the temporal correlations for the sequential measurements on a single system. So the violation of the LG inequalities witnesses the non-macrorealism, or the nonclassicality, of the system. Unlike the CHSH inequalities, there is no analog of Fine’s theorem for the LG inequalities \cite{5}, as the LG inequalities are only the necessary conditions for macrorealism. There have been some efforts to find the necessary and sufficient conditions for macrorealism, for example, using the no-signaling in time condition \cite{6,7} or using the LG inequalities plus some other inequalities \cite{8,9}. These necessary and sufficient conditions for macrorealism, however, are different from the LG inequalities. In fact, there could be many other effects than macrorealism that have negative influences on the violation of the LG inequalities.

Since the LG inequalities concern the time evolution of a single system and the effects of measurements on the system and on its dynamics, a natural setting is an open (quantum) system. But an open system could be influenced by many effects, in addition to the effects of measurements. Indeed, the effects of Markovian dynamics \cite{10,11} and the non-Markovian dynamics \cite{14,17} of the open quantum system on the LG inequalities have been extensively investigated in recent years. On the other hand, the equilibrium and non-equilibrium environments will have different effects on the violation of LG inequalities \cite{18,20}. Moreover, some combinations of the effects from either the open system dynamics or the environments also lead to new effects on the LG inequalities, cf. \cite{21,22}.

In view of such a plethora of influences on the LG inequalities, one might ask what the violation of LG inequalities implies. The recent work \cite{23} shows a one-to-one connection between the quantum coherence and the nonclassicality as witnessed by the violation of LG inequalities for Markovian processes. Therefore, the key message we learn from the LG inequalities’ violation is still the nonclassicality or quantumness of the system. In generalizing this result to non-Markovian processes, the authors of \cite{24} exploit the process tensors to describe the general non-Markovian quantum processes. The process tensors \cite{23,26} are powerful operational tools for studying various temporally extended properties of quantum processes. In particular, using process tensors we can distinguish the Markovian and non-Markovian quantum processes in an operationally clearer way \cite{27,28}. From this perspective, the process tensors are very useful tools for studying the influences of Markovian or non-Markovian dynamics. In spite of this good feature, we notice that the inequalities considered in \cite{24} are not the LG inequalities. So in this paper, we would like to study some aspects of LG inequalities by using a formalism similar to the process tensors, known as the operator-state formalism \cite{24,30}.
As has been partially introduced in [30], in the operator-state formalism operators are treated as states in a new Hilbert space and the temporally extended states, or the multipartite states for multitime processes can be expressed in a form similar to the process tensors. Therefore, many developments from the process tensor framework can be analogously considered in the operator-state formalism. In this work, we use the operator-state formalism to reconsider the LG inequalities and their violations. We define a new type of temporal quantum state which we call the process states. The process states can be obtained by acting the process tensors on maximally entangled states, and hence inherit lots of the structures of process tensors. In terms of the process states, we can derive the sufficient conditions on these process states for the LG inequalities to hold, and violating these conditions is also necessary for macrorealism. These conditions restrict the process states to a “quantum-classical” form. We find that these new conditions on the process states can provide us with a unified framework for considering the influences from the state disturbances and from the quantum memory effects on the violation of LG inequalities.

This paper is organized as follows. In section II, we first introduce the general framework of operator states and define a new type of temporally extended state called the process states. Then we rewrite the LG inequalities for two-time measurements using the two-time probabilities computed from the process states. In section III, we derive a set of sufficient conditions on the process states for the LG inequalities to hold. In section IV, the influences from the state disturbances and from the quantum memory effect on the violation of LG inequalities are considered in view of the new conditions the process states. We also study LG inequalities for processes with finite Markov order. These general conditions are exemplified in a simple model in section V. Section VI concludes.

II. LG INEQUALITIES USING PROCESS STATES

A. Operator states and process states

Let us introduce the operator state |O⟩ for an operator O on the Hilbert space H of quantum states of a system S, which belongs to a new Hilbert space H with an inner product defined by

\[ (O_1|O_2) = \text{Tr}(O_1^\dagger O_2). \] (1)

An orthonormal basis for H is |Π_{ij}⟩ where Π_{ij} = |i⟩⟨j|, as one can check that

\[ (Π_{ik}|Π_{ij}) = δ_{kj}δ_{il}. \] (2)

The completeness of this basis \{Π_{ij}\} is

\[ 1_H = \sum_{ij} |Π_{ij}\rangle⟨Π_{ij}|. \] (3)

Suppose the operators \( O_i \) are Hermitian operators for some physical observables, then we have the conjugate relation

\[ (O_1|O_2)^\dagger = \text{Tr}(O_1^\dagger O_2) = \text{Tr}(O_2^\dagger O_1) = (O_2|O_1). \] (4)

By using (3) and (4), we have

\[ (O^S) = \sum_{ij} (O^S|Π_{ij}^S)(Π_{ij}^S) = \sum_{ij} (Π_{ij}^O|O^A)^\dagger(Π_{ij}^O) = \sum_{ij} (Π_{ij}^A ⊗ Π_{ij}^O|O^A^*) = (Φ^AS|O^A^*) \] (5)

where in the second line we have changed the index from S to A without loss of generality and in the last line the matrix indices of Π_{ij} has been changed to Π_{ji} so that the Hermitian conjugate \dagger has been changed to the complex conjugate *. Here, Φ^AS is the maximally entangled state in \( H_A ⊗ H_S \), as A and S label the identical system but with (artificially) different indices. The normalization of Φ is hidden for simplicity. In effect, we have doubled the system Hilbert space \( H_S \) to \( H_S ⊗ H_S \equiv H_S ⊗ H_A \), and then projected out the A-part.

