

Exponential Clustering of Bipartite Quantum Entanglement at Arbitrary Temperatures

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Many inexplicable phenomena in low-temperature many-body physics are a result of macroscopic quantum effects. Such macroscopic quantumness is often evaluated via long-range entanglement, that is, entanglement in the macroscopic length scale. Long-range entanglement is employed to characterize novel quantum phases and serves as a critical resource for quantum computation. However, the conditions under which long-range entanglement is stable, even at room temperatures, remain unclear. In this regard, this study demonstrates the unstable nature of bipartite long-range entanglement at arbitrary temperatures, which exponentially decays with distance. The proposed theorem is a no-go theorem pertaining to the existence of long-range entanglement. The obtained results are consistent with existing observations, indicating that long-range entanglement at nonzero temperatures can exist in topologically ordered phases, where tripartite correlations are dominant. The derivation in this study introduces a quantum correlation defined by the convex roof of the standard correlation function. Further, an exponential clustering theorem for generic quantum many-body systems under such a quantum correlation at arbitrary temperatures is established, which yields the primary result by relating quantum correlation with quantum entanglement. Moreover, a simple application of analytical techniques is demonstrated by deriving a general limit on the Wigner-Yanase-Dyson skew and quantum Fisher information; this is expected to attract significant attention in the field of quantum metrology. Notably, this study reveals the novel, general aspects of low-temperature quantum physics and clarifies the characterization of long-range entanglement.

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I. INTRODUCTION

A. Background

In quantum many-body physics, macroscopic quantum effects such as superconductivity, Bose-Einstein condensation, quantum spin liquid, and quantum topological order are critical features of exotic quantum phenomena. In these phenomena, the length scale of the quantum effect is comparable to that in the real world. However, the clarification of such macroscopic quantum effects remains a crucial problem in modern physics, and various methods for characterizing quantumness in the macroscopic length scale have been proposed [1–4]. In particular, over the last two decades, quantum entanglement has become a representative measure for the quantumness [5,6]. Several studies have investigated the entanglement behaviors in quantum many-body systems from various perspectives

[7–16]. These advances in quantum entanglement have significantly contributed toward improving our understanding and establishing efficient classical and quantum algorithms to simulate quantum many-body systems [17–21].

A critical question regarding many-body quantum entanglement is whether entanglement can exist in the macroscopic length scale. Such entanglement is often referred to as long-range entanglement, which plays a crucial role not only in characterizing quantum phases [22,23] but also in realizing quantum computing [24–26]. It can be inferred that temperature plays an essential role in this context. Moreover, owing to the fragility of quantumness, thermal noise destroys the entanglement, making the length scale of the entanglement short range. Indeed, at a sufficiently high temperature where the possibility of thermal phase transition is eliminated, the quantum thermal state can be classified as the trivial phase [27] (i.e., generated by the finite-depth quantum circuit [22]). By contrast, at zero temperature, various quantum systems are known to exhibit long-range entanglement [28–32]. However, at nonzero but low temperatures, where thermal phase transition can occur, the effect of temperature on the entanglement remains highly unclear. In this case, the effect of thermal

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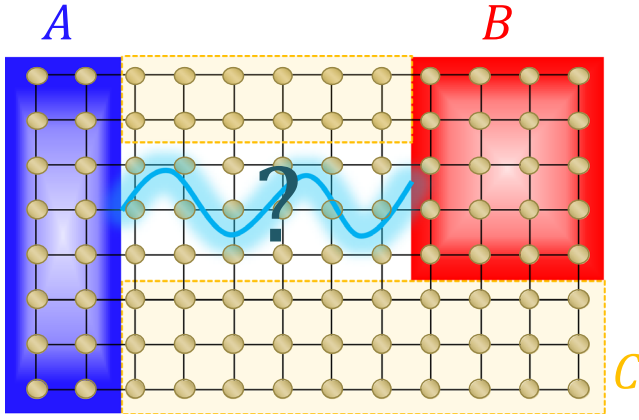


FIG. 1. Entanglement between two separated subsystems A and B . Considering the tripartite entanglement between subsystems A , B , and C , long-range entanglement at nonzero temperatures can be detected. It can also be observed in topologically ordered, quantum, many-body systems. This study aims to elaborate on the observation and prove that (more than) tripartite entanglement is required for long-range entanglement. The quantum entanglement between two systems is shown to decay exponentially with distance at arbitrary nonzero temperatures, in any quantum Gibbs state with short-range interacting Hamiltonians. Here, the entanglement-length scale, at most, grows in a polynomial manner with the inverse temperature β , as stated in inequalities (1)–(3).

noise is sufficiently suppressed, and it is possible to observe long-range entanglement in this temperature regime. Consequently, in such quantum systems, quantum phases protected by the topological order can exhibit long-range entanglement. It has been shown that, in the 4D toric code model [33], long-range entanglement can occur even at room temperatures [34,35] (see also Refs. [36,37]).

The purpose of this study is to identify the limitations associated with the structure of long-range entanglement at arbitrary nonzero temperatures. In the known example involving long-range entanglement, the protection afforded by the topological order plays an essential role. Moreover, the topological order is inherently a tripartite correlation [38–40]. However, these findings pose the following fundamental question: Can the long-range entanglement at nonzero temperatures only exist as (more than) tripartite correlations, or equivalently, does bipartite entanglement necessarily decay to zero at long distances under arbitrary temperatures? We conjecture that the answer to this question is yes (Fig. 1). The possibility of this conjecture being true can provide crucial information related to identifying the essence of long-range entanglement in the quantum phases at nonzero temperatures, which can further serve as a guideline in the search for candidate systems suitable for quantum devices. The conjecture is trivially true for arbitrary commuting Hamiltonians [41], where all the local interaction terms commute with each other. Hence, in the toric code model with the commuting Hamiltonian, bipartite long-range entanglement is strictly

prohibited, regardless of the existence of the tripartite long-range entanglement. Thus, as long as the commuting Hamiltonian is considered, the conjecture does not contradict the observations.