With the help of (5), we can consider the action of a quantum operation \( N^S \) on the state ρ^S of the system S:

\[ N^S|ρ^S⟩ = (ρ^A^*|N^S|Φ^AS) ≡ (ρ^A^*|Ψ^A^S) \] (6)

where \( N^S \) can be pulled into the round bracket because \( ρ^A^* \) acts only on the A which is treated differently than S. The state \( Ψ^A^S \equiv N^S|Φ^AS \) is nothing but the Choi state obtained from the Choi-Jamilkowski isomorphism. This way, we can also consider the successive actions of two quantum operations \( N^S \) and \( M^S \). Denote \( |σ^S⟩ = M^S|ρ^S⟩ \), then

\[ N^S ⊗ M^S|ρ^S⟩ = N^S|σ^S⟩ = (σ^A^*|Ψ^A^S) = (Ψ^SM^S|ρ^S)|Ψ^A^S⟩ = (Φ^AS|M^S|ρ^S ⊗ Ψ^A^S). \] (7)

The strangely looking indices of (7) are a feature of the operator-state formalism for multitime processes, cf. [30]. In fact, (7) is equivalent to

\[ (Ψ^SM^S|ρ^S)|Ψ^A^S⟩ = (Ψ^SM^S|Ψ^A^S)|ρ^S⟩ \] (8)

which can be expressed diagrammatically as

\[ \begin{array}{c}
N \\
M
\end{array} = S \begin{array}{c}
A' \\
A
\end{array} \] (9)
So, the seemingly wrong indices in the right hand side of (7) are actually telling us the same story as the left hand side of (7) with the help of two maximally entangled states (or Choi states).

For more actions of quantum operations, the expression will become more complicated. However, for computing the probabilities of multitime processes, we only need to use (7). Indeed, we can compute the trace of the state obtained from three quantum operations $\mathcal{M}_i, i = 1, 2, 3$ intersected with two unitary time evolutions $\mathcal{U}^{SE}$ of the initial state $\rho_0^{SE} = \rho_0^{S} \otimes \rho_0^{E}$ as

\[
P_{3:1} = (I^S \otimes I^E) [\mathcal{M}_3^S \circ \mathcal{U}_2^{SE} \circ \mathcal{M}_2^S \circ \mathcal{U}_1^{SE} \circ \mathcal{M}_1^S] (\rho_0^{S} \otimes \rho_0^{E}) =
\]
\[
= (I^S \otimes I^E) [\mathcal{M}_3^S \circ \mathcal{U}_2^{SE} \circ \mathcal{M}_2^S] \left [ (\Phi^{S_1,A'} | \mathcal{M}_1^{S_1} | \rho_0^{S_1} \otimes \mathcal{U}_1^{SE} [\Phi^{A'S} \otimes \rho_0^E]) \right ] =
\]
\[
= (I^S \otimes I^E) [\mathcal{M}_3^S (\Phi^{S_2,A''} \otimes \Phi^{S_1,A'} | \mathcal{M}_2^{S_2} \circ \mathcal{M}_1^{S_1} | \rho_0^{S_1} \otimes \mathcal{U}_2^{SE} \circ \mathcal{U}_1^{SE} [\Phi^{A'S} \otimes \Phi^{A'S_2} \otimes \rho_0^E]) =
\]
\[
= (I^S \otimes I^E) [\mathcal{M}_3^S (\Phi^{S_2,A''} \otimes \Phi^{S_1,A'} | \mathcal{M}_2^{S_2} \circ \mathcal{M}_1^{S_1} (I^E | \mathcal{U}_2^{S_1} \circ \mathcal{U}_2^{SE} | \rho_0^{S_1} \otimes \Phi^{A'S_3} \otimes \Phi^{A'S_2} \otimes \rho_0^E)]) ,
\]

where the labels $S_i, i = 1, 2, ..., n$ (which are ordered as $S_1 \rightarrow S_2 \rightarrow \ldots \rightarrow S_n$) label the input state for each operation. We observe that (10) contains two parts: one part is the evolution of the state (on the right) and the other is the quantum operations (on the left). Diagrammatically, this type of algebraic manipulation means connecting $(n - 1)$ segments of the curved lines of (9). By repeating this manipulation up to the $n$-th operation, we can obtain the corresponding $n$-point probability. In the general $n$-point case, we define the process state as

\[
|S_{n:1} := (I^E | \mathcal{U}_{n-1}^{S_1} \circ \ldots \circ \mathcal{U}_{1}^{S_n} | \rho_0^{S_1} \otimes (\bigotimes_{j=2}^{n} \Phi^{A^{(j-1)} S_j} | \otimes \rho_0^E). \]

We also define the $n$-point operation as

\[
(O_{n:1}^{(x_1, \ldots, x_n}) := (I^{S_1} \otimes (\bigotimes_{i=1}^{n-1} \Phi^{S_i A^{(i)}} | | \mathcal{M}_{n:1}^{(x_n)} \otimes \ldots \otimes \mathcal{M}_{1:1}^{(x_1)} , \]

where the operation $\mathcal{M}_{i:1}^{(x_i)}$ acts on $S_i$. The quantum operations of (selective) projective quantum measurements act as

\[
\mathcal{M}_{j:1}^{(x_j)} | \rho^S \rangle = | \Pi_{x_j} | | \rho^S | \Pi_{x_j} \rangle = | \Pi_{x_j} | | \Pi_{x_j} | \rho^S \rangle , \]

so the $| \Pi_{x_j} \rangle$ in (13) projects the maximally entangled states in (12) to the bipartite classical states. In this case, the $n$-point operation (12) can be briefly denoted as

\[
(\Pi_{x_n} \otimes | \Pi_{x_{n-1}} \otimes \Pi_{x_{n-1}}^{(n-1)} | \ldots \otimes | \Pi_{x_1} \otimes | \Pi_{x_1}^{(1)} |). \]

With these notations in hand, the joint probability for $n$-point measurements can be expressed as

\[
P_{n:1}(x_{n:1} | \mathcal{M}_{n:1} = (O_{n:1}^{(x_n; \ldots; x_1)} | | S_{n:1}) . \]

It is helpful to compare the process states with the process tensors; we do this in Appendix A. Importantly, a process state can be rewritten as the action of a process tensor on the tensor product of maximally entangled states.

\[
|S_{n:1} := | T_{n:1} (\bigotimes_{j=2}^{n} \Phi^{A^{(j-1)} S_j} | , \]

\[
cf. (A6). In this sense, many results obtained in the process tensor formalism can be translated into the process states formalism.