Thus far, rigorous and general studies on low-temperature phases remain scarce. At low temperatures, in contrast to high-temperature phases, the structures of quantum many-body systems are considerably influenced by the system details. Therefore, analyses of the low-temperature properties are often considered as computationally hard problems [43,44]. In such situations, all the long-range quantum effects are not strictly prohibited (e.g., off-diagonal long-range order [1]), with only a fraction of them being forbidden at low temperatures. In the latter example, the thermal area law is known as a representative characterization of the low-temperature phases of many-body systems, which is universally true at arbitrary temperatures [11,45,46]. It states that the entanglement between two adjacent subsystems can reach the maximum of the size of their boundaries. In other words, the area law implies that entanglement should be localized around the boundary and thus indirectly supports the argument presented.

B. Brief description of main results

Here, we provide an overview of the contributions of this study. The quantum Gibbs state is denoted as ρ_β at inverse temperature β , where a short-range interacting Hamiltonian is considered (further details are provided in Sec. II A). Let $\rho_{\beta,AB}$ be a reduced density matrix on the subsystems A and B , which are separated by distance R . For an arbitrary choice of A and B , we focus on the entanglement between A and B (Fig. 1).

First, the primary challenge faced when addressing the main problem is that the entanglement for a mixed state cannot be described in an analytically tractable form [e.g., Eqs. (20) and (79)]. Moreover, owing to the computational hardness [47,48], the entanglement cannot be computed even at numerical levels, except for specific cases [49]. However, in free fermion and harmonic chains, analytical forms of entanglement negativity [50] [see Eq. (G1)] have been obtained [51–53] at finite temperatures. These studies considered the entanglement negativity between adjacent subsystems A and B (i.e., $R = 0$) on one-dimensional chains and consequently analyzed the manner in which the negativity is saturated with an increase in the sizes of A and B (e.g., setting $|A| = |B| = \ell$ and tuning length ℓ). In these systems, the saturation rate is approximately expressed as $e^{-\ell/\mathcal{O}(\beta)}$, and Ref. [53] concluded that quantum coherence can only be maintained for length scales of $\mathcal{O}(\beta)$. Similar observations have been numerically obtained for a more general class of many-body systems [54,55]. Thus, these results strongly support the clustering of bipartite entanglement in specific models.

To overcome the difficulties in the analysis of the entanglement, first, a quantum correlation $\text{QC}_\rho(O_A, O_B)$

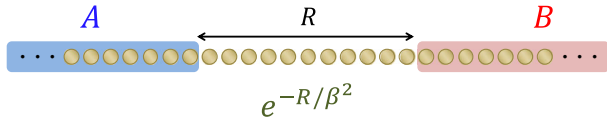


FIG. 2. Schematic of 1D entanglement clustering. In the obtained bound (2), the subset dependence $e^{\mathcal{O}(|A|+|B|)}$ prohibits its application to the upper bound of the entanglement between two large blocks. In one-dimensional systems, this problem can be resolved to obtain better subset dependence, as in Eq. (3). Here, the characteristic length of bipartite entanglement becomes $\mathcal{O}(\beta^2)$ instead of $\mathcal{O}(\beta)$.

is introduced, which is defined based on the analogy of the entanglement measure and obtained from the convex roof of the standard correlation function $C_\rho(O_A, O_B) = \text{tr}(\rho O_A O_B) - \text{tr}(\rho O_A)\text{tr}(\rho O_B)$, as in Eq. (33). The quantum correlation $\text{QC}_\rho(O_A, O_B)$ is strongly associated with entanglement (see Sec. III). In particular, the upper bound of the quantum correlation yields an upper bound for the entanglement measure of the positive-partial-transpose (PPT) relative entanglement (Proposition 9). In general, the exponential clustering of the quantum correlation at arbitrary temperatures of arbitrary dimensions can be proven (see Theorem 10):

$$\text{QC}_{\rho_\beta}(O_A, O_B) \lesssim (|\partial A| + |\partial B|)e^{-R/\xi_\beta}, \quad (1)$$

with $\xi_\beta = \mathcal{O}(\beta)$, whose explicit form is expressed as Eq. (54), where O_A and O_B are supported on subsets A and B , respectively. The inequality (1) provides a quantum version of the clustering theorem that generally holds at arbitrary temperatures.

Based on the upper bound (1), it may be possible to avoid the intractability of the quantum entanglement. Further, using the association between the quantum correlation and the entanglement, the following statement on entanglement clustering is proven (see Corollary 11):

$$E_R^{\text{PPT}}(\rho_{\beta,AB}) \lesssim e^{-R/\xi_\beta + \mathcal{O}(|A|+|B|)}, \quad (2)$$

where $E_R^{\text{PPT}}(\rho_{AB})$ is the PPT relative entanglement (50). Herein, two points can be improved: (i) A bound is obtained for E_R^{PPT} instead of the standard relative entanglement E_R , and (ii) the subset dependence is exponential (i.e., $e^{\mathcal{O}(|A|+|B|)}$) instead of polynomial [i.e., $\text{poly}(|A|, |B|)$]. To address the first point, the zero-quantum correlation must be related to the separable condition instead of the PPT condition (Lemma 8). However, this point remains to be addressed (Conjecture 7). Regarding the second point, the inequality (2) in one-dimensional systems (Theorem 12, Fig. 2) can be improved by refining the analyses based on the belief propagation [56,57]:

$$E_R^{\text{PPT}}(\rho_{\beta,AB}) \lesssim (|A| + |B|)e^{-\mathcal{O}(R/\xi_\beta^2)}. \quad (3)$$

Thus, a significantly improved clustering theorem for the bipartite entanglement measure in one-dimensional systems can be obtained.

Finally, as a related quantity, another type of quantum correlation that is based on the Wigner-Yanase-Dyson (WYD) skew information [58,59] is considered: $\bar{Q}_\rho(O_A, O_B) := \int_0^1 Q_\rho^{(\alpha)}(O_A, O_B) d\alpha$, with $Q_\rho^{(\alpha)}(O_A, O_B) := \text{tr}(\rho O_A O_B) - \text{tr}(\rho^{1-\alpha} O_A \rho^\alpha O_B)$. In a previous study [58], it was numerically verified that the quantity $\bar{Q}_\rho(O_A, O_B)$ exhibits an exponential decay with distance, even at the critical point. Because the WYD skew information is considered as a measure of quantum coherence [60], the decay rate of $\bar{Q}_\rho(O_A, O_B)$ has been dubbed as the ‘‘quantum coherence length’’ [58]. Consequently, using a similar analysis for the proof of Eq. (1), it is proven that the numerical observations in Refs. [58,59] are universally true (Theorem 13):

$$Q_{\rho_\beta}^{(\alpha)}(O_A, O_B) \lesssim (|\partial A| + |\partial B|)e^{-R/\xi'_\beta} \quad (4)$$

for arbitrary α , where $\xi'_\beta = \mathcal{O}(\beta)$ is explicitly expressed as Eq. (62). The above inequality also yields the general limits on the WYD skew information as well as the quantum Fisher information:

$$\mathcal{I}_{\rho_\beta}^{(\alpha)}(K) \lesssim \beta^D n \quad \text{and} \quad \mathcal{F}_{\rho_\beta}(K) \lesssim \beta^D n, \quad (5)$$

with K being an arbitrary operator in the form of $K = \sum_{i \in \Lambda} O_i$ (Λ : total set of sites), where $\mathcal{I}_{\rho_\beta}^{(\alpha)}(K)$ and $\mathcal{F}_{\rho_\beta}(K)$ are the WYD skew (58) and quantum Fisher (65) information, respectively. These general limits provide useful information related to the application of quantum many-body systems to quantum metrology [61–65].

The remainder of this paper is organized as follows. In Sec. II, the precise setting and notations used throughout the paper are formulated, coupled with the introduction to certain preliminaries such as the Lieb-Robinson bound and entanglement measure. In Sec. III, the quantum correlation $\text{QC}_\rho(O_A, O_B)$ is introduced as the convex roof of the standard correlation function. In addition, several rigorous results on the relationships between the quantum correlation and quantum entanglement are provided. Further, in Sec. IV, the main results on the clustering theorem for the quantum correlation [Eq. (1)] and the PPT relative entanglement [Eqs. (2) and (3)] are provided. Thereafter, in Sec. V, the obtained results are demonstrated on the WYD skew and quantum Fisher information [Eqs. (4) and (5)]. In Sec. VI, the following topics relevant to the obtained results are discussed: (i) the relationship between the macroscopic quantum effect and quantum entanglement (Sec. VI A), (ii) the relationship between entanglement clustering and the quantum Markov property (Sec. VI A), (iii) the relationship between the quantum correlation and entanglement of formation (Sec. VI C), (iv) optimality of the proposed main theorems (Sec. VI D), and (v) extension of the results

obtained to more general quantum states based on the Bernstein-Widder theorem (Sec. VI E). Finally, in Sec. VII, the study is summarized, along with a discussion regarding the scope for future work.

II. SETUP AND PRELIMINARIES

Consider a quantum system on a D -dimensional lattice with n sites. On each of the sites, the Hilbert space with dimension d_0 is assigned. Let Λ be the set of total sites. Further, for an arbitrary subset $X \subseteq \Lambda$, the cardinality (the number of sites contained in X) is denoted as $|X|$. In addition, a complementary subset of X is denoted as $X^c := \Lambda \setminus X$. For an arbitrary subset $X \subseteq \Lambda$, \mathcal{D}_X is defined as the dimension of the Hilbert space on X , that is, $\mathcal{D}_X = d_0^{|X|}$. Finally, $X \cup Y$ is denoted as XY .

For arbitrary subsets $X, Y \subseteq \Lambda$, $d_{X,Y}$ is defined as the shortest path length on the graph connecting X and Y , and hence if $X \cap Y \neq \emptyset$, $d_{X,Y} = 0$. However, when X comprises only one element (e.g., $X = \{i\}$), the distance $d_{\{i\},Y}$ is denoted as $d_{i,Y}$ for simplicity. In addition, the surface subset of X is denoted as $\partial X := \{i \in X | d_{i,X^c} = 1\}$.