B. LG inequalities

The general statement of macrorealism can be made operational by the following postulates [4, 31]:

1. Macrealism per se: A macroscopic object should have two or more macroscopically distinct states and at any time the object is in one of these states.

2. Non-invasive measurability: It is possible to measure the state without disturbing the subsequent dynamics.

3. Induction: The present state and the measurement outcome of the present state cannot be affected by future measurements.

Based on these postulates, we can derive the LG inequalities for the two-point correlations of two-time measurements.

Let us consider a two-time measurement, or two measurements at times $t_i$ and $t_j$, with outcomes $Q_i$ and $Q_j$ respectively. The joint pair probability for this two-time measurement to happen is $P(Q_j, t_j; Q_i, t_i)$. Then the corresponding two-time correlation function is

\[
C(t_j, t_i) = \sum_{Q_j, Q_i} Q_j Q_i P(Q_j, t_j; Q_i, t_i). \]

This $C(t_j, t_i)$ is a correlation function in the sense of classical probability theory. In quantum theory, we should consider instead the quantum measurements on the quantum system represented by the measurement operators $\mathcal{M}_i$. Let $\rho$ be the density matrix of the quantum system which has the open quantum dynamics dictated by a superoperator $\mathcal{L}$. That is, we have the time evolution equation $\frac{d\rho}{dt} = \mathcal{L}\rho$ with a formal solution $\rho(t_j) = e^{\mathcal{L}(t_j-t_i)\rho(t_i)}$. If the quantum measurements are projective, i.e., $\mathcal{M} = \sum_m a_m \Pi_m$, where $a_m = \pm 1$ for simplicity and $\Pi_m$ are projection operators, then the quantum correlation function for the two-time measurement is

$$C_q(t_j, t_i) = \sum_{m,n} a_m a_n \text{Tr}[\Pi_m e^{\mathcal{L}(t_j-t_i)}(\Pi_n \rho(t_i) \Pi_n)] = \text{Tr}[\mathcal{M}(t_j)\mathcal{M}(t_i)\rho(t_i)],$$

where the $\mathcal{M}(t_j)$ are written in the Heisenberg picture and in particular for $\mathcal{M}(t_i)\rho(t_i)$ the evolution operator is simply an identity. In general, $C_q(t_j, t_i)$ is complex, and its imaginary part measures the noncommutativity of $\mathcal{M}(t_j)$ and $\mathcal{M}(t_i)$. By Lüders’ theorem [22], we know that the non-invasiveness of measurements is equivalent to the commutativity of the measurement operators, so we should consider only the real part

$$C_{ji} = \frac{1}{2} \text{Tr}((\mathcal{M}(t_j), \mathcal{M}(t_i))\rho).$$

To obtain the LG inequalities in the simplest form, we consider only the two-time measurements, that is, $n = 2$ in [11] and [12]. So the two-time joint probability is

$$P_{i,j}(x_i, x_j | M_{i,j}) = \langle \mathcal{O}_{i,j}(x_i, x_j) | S_{n,1} \rangle, \quad i \leq j.$$  

(20)

Since the quantum measurements affect both the quantum coherence of the system’s state and its subsequent dynamics, the classical Kolmogorov consistency condition could be violated, to wit,

$$P_{i,j}(x_i, x_j | M_{i,j}) \neq \sum_{x_{j+1}, \ldots, x_n} P_{n,1}(x_{n+1} | M_{n,1})$$

(21)

where the $x_i$ are not summed over. In contrast, if the measurements do not affect the state of the system (i.e., macrorealism per se) and do not disturb the following dynamics of the system (i.e., noninvasive measurability), then we can obtain the two-time probabilities from the $n$-time joint probabilities and also the LG inequalities for the two-time probabilities. Notice that the induction condition is naturally satisfied in the present framework,

$$P_{i,j}(x_i, x_j | M_{i,j}) = \sum_{x_{j+1}, \ldots, x_n} P_{n,1}(x_i, x_{n+1} | M_{i,j} \otimes M_{n,j})$$

(22)

as the order of quantum operations matters.

In terms of the two-time probabilities [12], the two-time correlation are

$$C_{ij} = \sum_{x_i, x_j} x_i x_j P_{i,j}(x_i, x_j | M_{i,j}).$$

(23)

Taking $n = 3$ for example, we can obtain all the two-time probabilities from the three-time joint probability. It is then obvious that

$$K_3 \equiv C_{12} + C_{23} - C_{13} = 1 - \sum_{x_i, x_j, x_k} (x_j - x_k)(x_j - x_i)P_{3,1}(x_i, x_j, x_k).$$

(24)

When $x_i, x_j, x_k = \pm 1$, we have

$$K_3 \leq 1$$

(25)

which are the LG inequalities.

### III. NEW CONDITIONS FOR LG INEQUALITIES

As mentioned above, the violation of LG inequalities could be influenced by different types of dynamics and the decoherence of the open system. In order to see these influences clearly, we consider here the conditions on the process states for the LG inequalities to hold.

Consider again the case of three-time measurements with joint probability

$$P_{3,1} = (\Pi_{S_1}^S \otimes \Pi_{S_2}^S \otimes \Pi_{A''}^S) \otimes (\Pi_{S_1}^A \otimes \Pi_{A''}^A) | S \rangle$$

(26)

where $S$’s indices can be recovered as $S_{S_1 S_2 A'' S_1 A'}$. We also have the probabilities for two-time measurements:

$$P_{1,2} = \sum_{x_3} (\Pi_{S_3}^S \otimes \Pi_{S_2}^S \otimes \Pi_{A''}^S) \otimes (\Pi_{S_1}^A \otimes \Pi_{A''}^A) | S \rangle,$$

$$P_{2,3} = \sum_{x_{1,y_1}} (\Pi_{S_3}^S \otimes \Pi_{S_2}^S \otimes \Pi_{A''}^S) \otimes (\Pi_{S_1}^A \otimes \Pi_{A''}^A) | S \rangle,$$

$$P_{1,3} = \sum_{x_{2,y_2}} (\Pi_{S_3}^S \otimes \Pi_{S_2}^S \otimes \Pi_{A''}^S) \otimes (\Pi_{S_1}^A \otimes \Pi_{A''}^A) | S \rangle,$$