For a subset $X \subseteq \Lambda$, the extended subset $X[r]$ is defined as

$$X[r] := \{i \in \Lambda | d_{X,i} \leq r\}, \quad (6)$$

where $X[0] = X$, and r is an arbitrary positive number (i.e., $r \in \mathbb{R}^+$). Based on the notation, for $i \in \Lambda$, it is concluded that the subset $i[r]$ is a ball region with radius r centered at the site i . A geometric parameter γ is introduced, which is determined based on the lattice structure alone. Further, $\gamma \geq 1$ is defined as a constant of $\mathcal{O}(1)$ that satisfies the following inequalities:

$$\max_{i \in \Lambda} (|\partial i[r]|) \leq \gamma r^{D-1}, \quad \max_{i \in \Lambda} (|i[r]|) \leq \gamma r^D, \quad (7)$$

where $r \geq 1$.

A. Hamiltonian and quantum Gibbs state

Throughout the study, generic Hamiltonians with few-body interactions are considered. Here, the Hamiltonian is expressed in the following k -local form:

$$H = \sum_{|Z| \leq k} h_Z, \quad \max_{i \in \Lambda} \sum_{Z: Z \ni i} \|h_Z\| \leq g, \quad (8)$$

where each of the interaction terms $\{h_Z\}_{|Z| \leq k}$ acts on the spins on $Z \subset \Lambda$. For an arbitrary subset $L \subset \Lambda$, the subset Hamiltonian, which includes interactions in a subset L , is denoted as H_L :

$$H_L = \sum_{Z: Z \subset L} h_Z. \quad (9)$$

To characterize the interaction strength of the Hamiltonian, the following assumption is imposed:

$$\max_{\{i,j\} \subset \Lambda} \sum_{Z \supset \{i,j\}} \|h_Z\| \leq J(d_{i,j}), \quad (10)$$

where $J(x)$ is a function that monotonically decreases with $x \geq 0$. Here, the short-range interaction is primarily considered, where the decay of the function $J(x)$ is faster than the exponential decay; in other words,

$$J(x) \leq g_0 e^{-\mu_0 x} \quad (\text{short-range interaction}) \quad (11)$$

with $g_0 = \mathcal{O}(1)$ and $\mu_0 = \mathcal{O}(1)$. The results can be generalized to a broader class of interactions, as discussed in the Appendix B.

Using the Hamiltonian, the quantum Gibbs state can be defined as follows:

$$\rho_\beta = \frac{e^{-\beta H}}{Z_\beta}, \quad Z_\beta = \text{tr}(e^{-\beta H}), \quad (12)$$

where β is the inverse temperature. Throughout the paper, by appropriately choosing the energy origin, $Z_\beta = 1$ is enforced, that is,

$$\rho_\beta = e^{-\beta H}. \quad (13)$$

However, when considering a reduced density matrix on a region L ($L \subset \Lambda$), it is denoted as $\rho_{\beta,L}$:

$$\rho_{\beta,L} := \text{tr}_{L^c}(\rho_\beta), \quad (14)$$

where tr_{L^c} implies the partial trace for the Hilbert space on the subset L^c .

B. Lieb-Robinson bound

Herein, we present the Lieb-Robinson bound that characterizes the quasilocality via time evolution [66–69]. The Lieb-Robinson bound is central to most of the derived results in this study, and it is formulated as follows:

Lemma 1. (Lieb-Robinson bound [70]) For arbitrary operators O_X and O_Y with unit norm and $d_{X,Y} = R$, the norm of the commutator $[O_X(t), O_Y]$ satisfies the following inequality:

$$\| [O_X(t), O_Y] \| \leq C \min(|\partial X|, |\partial Y|) (e^{v|t|} - 1) e^{-\mu R}, \quad (15)$$

where C , v , μ are constants of $\mathcal{O}(1)$, which depend on the system parameters, that is, k , g , g_0 , μ_0 , D , and γ .

Using the Lieb-Robinson bound (15), the approximation of $O_X(t)$ onto a local region $Y \supset X$ can be obtained. We define $O_X(t, Y)$ as

TABLE I. Fundamental parameters in our statements.

Definition	Parameters
Spatial dimension	D
Local Hilbert space dimension	d_0
Structure parameter of the lattice [see Eq. (7)]	γ
Maximum number of sites involved in interactions [see Eq. (8)]	k
Upper bound on the one-site energy [see Eq. (8)]	g
Parameters in the Lieb-Robinson bound [see Eq. (15)]	C, v, μ

$$O_X(t, Y) := \frac{1}{\text{tr}_{Y^c}(\hat{1})} \text{tr}_{Y^c} [O_X(t)] \otimes \hat{1}_{Y^c}, \quad (16)$$

where $\text{tr}_{Y^c}(\dots)$ is the partial trace for subset Y^c ; hence, the operator $O_X(t, Y)$ is supported on the subset $Y \subseteq \Lambda$. Note that $O_X(t, \Lambda) = O(t)$. As shown in Ref. [71], for arbitrary subsets $Y \supseteq X$, the following can be derived:

$$\|O_X(t) - O_X(t, Y)\| \leq \inf_{U_{Y^c}} \| [O_X(t), U_{Y^c}] \|, \quad (17)$$

where $\inf_{U_{Y^c}}$ accepts all unitary operators U_{Y^c} that are supported on Y^c . On selecting $Y = X[R]$ with $R \in \mathbb{N}$, the following inequality can be obtained using the Lieb-Robinson bound (15):

$$\|O_X(t) - O_X(t, X[R])\| \leq C|\partial X|(e^{v|R|} - 1)e^{-\mu R}, \quad (18)$$

where the inequality (15) is applied to $[O_X(t), U_{X[R]^c}]$ with $U_{X[R]^c}$ an arbitrary unitary operator. Based on the above inequality, it can be ensured that $O_X(t) \approx O_X(t, X[R])$ for $R \gtrsim (v/\mu)t$. Often, (v/μ) is referred to as the ‘‘Lieb-Robinson velocity’’: $v_{\text{LR}} = v/\mu$. In Table I, the fundamental parameters used are summarized.

Provided the Lieb-Robinson bound holds, the primary results of this study can be extended to more general quantum systems such as long-range interacting systems with power-law decaying interactions (see also Appendix B).

C. Quantum entanglement

Here, the basic definition of quantum entanglement [5,72] is presented. First, $\text{SEP}(A:B)$ is defined as a set of separable quantum states on the subset AB . For an arbitrary quantum state ρ , the reduced density matrix ρ_{AB} satisfies $\rho_{AB} \in \text{SEP}(A:B)$ if and only if the following decomposition exists:

$$\rho_{AB} = \sum_s p_s \rho_{s,A} \otimes \rho_{s,B}. \quad (19)$$

When ρ_{AB} is a pure state, $\rho_{AB} \in \text{SEP}(A:B)$ implies that ρ_{AB} is given by the product state. Further, a quantum state ρ_{AB} is defined to be entangled if and only if $\rho_{AB} \notin \text{SEP}(A:B)$.

In quantifying the entanglement, the relative entanglement [73–75] can be adopted as follows:

$$E_R^{\mathcal{X}}(\rho_{AB}) := \inf_{\sigma_{AB} \in \mathcal{X}} S(\rho_{AB} \| \sigma_{AB}), \quad (20)$$

where \mathcal{X} is the arbitrary class of quantum states (focus of this study) and $S(\rho_{AB} \| \sigma_{AB})$ is the relative entropy:

$$S(\rho_{AB} \| \sigma_{AB}) := \text{tr}[\rho_{AB} \log(\rho_{AB})] - \text{tr}[\rho_{AB} \log(\sigma_{AB})]. \quad (21)$$

In particular, on choosing $\mathcal{X} = \text{SEP}(A:B)$, the following is denoted,

$$E_R(\rho_{AB}) := \inf_{\sigma_{AB} \in \text{SEP}(A:B)} S(\rho_{AB} \| \sigma_{AB}), \quad (22)$$

for simplicity.

The relative entanglement $E_R(\rho_{AB})$ is also related to the closeness of the target state to the zero-entangled state. Pinsker’s inequality entails

$$\|\rho_{AB} - \sigma_{AB}\|_1 \leq \sqrt{2S(\rho_{AB} \| \sigma_{AB})} \quad (23)$$

for an arbitrary σ_{AB} . Hence, definition (22) immediately yields

$$\delta_{\rho_{AB}} := \inf_{\sigma_{AB} \in \text{SEP}(A:B)} \|\rho_{AB} - \sigma_{AB}\|_1 \leq \sqrt{2E_R(\rho_{AB})}. \quad (24)$$

The quantity $\delta_{\rho_{AB}}$ yields meaningful upper bounds for various entanglement measures. Using the continuity of the information measures [76,77], most of the entanglement measures are upper bounded by $\mathcal{O}(\delta_{\rho_{AB}}) \times \log(D_{AB})$, such as the entanglement of formation [78], the entanglement of purification [77], the relative entanglement [79], and the squashed entanglement [76,80].

D. Clustering theorem at high temperatures: Known results

This section reviews an established clustering theorem that holds above a threshold temperature, which is usually determined by the convergence of the cluster expansion. In high-temperature regimes, clustering of the entanglement can be immediately derived by combining Pinsker’s inequality and the exponential decay of the mutual information (Corollary 4 below).

For an arbitrary quantum state ρ , the standard correlation function $C_\rho(O_A, O_B)$ between observables O_A and O_B can be defined as

$$C_\rho(O_A, O_B) := \text{tr}(\rho O_A O_B) - \text{tr}(\rho O_A) \cdot \text{tr}(\rho O_B). \quad (25)$$

As a stronger concept of the bipartite correlation, the mutual information $\mathcal{I}_\rho(A:B)$ between two subsystems A and B can be defined as follows:

$$\mathcal{I}_\rho(A:B) := S_\rho(A) + S_\rho(B) - S_\rho(AB), \quad (26)$$

where $S_\rho(A)$ is the von Neumann entropy for the reduced density matrix on subset A , that is, $S_\rho(A) := \text{tr}[-\rho_A \log(\rho_A)]$, with ρ_A being the reduced density matrix on A [see Eq. (14)].

Previous studies [81,82] have provided the following clustering theorem, which holds at arbitrary temperatures as $\beta \lesssim \log(n)$ (see also Ref. [83]):

Lemma 2. (1D clustering theorem) Let O_A and O_B be arbitrary operators supported on subsets A and B , respectively. When a quantum Gibbs state ρ_β as in Eq. (13) with $D = 1$ is considered, the following inequality holds at arbitrary temperatures $\beta \lesssim \log(n)$ (n : system size) [81]:

$$C_{\rho_\beta}(O_A, O_B) \leq \text{poly}(|A|, |B|) \exp\left(-\frac{R}{e^{\Omega(\beta)}}\right), \quad (27)$$

where $d_{A,B} = R$, and the notation $\Omega(\beta)$ denotes $\Omega(\beta) \propto \beta^{1+z}$ ($z \geq 0$). In addition, the mutual information $\mathcal{I}_\rho(A:B)$ decays exponentially with distance [82]:

$$\mathcal{I}_\rho(A:B) \leq \text{poly}(|A|, |B|) \exp\left(-\frac{R}{e^{\Omega(\beta)}}\right). \quad (28)$$