(27)

where the double sum $\sum_{x,y}$ means that no projective measurement has been done. Compared to [14], in the absence of a measurement the corresponding state remains to be a maximally entangled state $(\sum_{x,y} \Pi_{S_3}^S \otimes \Pi_{A''}^A)$. Now suppose the two-time probabilities can be obtained from the three-time joint probability [20] as marginals, then we see that the conditions in [27] are equivalent to satisfying one of

$$(\Pi_{x_1 y_1}^A | S_{S_1 S_2 A'' S_1 A'} ) = \delta_{x_1 y_1} (\Pi_{x_1}^A | S_{S_1 S_2 A'' S_1 A'} ),$$

(28)

$$(\Pi_{x_1 y_1}^A | S_{S_1 S_2 A'' S_1 A'} ) = \delta_{x_1 y_1} (\Pi_{x_1}^A | S_{S_1 S_2 A'' S_1 A'} ),$$

(29)

and one of

$$(\Pi_{x_2 y_2}^A | S_{S_1 S_2 A'' S_1 A'} ) = \delta_{x_2 y_2} (\Pi_{x_2}^A | S_{S_1 S_2 A'' S_1 A'} ),$$

(30)

$$(\Pi_{x_2 y_2}^A | S_{S_1 S_2 A'' S_1 A'} ) = \delta_{x_2 y_2} (\Pi_{x_2}^A | S_{S_1 S_2 A'' S_1 A'} ),$$

(31)
where $|S_{S_1S_2A''}^S| = (\mathcal{P}_{x_1}^{S_1} \otimes \mathcal{P}_{x_2}^{A'}|S)$ is the reduced process state after the first measurement. We only need one condition from two conditions because in the operation part of the states, e.g., $\Phi^{S_1A'}$, are maximally entangled states.

The conditions (25) restricts the initial state $\rho_{S_1}$ to be a classical state with diagonal density matrix. That is, the process state should take the form of a “quantum-classical” state

$$
|S_{S_1S_2A''S_2A'}^S| = \sum_{x_1} |S_{x_1}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_1}^{S_1}|.
$$

If the conditions (29), (30) and (31) are furthermore satisfied, we have

$$
|S_{S_1S_2A''S_2A'}^S| = \sum_{x_1,x_2} |S_{x_1,x_2}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_2}^{S_2} \otimes |\mathcal{P}_{x_1}^{A'}| \otimes |\mathcal{P}_{x_1}^{S_1}|.
$$

Recalling the definition of process states (or the diagrammatic rule (9)), we know that from $A'$ to $S_2$ the system undergoes a time evolution $U_1$, so that the particular form of (33) means this time evolution $U_1$ should be a classical time evolution without generating quantum coherence on the system. This is a very strong requirement for the time evolutions.

On the other hand, when only (29) and (30) are satisfied, the allowable process state takes the form

$$
|S_{S_1S_2A''S_2A'}^S| = \sum_{x_1,x_2} |S_{x_1,x_2}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_2}^{S_2} \otimes |\mathcal{P}_{x_1}^{A'}| \otimes |\mathcal{P}_{x_1}^{S_1}| + \sum_{x_1} \left( |S_{x_1}^{S_1S_2A''S'} \otimes |\mathcal{P}_{x_1}^{S_1}| - |S_{x_1}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_1}^{S_1}| \right) \otimes |\mathcal{P}_{x_1}^{A'}|,
$$

The first summation term of (34) corresponds to a stronger condition $(\mathcal{P}_{x_1}^{S_2} |S_{S_2A''S_2A'}| = \delta_{x_2,y_2} (\mathcal{P}_{x_2}^{S_2} |S_{S_2A''S_1A'}|)$ which is independent on the first measurement. The second summation term of (34) is then the difference between two situations without and with the first measurement on $S_1$: after taking the trace $(\mathcal{P}_{x_1}^{S_1} \otimes |\mathcal{P}_{x_1}^{A'}| |S|)$, the second summation term vanishes. Compared to (33), the process state (34) allows arbitrary evolutions after the first measurement. If (28) and (30) are satisfied, we have

$$
|S_{S_1S_2A''S_2A'}^S| = \sum_{x_1,x_2} |S_{x_1,x_2}^{S_1A''A'} \otimes |\mathcal{P}_{x_2}^{S_2} \otimes |\mathcal{P}_{x_1}^{A'}| \otimes |\mathcal{P}_{x_1}^{S_1}| + \sum_{x_1} \left( |S_{x_1}^{S_1S_2A''S'} \otimes |\mathcal{P}_{x_1}^{S_1}| - |S_{x_1}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_1}^{S_1}| \right) \otimes |\mathcal{P}_{x_1}^{A'}|,
$$

the first term of which means that the state is a classical state, and the second term means that the state fed into the second measurement is a classical state. Likewise, we have other two possible process states: If (29) and (31) are satisfied, we have

$$
|S_{S_1S_2A''S_2A'}^S| = \sum_{x_1,x_2} |S_{x_1,x_2}^{S_1A'\prime A'} \otimes |\mathcal{P}_{x_2}^{S_2} \otimes |\mathcal{P}_{x_1}^{A'}| + \sum_{x_1} \left( |S_{x_1}^{S_1S_2A''S'} \otimes |\mathcal{P}_{x_1}^{S_1}| - |S_{x_1}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_1}^{S_1}| \right) \otimes |\mathcal{P}_{x_1}^{A'}|,
$$

and if (28) and (31) are satisfied, we have

$$
|S_{S_1S_2A''S_2A'}^S| = \sum_{x_1,x_2} |S_{x_1,x_2}^{S_1A''A'} \otimes |\mathcal{P}_{x_2}^{S_2} \otimes |\mathcal{P}_{x_1}^{A'}| + \sum_{x_1} \left( |S_{x_1}^{S_1S_2A''S'} \otimes |\mathcal{P}_{x_1}^{S_1}| - |S_{x_1}^{S_1S_2A''A'} \otimes |\mathcal{P}_{x_1}^{S_1}| \right) \otimes |\mathcal{P}_{x_1}^{A'}|.
$$

Thus, satisfying different sets of the conditions (28)–(31) gives rise to four types of “quantum-classical” process states (34)–(37), which we denote by $|S_{QC}|$.