A similar result holds in arbitrary-dimensional systems:

Lemma 3. (high-dimensional clustering theorem) Under the same setup as in Lemma 2, the following inequality holds at arbitrary temperatures, such that $\beta < \beta_c$ in arbitrary-dimensional systems [84–88]:

$$C_{\rho_\beta}(O_A, O_B) \leq \text{poly}(|A|, |B|) \exp\left(-\frac{R}{\mathcal{O}(1)}\right), \quad (29)$$

where β_c is a constant that does not depend on the system size. Furthermore, the mutual information $\mathcal{I}_\rho(A:B)$ decays exponentially with distance [27]:

$$\mathcal{I}_\rho(A:B) \leq \text{poly}(|A|, |B|) \exp\left(-\frac{R}{\mathcal{O}(1)}\right). \quad (30)$$

Lemmas 2 and 3 immediately imply the exponential decay of the bipartite quantum entanglement. Consequently, using Pinsker's inequality (23) and the equation

$$\mathcal{I}_\rho(A:B) = S(\rho_{AB} \| \rho_A \otimes \rho_B), \quad (31)$$

the following corollary is obtained:

Corollary 4. In the temperature regimes $\beta \lesssim \log(n)$ (1D) and $\beta < \beta_c$ (high dimensions), the trace distance of $\|\rho_{AB} - \rho_A \otimes \rho_B\|_1$ exponentially decays with the distance between regions A and B :

$$\|\rho_{AB} - \rho_A \otimes \rho_B\|_1 \leq \text{poly}(|A|, |B|) e^{-\mathcal{O}(R)}. \quad (32)$$

Owing to $\rho_A \otimes \rho_B \in \text{SEP}(A:B)$, the above corollary implies $\delta_{\rho_{AB}} \lesssim e^{-\mathcal{O}(R)}$. For the relative entanglement (22), $E_R(\rho_{AB}) \leq \text{poly}(|A|, |B|) e^{-\mathcal{O}(R)}$ is obtained from the continuity bound [79]. Therefore, in high-temperature regimes, the problem of bipartite entanglement clustering can be easily proved using the established results [89]. Consequently, this study focuses on the low-temperature regimes, where thermal phase transitions can occur and the clustering of bipartite correlations may no longer be satisfied.

III. QUANTUM CORRELATION

Before discussing the entanglement clustering theorem, the quantum correlation function, defined as a convex roof of the standard correlation function $C_\rho(O_A, O_B)$ in Eq. (25), must be considered. Quantum correlation is a natural quantum analog of the standard correlation function and has a significant relationship with quantum entanglement (Sec. III B). Quantum correlation is introduced for two primary reasons:

- (1) The clustering theorem for quantum correlation can be proved in a completely general manner (Theorem 10).
- (2) The clustering of quantum correlation is also utilized to prove the entanglement clustering theorems (Corollary 11 and Theorem 12).

A. Definition

For an arbitrary many-body quantum state ρ , the quantum correlation for observables O_A and O_B can be defined by the convex roof of the standard correlation function (25), that is, $C_\rho(O_A, O_B) [= \text{tr}(\rho O_A O_B) - \text{tr}(\rho O_A) \cdot \text{tr}(\rho O_B)]$:

$$\text{QC}_\rho(O_A, O_B) := \inf_{\{p_s, \rho_s\}} \sum_s p_s |C_{\rho_s}(O_A, O_B)|, \quad (33)$$

where minimization is performed for all possible decompositions of ρ such that $\rho = \sum_s p_s \rho_s$ with $p_s > 0$, and ρ_s is a quantum state. Herein, the mixed convex roof was adopted instead of the pure convex roof, for which decomposed states $\{\rho_s\}$ are restricted to the pure state; in other words, $\rho_s = |\phi_s\rangle\langle\phi_s|$ for $\forall s$. This is because using it ensures inequality (37) in Lemma 5. For example, the mixed convex roof has been considered in Refs. [91–94].

Subsequently, the definition immediately implies

$$\text{QC}_\rho(O_A, O_B) = |C_\rho(O_A, O_B)| \quad (34)$$

when ρ is given by the pure state.

The quantum correlations for a density matrix ρ may be different from those for a reduced density matrix ρ_L ($L \subset \Lambda$), that is, $\text{QC}_{\rho_L}(O_A, O_B) \neq \text{QC}_\rho(O_A, O_B)$ [Eq. (37)]. For example, consider the case wherein ρ is given by the Greenberger-Horne-Zeilinger (GHZ) state as follows:

$$\frac{1}{2}(|0_\Lambda\rangle + |1_\Lambda\rangle)(\langle 0_\Lambda| + \langle 1_\Lambda|), \quad (35)$$

where $|0_\Lambda\rangle$ ($|1_\Lambda\rangle$) is the product state of $|0_i\rangle$ ($|1_i\rangle$) states ($i \in \Lambda$). Then, the quantum state ρ has a nonzero quantum correlation, based on Eq. (34), while the reduced density matrices in arbitrary subsystems $L \subset \Lambda$ are given by a mixed state of $|0_L\rangle$ and $|1_L\rangle$, each of which exhibits no correlations. Hence, no quantum correlations exist in the reduced density matrix of the GHZ state.