As long as the process state satisfies one of these $|S_{QC}|$, the two-time probabilities can be obtained from a three-time probability as marginals, and one can derive the LG inequalities. If the process state is not any of the four types, then by the induction condition, we have

$$
K_3 = 1 - \sum_{x_1,x_2,x_3} (x_j - x_k)(x_j - x_1) \mathcal{P}_{3;1}(x_i, x_j, x_k) + \sum_{x_1,y_1,x_2,x_3} x_2 x_3 (\mathcal{P}_{x_3}^{S_3} \otimes |\mathcal{P}_{x_2}^{S_2} \otimes |\mathcal{P}_{x_2}^{A''} \otimes |\mathcal{P}_{y_1}^{S_1} \otimes |\mathcal{P}_{y_1}^{A'}| |\Delta S| - \sum_{x_1,x_2,y_2,x_3} x_1 x_3 (\mathcal{P}_{x_3}^{S_3} \otimes |\mathcal{P}_{y_2}^{S_1} \otimes |\mathcal{P}_{x_2}^{A''} \otimes |\mathcal{P}_{y_1}^{S_1} \otimes |\mathcal{P}_{y_1}^{A'}| |\Delta S|)
$$

where $\Delta S = S - S_{QC}$ is the deviation of the process state from the “quantum-classical” process state. Therefore,
we can use this deviation $\Delta S$ to study the violation of LG inequalities.

We remark that the conditions (25)–(31) together with the induction condition is in the same spirit of the no-signaling in time conditions (plus the induction condition) [11]. Here, we have transferred the no-signaling in time conditions to the “quantum-classical” conditions on process states. These conditions are imposed on the maximally entangled states or Choi states in the process states, so they do not have counterparts in the process tensor formalism.

IV. VIOLATION OF LG INEQUALITIES VIA DEVIATION OF PROCESS STATE

In this section, we consider different influences on the violation of LG inequalities by looking at the deviations from the “quantum-classical” conditions on process states introduced above. We split the violation of noninvasive measurability into two positive influences on the violation of LG inequalities: one from the state disturbance by quantum operations and the other from the memory effects induced by dynamics.

A. Violation of LG inequalities by state disturbance

We first show that, in the absence of memory effect, the violation of LG inequalities is clearly influenced by the disturbance on the system’s state caused by measurements.

Let us consider general quantum processes generated by a series of quantum operations $N_i$, so that the corresponding open system evolution is $|\rho_0^S\rangle = N_2\otimes \ldots \otimes N_1|\rho_0^S\rangle$. In the absence of memory effects, the overall quantum process is a Markovian process. Now recall the Markovian condition for process tensors [27]: A process tensor $|T_{n:1}\rangle$ is Markovian if it can be written as

$$|T_{n:1}\rangle = |T_{n:n-1} \otimes \ldots \otimes T_{2:1}\rangle.$$  \hspace{1cm} (39)

Since this condition only concerns the process tensors, by (19) or (A6), we see that this Markovian condition transfers to the following condition on process states

$$|S_{n:1}\rangle = |S_{n:n-1}^A S_n \otimes \ldots \otimes S_{2:1}^A S_2 \otimes \rho_0^S\rangle.$$  \hspace{1cm} (40)

where $S_{i:i-1}^A = N_i^A S_i$. As the quantum operation at each step is fixed, the particular form (40) restricts the quantum process to follow a fixed form of dynamics. In other words, the influence here comes from the disturbance on the states. Because the process state Eq. (40) is formally closed to the “quantum-classical” state (35), it is appropriate to study the influence from the disturbance on states using the deviations between them.

As before, by comparing Eq. (40) and (55), we see that, for these two states to coincide upon the first two measurements, we require

$$\rho_0^S = \sum_{x_1} P_1(x_1)\Pi_{x_1}^S,$$  \hspace{1cm} (41)

$$(\Pi_{x_1}^A|N_1^A S_2\rangle = \sum_{x_2} P_2(x_2)\Pi_{x_2}^S,$$  \hspace{1cm} (42)

where $P_1(x_1) = (\Pi_{x_1}^S|\rho_0^S\rangle$ and $P_2(x_2) = (\Pi_{x_2}^A\otimes \Pi_{x_2}^S|N_1^A S_2\rangle$. The condition (41) means that the input state for the first measurement $M_1$ is a diagonal classical state. Similarly, the condition (42) requires that the input state for the second measurement $M_2$ is a diagonal classical state, after the first trace $(\Pi_{x_1}^S \otimes \Pi_{x_1}^A|S\rangle$ is taken. Thus, we conclude that there is a positive influence on the violation of LG inequalities for an open system from the state changes (e.g., the coherence generation) caused by the quantum operations.

B. Violation of LG inequalities by memory effect

Now let us turn to the influence on LG inequalities from the memory effects. In the presence of memory effects, the process state cannot be written in the form of (40). Generally speaking, $|S^{A^{(j)}} S_{j+1}\rangle$ and $|S^{A^{(j-1)}} S_j\rangle$ are quantum correlated, thereby making it difficult for the total process state to conform to the “quantum-classical” form. Therefore, the memory effects have positive influences on the violation of LG inequalities, which is consistent with the results of previous work [14].

We can see the influence from memory effects more clearly by discarding the influence from the state disturbance. To this end, we consider the input state $\rho^S_j$ for the $j$-th operation in a particularly chosen basis such that $\rho^S_j = \sum_{x_j} P_j(x_j)\Pi_{x_j}^S$, i.e., diagonal in this basis. Then, the measurement $M_j^{(x_j)}$ in this basis does not affect the coherence of $\rho^S_j$, i.e.,

$$\sum_{x_j} M_j^{(x_j)}(\rho^S_j) = \rho^S_j.$$  \hspace{1cm} (43)

But this measurement can still change the system-environment quantum correlations, making this relation invalid. Consequently, the measurement still disturbs the subsequent dynamics of the open system, thereby violating the LG inequalities.

For classical processes, the measurement is expected to affect neither the state nor the subsequent dynamics, in
line with the non-invasive measurability, and hence the classical memory effect should not contribute positively to the violation of LG inequalities. However, there exists special cases of classical process in which the classical non-Markovian effects lead to the violation of temporal inequalities similar to the LG inequalities [33]. Even if there exist quantum memories, it is still possible for the process to be Markovian [34]. So, to avoid confusions, we only focus on the quantum memory effects, without emphasizing the non-Markovianity.

To characterize the influence of quantum memories on LG inequalities, we consider here the system-environment joint states. For the measurements not to disturb the state, the states to be measured must be diagonal classical states in the measurement basis. In such a situation, the system-environment input states $\rho^{S,E}$ for the $j$-th measurement operation should be classical-quatum states $\rho^{S,E}_{CQ}$. Suppose there is no other influences than the quantum memory, then we can use the deviation $|\rho^{SE} - \rho^{SE}_{CQ}|$ of the total state $\rho^{SE}$ from the classical-quantum state $\rho^{SE}_{CQ}$ to characterize the influence from the quantum memory.

In the three-time measurement case, if the first measurement $M_1$ is done in the basis where the input state $\rho^{S_1}$ is classical, then by eq. (43) we have

$$\mathcal{P}_{2,3}(x_2, x_3 | M_{2,3}) = \sum_{x_1} [\mathcal{P}_{3,1}(x_3 | M_{3,1})]. \tag{44}$$

But due to the relation $M_1^{S}(\rho^{SE}) = |\rho^{SE}_{CQ}| - |\rho^{SE} - \rho^{SE}_{CQ}|$, we have

$$\mathcal{P}_{1,3}(x_1, x_3 | M_{1,3}) = \sum_{x_2} [\mathcal{P}_{3,1}(x_3 | M_{3,1}) + \mathcal{P}_{2,3}(x_2, x_3 | M_{2,3})] + \mathcal{M}_{2}^{S}(\rho^{SE}_{CQ}) - \rho^{SE}_{CQ}(|\Pi_{x_1}^{S} \rho^{S_1}_0|) \tag{45}$$

where $\rho^{SE}_{CQ} = \mathcal{U}^{SE}(\Pi_{x_1}^{S} \otimes \rho^{S_1}_0)$ and $\rho^{SE}_{CQ} = \mathcal{M}_2(\rho^{SE}_{x_1})$. Thus, the second line of eq. (45) clearly shows the influence from the quantum memories.

C. The case with Markov order

An interesting intermediate case between the memoryless and mnemonic processes is the process with finite Markov order, i.e. memories of finite length. The quantum Markov order has been characterized in the process tensor framework [33, 36], where a quantum process with finite-length Markov order has the process tensor of the following form

$$|\mathcal{T}_{HM F}| = \sum_{x} P(x)|\mathcal{T}_{H}^{(x)} \otimes \Delta_{M}^{(x)} \otimes \mathcal{T}_{F}^{(x)}| \tag{46}$$

where the subscripts $H, M, F$ label respectively the history, Markov order, and future parts of the quantum process. The $\Delta_{M}^{(x)}$ is a particular quantum instrument such that $(O_{M}^{(x)} | \Delta_{M}^{(y)} |) = \delta_{xy}$. This form of process tensors allows a non-vanishing conditional mutual information $I(F : H| M) > 0$, thereby indicating the quantum memory effect. Using again (10) or (A6), we obtain the similar structure for process states

$$|\mathcal{S}_{HM F}| = \sum_{x} P(x)|\mathcal{S}_{H}^{(x)} \otimes \mathcal{S}_{M}^{(x)} \otimes \mathcal{S}_{F}^{(x)}| \tag{47}$$

with $\mathcal{S}_{M}^{(x)}$ induced by the instrument $\Delta_{M}^{(x)}$.

To see the influence from the Markov order part $M$ on LG inequalities, let us suppose the non-invasive measurability is satisfied in the $H, F$ parts. In the three-time measurement case with now the Markov order-1 (i.e., the memory extends to the second-step time evolution), we have the following property of the marginal probabilities [35, 36]

$$\frac{\mathcal{P}_{2,3}(x_2, x_3 | M_{2,3})}{\mathcal{P}_{2}(x_2 | M_{2})} = \frac{\mathcal{P}_{3,1}(x_3 | M_{3,1})}{\mathcal{P}_{1,2}(x_1, x_2 | M_{1,2})} \tag{48}$$

Since the instrument in the Markov order part $M$ is chosen such that $(O_{M}^{M} | \mathcal{S}_{M}^{(x)} |) = \delta_{xy}$, the second measurement in $M$ effectively acts like an identity matrix (cf. the double summation in eq. (27)), that is

$$\sum_{x} \Pi_{x}^{M} |\mathcal{S}_{3,1}^{(M)}| = \sum_{x,y} \Pi_{x,y}^{M} |\mathcal{S}_{3,1}^{(M)}| = |1_{M}^{M} |\mathcal{S}_{3,1}^{(M)}| \tag{49}$$

Therefore, $\mathcal{P}_{1,3}$ can still be derived from $\mathcal{P}_{3,1}$ as marginal

$$\mathcal{P}_{1,3}(x_1, x_3 | M_{1,3}) = \sum_{x_2} \mathcal{P}_{3,1}(x_3 | M_{3,1}) \tag{50}$$