As the basic properties of $\text{QC}_\rho(O_A, O_B)$, the following lemma is proven:

Lemma 5. Let O_A and O_B be arbitrary operators supported on A and B , respectively. Subsequently, the following inequalities are obtained:

$$\text{QC}_\rho(O_A, O_B) \leq |C_\rho(O_A, O_B)| \quad (36)$$

and

$$\text{QC}_{\rho_L}(O_A, O_B) \leq \text{QC}_\rho(O_A, O_B), \quad (37)$$

where $A \subseteq L$ and $B \subseteq L$. The second inequality is consistent with the example of the GHZ state (35).

In addition, the quantum correlation satisfies the following continuity bound. For two arbitrary quantum states ρ and σ , the difference between $\text{QC}_\rho(O_A, O_B)$ and $\text{QC}_\sigma(O_A, O_B)$ is upper bounded as

$$|\text{QC}_\sigma(O_A, O_B) - \text{QC}_\rho(O_A, O_B)| \leq 7\sqrt{2}\epsilon^{1/2}, \quad (38)$$

where $\|O_A\| = \|O_B\| = 1$ and $\epsilon = \|\sigma - \rho\|_1$ are set.

Proof.—The proof of inequality (36) is obtained by choosing the decomposition as $\rho = p_1\rho_1$ with $p_1 = 1$ and $\rho_1 = \rho$ in definition (33). Regarding the second inequality, the decomposition $\{\rho_s, \rho_s\}$ is considered such that

$$\sum_s p_s |C_{\rho_s}(O_A, O_B)| = \text{QC}_\rho(O_A, O_B). \quad (39)$$

For the reduced density matrix ρ_L , the decomposition using $\{\rho_s, \rho_s\}$ is chosen as

$$\rho_L = \sum_s p_s \rho_{s,L}, \quad \rho_{s,L} = \text{tr}_{L^c}(\rho_s). \quad (40)$$

Subsequently, $|C_{\rho_s}(O_A, O_B)| = |C_{\rho_{s,L}}(O_A, O_B)|$ is obtained, and hence, inequality (37) is derived as

$$\begin{aligned} \text{QC}_{\rho_L}(O_A, O_B) &\leq \sum_s p_s |C_{\rho_{s,L}}(O_A, O_B)| \\ &= \text{QC}_\rho(O_A, O_B). \end{aligned} \quad (41)$$

Finally, the inequality (38) is proven via the application of the method in Ref. [91] (Proposition 5). For the standard correlation $C_\rho(O_A, O_B)$, straightforward calculations yield

$$|C_\rho(O_A, O_B)| \leq 1 \quad (42)$$

and

$$|C_\rho(O_A, O_B) - C_\sigma(O_A, O_B)| \leq 3\|\rho - \sigma\|_1, \quad (43)$$

where $\|O_A\| = \|O_B\| = 1$. Hence, we can choose parameters K and M in Eqs. (29) and (30) of Ref. [91] as $K = 3/\log(d_X)$ and $M = 1/\log(d_X)$, where d_X is the total Hilbert space dimension for ρ , that is, $d_X = \mathcal{D}_\Lambda$ according to this study's notations. Thus, inequality (38) can be obtained from Eqs. (31) and (51) and Proposition 5 of Ref. [91]. This completes the proof. ■

B. Condition for zero quantum correlation

As a trivial statement, we first prove the following lemma:

Lemma 6. For a quantum state ρ_{AB} supported on $A \cup B$, the quantum correlation $\text{QC}_{\rho_{AB}}(O_A, O_B)$ is equal to zero for arbitrary operators O_A and O_B if ρ_{AB} is not entangled between the subsystems A and B [i.e., $\rho_{AB} \in \text{SEP}(A:B)$]:

$$\rho_{AB} \in \text{SEP}(A:B) \rightarrow \text{QC}_{\rho_{AB}}(O_A, O_B) = 0 \quad (44)$$

for arbitrary pairs of O_A, O_B . Considering the contraposition of statement (44), it can be concluded that

$$\begin{aligned} \text{QC}_{\rho_{AB}}(O_A, O_B) \neq 0 &\text{ for a pair of } O_A, O_B \\ &\rightarrow \rho_{AB} \notin \text{SEP}(A:B). \end{aligned} \quad (45)$$

Proof.—Considering definition (19) for $\text{SEP}(A:B)$, there exists a decomposition of

$$\rho_{AB} = \sum_s p_s \rho_{s,A} \otimes \rho_{s,B} \quad (46)$$

when the quantum state ρ_{AB} is not entangled. For such a decomposition, the state ρ_{AB} exhibits no quantum correlations for operators O_A or O_B :

$$\text{QC}_{\rho_{AB}}(O_A, O_B) \leq \sum_s p_s |C_{\rho_{s,A} \otimes \rho_{s,B}}(O_A, O_B)| = 0. \quad (47)$$

This completes the proof. ■

Thus, zero entanglement has been proven to be a sufficient condition for the zero-quantum correlation, as in Eq. (44). However, this leads to the immediate question of whether the converse is also true, that is,

$$\begin{aligned} \text{QC}_{\rho_{AB}}(O_A, O_B) = 0 &\text{ for arbitrary pairs of } O_A, O_B \\ &\stackrel{?}{\longrightarrow} \rho_{AB} \in \text{SEP}(A:B). \end{aligned} \quad (48)$$

To address this question, the following conjecture is proposed:

Conjecture 7. Statement (48) is true. In other words, the zero-quantum correlation for arbitrary pairs of O_A, O_B is necessary and sufficient for zero entanglement. The reason for considering the conjecture to be true is that the following relationship exists for the standard correlation function:

$$C_{\rho_{AB}}(O_A, O_B) = 0 \quad \text{for arbitrary pairs of } O_A, O_B \\ \Leftrightarrow \rho_{AB} \text{ is a product state.} \quad (49)$$

Hence, it is natural to expect that the quantum version of the above relationship is true as well. Regarding the above conjecture, at the very least, the following statement can be proven:

Lemma 8. If $\text{QC}_{\rho_{AB}}(O_A, O_B) = 0$ for arbitrary pairs of O_A, O_B , the Peres-Horodecki separability criterion [95,96], i.e., the PPT condition, is satisfied. Thus, the operator $\rho_{AB}^{T_A}$ has no negative eigenvalues, where T_A is the partial transpose with respect to the Hilbert space on the subset A .