$\mathcal{P}_{2,3}$, on the other hand, can be obtained from $\mathcal{P}_{1,3}$ and $\mathcal{P}_{1,2}$ with the help of eq. (48). Using these probabilities, we can obtain

$$K_{3} = \sum_{x_1, x_1, x_2, x_3, x_k} \left[ x_i x_j P_{3,1}(x_i, x_j, x_k) + x_i x_k \frac{P_{3,1}(x_i, x_j, x_k)}{P_{1,2}(x_i, x_j)} P_{2}(x_j) - x_i x_k P_{3,1}(x_i, x_j, x_k) \right] \tag{51}$$
where we have used in the second line (with \( \doteq \)) the relation
\[
\sum_{x_j} x_j^2 P_{2,3}(x_j, x_k) = \sum_{x_j} P_{2,3}(x_j, x_k) = 1
\]
for dichotomic outcomes \( x_j = \pm 1 \). Thus, the violation of LG inequalities depends on \( P_2(x_j) \) and \( P_{1,2}(x_i, x_j) \).
It is not difficult to see from (51) that, when \( P_2(x_j) \geq P_{1,2}(x_i, x_j) \), the LG inequalities must be satisfied. This happens, for example, when the first operation \( N_1 \) is a quantum channel, so that
\[
P_{1,2} = (\Pi_{x_2} |N_1| \Pi_{x_2})(\Pi_{x_1} |\rho_0),
\]
\[
P_2 = \sum_{x_1, y_1} (\Pi_{x_2} |N_1| \Pi_{x_1, y_1})(\Pi_{x_1, y_1} |\rho_0), \quad (52)
\]
As both of them are positive, we have then \( P_2(x_j) \geq P_{1,2}(x_i, x_j) \). When \( P_2(x_j) < P_{1,2}(x_i, x_j) \), the LG inequalities could be violated.

V. AN EXAMPLE

To exemplify the above general considerations, we consider here a simple noisy model with two-qubits which has been previously considered in [17]. In this model, the initial state of the system is \( \rho_0 \), and the initial state vector of the environment is also \( |\psi_E = (|+\rangle - |\rangle)/\sqrt{2} \), where the \(|\pm\rangle\) are just the qubit states. The total Hamiltonian for the \( \rho^{SE} \) is
\[
H = \omega(|+-\rangle \langle++| + |+\rangle \langle-+|). \quad (53)
\]
Let us consider two steps of time evolutions generated by \( H \): The time interval for the first step is \([0, t_1 = \tau_1]\), and the time interval for the second step is \([t_1, t_2 = t_1 + \tau_2]\). Suppose the measurements at \( t_1 \) and \( t_2 \) are projective measurements. Then the process state for this two-time measurement is
\[
|S_{S_3 S_2 A'' S_1 A'}\rangle = |\rho_0^{S_1} \otimes \frac{1}{2} [\Pi_{\psi_+}^{S_3 S_2 A''} + \Pi_{\psi_-}^{S_3 S_2 A''}]\rangle \quad (54)
\]
where \( \Pi_{\psi_+}^{S_3 S_2 A''} \) is the density matrix of the state
\[
2\sqrt{2} |\psi_+^{S_3 S_2 A'' S_1}\rangle = |(++) + (1)^k |(++)\rangle \leq |(+\rangle + |\rangle)(++) + i(-1)^k \sin \theta_2 |(++)\rangle,
\]
and \( \Pi_{\psi_+}^{S_3 S_2 A'' A'} \) is the density matrix of
\[
2\sqrt{2} |\psi_+^{S_3 S_2 A'' S_1}\rangle = |(++) + (1)^k |(++)\rangle \leq |(+\rangle + |\rangle)(++) + i(-1)^k \sin \theta_2 |(++)\rangle,
\]
Here, \( \theta_1 = \omega \tau_1 \) and we have decomposed the time evolutions \( e^{-iHt} \) into the triangular functions.

Generally speaking, this process state cannot be written in a Markovian form (40), except for the case with \( \theta_1 = k\pi \) in which we have
\[
2\sqrt{2} |\psi_{S_3 S_2 A'' S_1}\rangle = ((-\rangle + (1)^k |(++)\rangle) \leq (|\rangle + \cos \theta_2 |(++)\rangle + i(-1)^k \sin \theta_2 |(++)\rangle),
\]
and hence the corresponding process state
\[
|S_{S_3 S_2 A'' S_1 A'}\rangle = |\rho_0^{S_1} \otimes \Phi_k^{S_2 A'} \otimes \frac{1}{2} [\Pi_{\psi_+}^{A''} + \Pi_{\psi_-}^{A''}]\rangle, \quad (58)
\]
with \( |\Phi_k^{S_2 A'}\rangle = (|\rangle + (1)^k |(++)\rangle)/\sqrt{2} \), takes the form of (40). So we let \( \rho_0^{S_1} = \sum_{x_1} P(x_1) \Pi_{x_1}^{S_1} \) in this case, then after the first step it becomes \( \rho_0^{S_2} = (\Phi_k^{S_1 A'} |S_{S_2 A''} S_1 A') = \sum_{x_1} P(x_1) \Pi_{x_1}^{S_2} \) with \( \Pi_{x_1}^{S_2} = (\Pi_{x_1}^{A'} |\Phi_k^{S_2 A'} \rangle \). Therefore, we can rewrite (58) as
\[
|S_{S_3 S_2 A'' S_1 A'}\rangle = \sum_{x_1} P(x_1) P'(x_1) |\Pi_{x_1}^{S_1} \otimes \Pi_{x_1}^{S_2} \otimes \Pi_{x_1}^{A'} \otimes S_{S_3 A''}\rangle + \sum_{x_1} P(x_1) |\Pi_{x_1}^{S_1} \otimes (\Phi_k^{S_2 A'} - P'(x_1) \Pi_{x_1}^{S_2} \otimes \Pi_{x_1}^{A'} \otimes S_{S_3 A''}\rangle, \quad (59)
\]
where \( P'(x_1) = (\Pi_{S_1}^2 \otimes \Pi_{A'}^2) |\Phi_{S_2}^{S_2'}\rangle \). If we choose the measurement basis for two measurements as \( \{|x_1\rangle_{S_1}\} \) and \( \{|x_1\rangle_{S_2}\} \) respectively, the state has the “quantum-classical” form, thereby satisfying the LG inequalities.

When \( \theta_1 \neq k\pi \), for example, \( \theta_1 = \theta_2 = (k + 1/2)\pi \), we have

\[
2 |\psi^{A}_1 S_2 A'' S_3\rangle = i(-1)^{k-1} |+-\rangle_{S_2 A''} \otimes |\Phi_0\rangle_{A'S_3} + |--\rangle_{S_2 A''} \otimes |\Phi_1\rangle_{A'S_3} .
\]

Thus we have

\[
K_3 = 2 \cos 2\theta - \cos 4\theta,
\]

which gives the maximum value 3/2 when setting \( \theta = \pi/6 \).

VI. CONCLUSION AND DISCUSSION

In this paper, we have studied the LG inequalities in the framework of the operator-state formalism. We have introduced a class of new temporal quantum states called the process states to investigate the LG inequalities. In particular, we have derived a set of sufficient conditions on the process states for the LG inequalities to hold. Since the process states share many structures of the process tensors, we have exploited these conditions on the process states to investigate different influences on the violations of LG inequalities. It turns out that in this new framework we are able to study the influences from the environments in a unified way.

The use of process states highlights the state structure in testing macrorealism. In spite of the existence of various influences from environment on the LG inequalities for the open system, it is found that the violation of LG inequalities (or other inequalities alike) is still a witness for the existence of quantum coherence in the open system [23, 24]. In terms of the “quantum-classical” process states, we can clearly see whether there is quantum coherence in this temporal setting.

The problem of the existence of a joint probability over time, when the marginals at each time are known, is not an easy one in quantum theory. There exists a no-go result [37] stating that it is impossible to do so in quantum theory. Recently in [38], a new type of quantum states over time allowing the existence of joint probability over time is constructed by using the Jordan product of two Choi states in the forward and backward time directions. Here, instead of Jordan product, we use the Choi states in two time directions to rewrite the process tensors as a multipartite quantum state. This way, the temporally extended quantum states are rewritten as a zigzag-time-ordered quantum state. Whether the process states evade the no-go arguments deserves further consideration.

We finally remark that both the violation of LG inequalities [39] and the process tensors [40] can be experimentally realized in the quantum optical platform. So, the process states considered in this work are also experimentally realizable.
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Appendix A: Process tensors and comparison with Process states

A process tensor [23, 26] is a multilinear map \( T_{n:0} : A_{n-1:0} \mapsto \rho_n \) from a set \( A_{n-1:0} \) of \((n-1)\) quantum operations to the final state \( \rho_n \) obtained after these \((n-1)\) operations. Let us denote by \( A_i \in A_{n-1:0} \) the quantum operation at the \( i \)-th step/time and by \( U_{j} \) the unitary operation \( U_{j:i} \). Then the process tensor \( T_{n:0} \) corresponds to the global evolution \( \rho_n^{SE} = U_{n,n-1}A_{n-1}U_{n-1,n-2}...A_1U_0A_0\rho_0^{SE} \), so

\[
\rho_n = \text{tr}_E(\rho_n^{SE}) = T_{n:0}[A_{n-1:0}] = \sum_{s,x} T_{s,x} A_{s,x}, \quad (A1)
\]

where

\[
T_{s,x} = \sum_e \prod_{j=0}^{k-1} \left( U_{j+1:j} \rho_0^{SE} \right)_{s,x}, \quad A_{s,x} = \prod_{j=0}^{k-1} \left( A_j \right)_{s,x}
\]

with the collections \( s, x, e \) standing for the system, operation, environment (matrix) indices respectively. By the Choi-Jamiolkowski isomorphism, the quantum operations \( A_j : \mathcal{H}_i \to \mathcal{H}_o \) can be transformed into the corresponding Choi states \( O_j = A_j \otimes I(\Phi) \), where \( \Phi \) is a projection to the maximally entangled states \( \sum_i |ii\rangle \) in the Hilbert space \( \mathcal{H}_o \otimes \mathcal{H}_i \). Denote the nested sequence of Choi states by \( O_{k:0}^{E,s} \), then the joint probability of the whole quantum process producing outcomes \( \{x_j\} \equiv x_{k:0} \) is

\[
P_{k:0}(x_{k:0}|A_{k-1:0}) = \text{tr}(O_{k:0}^{E,s} T_{k:0}). \quad (A2)
\]

This is a generalization of the familiar Born rule \( P_i = \text{tr}(\Pi_i \rho) \) with projector \( \Pi_i \).

The process tensor for \((n-1)\) steps of evolutions, as defined in (A1), can be expressed as an operator/tensor state

\[
|T_{n:1} \rangle = (I^E U_{n,n-1} \circ \cdots \circ U_{2:1}) |\rho_n^{SE} \rangle, \quad (A3)
\]

where \((I^E) \) means taking the trace over the environment \( E \). The operator state for \((n-1)\)-time measurements with outcomes \( x_i, i = 1, ..., n - 1 \) is

\[
|O_{n:1}^{(x_{n-1})} \rangle = O_{n,n-1}^{(x_{n-1})} \circ \cdots \circ O_{2:1}^{(x_1)} |\rho_n^{S} \rangle = (M_{n-1}^{(x_{n-1})} \otimes I_{n-1}) \circ \cdots \circ (M_1^{(x_1)} \otimes I_1) |\rho_n^{S} \rangle \quad (A4)
\]

where \( O_j^{(x_j)} = M_j^{(x_j)} \otimes I(\Phi) \). Finally, the joint probability \( \{A2\} \) can be expressed as

\[
\mathcal{P}_{n:1}(x_{n:1}|M_{n:1}) = \langle O_{n:1}^{(x_{n:1})} | T_{n:1} \rangle \quad (A5)
\]

Comparing the process tensors with the process states defined in the main text, we see that they are different in general. For example, the process tensor state \( (A3) \) is still a state in \( \mathcal{H}_S \), while the process state \( (A1) \) is a state in \( \mathcal{H}_{S}^{SE} \). But the final \( n \)-point probabilities have the same structure. The difference lies in the different splitting of state and operator in the temporal generalization of the Born rule in usual quantum mechanics. In fact, a process state can be considered as a process tensor acting the tensor product of maximally entangled states,

\[
|S_{n:1} \rangle = |T_{n:1}^{n} | \otimes \Phi^{[A_{j-1}]}(S_j) \rangle \quad (A6)
\]

if \( S_j \) denotes the system before an operation \( O \) and \( A_{j}^t \) denotes the system after an operation \( U \). Namely, we pull the curves in (9) straight for (A6) to hold.

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