Proof.—The statement is immediately followed by Proposition 9 below. The condition that $\text{QC}_{\rho_{AB}}(O_A, O_B) = 0$ for arbitrary pairs of O_A, O_B implies $\epsilon = 0$ in Eq. (51). Hence, by applying $\epsilon = 0$ to inequality (52), $\rho_{AB} \in \text{PPT}$ is obtained, where PPT is a set of states such that the PPT condition is satisfied [Eq. (50) below]. This completes the proof. ■

The above lemma shows that Conjecture 7 rigorously holds for a certain class of quantum systems, such as $2 \times 2, 2 \times 3$ quantum systems [96,97]. Thus, any attempt to prove or disprove the conjecture in general cases must consider the existence of the bound entanglement [98,99]. A possible route to proving Conjecture 7 relies on the entanglement witness [100–103]. However, appropriately reducing the calculations of the witness to those of quantum correlations is a challenging task. As shown in the proofs of Proposition 9 and Lemma 25 below, the calculation of the partial transpose can be related to the quantum correlations.

C. PPT relative entanglement

Finally, in this section, quantum correlation is related to the PPT relative entanglement. As shown in Lemma 8, quantum correlation is proven to be strongly related to the PPT condition. Consequently, using this property, quantum correlations can be related to the following PPT relative entanglement [104–107]:

$$E_R^{\text{PPT}}(\rho_{AB}) := \inf_{\sigma_{AB} \in \text{PPT}} S(\rho_{AB} \| \sigma_{AB}), \quad (50)$$

where $\mathcal{X} = \text{PPT}$ is used in Eq. (20) with PPT a set of the quantum states σ_{AB} that satisfy the PPT condition, that is, $\sigma_{AB}^{T_A} \geq 0$ for $\sigma_{AB} \in \text{PPT}$. Because the PPT set includes the separable set SEP ($\text{PPT} \supseteq \text{SEP}$), $E_R^{\text{PPT}}(\rho_{AB})$ is smaller than or equal to $E_R(\rho_{AB})$, except for special cases. As shown in Ref. [74], the PPT relative entanglement satisfies all basic

conditions for the entanglement measure (i.e., the four conditions in Ref. [72]). In addition, it provides an upper bound for Rains' bound [108,109], which is strongly related to the distillable entanglement [104,108].

As shown in the following proposition, the quantum correlation (33) provides an upper bound for the PPT relative entanglement (see Appendix E for the proof):

Proposition 9. Let ρ_{AB} be an arbitrary quantum state such that

$$\text{QC}_{\rho_{AB}}(O_A, O_B) \leq \epsilon \|O_A\| \cdot \|O_B\| \quad (51)$$

for two arbitrary operators O_A and O_B . Thus,

$$E_R^{\text{PPT}}(\rho_{AB}) \leq 4\mathcal{D}_{AB}\bar{\delta} \log(1/\bar{\delta}) \leq 4\mathcal{D}_{AB}\bar{\delta}^{1/2}, \\ \bar{\delta} := 4\epsilon \min(\mathcal{D}_A, \mathcal{D}_B), \quad (52)$$

where the second inequality is trivially derived from $x \log(1/x) \leq x^{1-1/e} \leq x^{1/2}$ for $0 \leq x \leq 1$. Recall that \mathcal{D}_{AB} is the Hilbert space dimension in the region AB . Based on the proposition, if there are no quantum correlations, that is, if $\epsilon = 0$ in Eq. (51), it can be ensured that $E_R^{\text{PPT}}(\rho_{AB}) = 0$, which also yields Lemma 8. Consequently, the clustering theorem for the quantum correlation can be associated with that for quantum entanglement. In the following section, the generic quantum Gibbs states are presented to satisfy the exponential clustering for quantum correlations at arbitrary temperatures, thereby indicating that the entanglement clustering theorem also holds.

IV. EXPONENTIAL CLUSTERING FOR QUANTUM CORRELATIONS

In this section, the main theorems of this study on the exponential clustering of the quantum correlations as well as quantum entanglement are presented. The theorems capture the universal structures of generic quantum Gibbs states at arbitrary temperatures.

First, consider the following theorem on quantum correlation (see Appendix D for the proof):

Theorem 10. Let O_A and O_B be arbitrary operators with the unit norm that are supported on the subsets $A \subset \Lambda$ and $B \subset \Lambda$, respectively ($d_{A,B} = R$). Then, when a quantum state ρ is given by a quantum Gibbs state with the short-range Hamiltonian (11) ($\rho = \rho_\beta$), the quantum correlation $\text{QC}_{\rho_\beta}(O_A, O_B)$ is upper bounded as follows:

$$\text{QC}_{\rho_\beta}(O_A, O_B) \\ \leq C_\beta (|\partial A| + |\partial B|) (1 + \log |AB|) e^{-R/\xi_\beta}, \quad (53)$$

where $C_\beta = c_{\beta,1} + c_{\beta,2}$, and the parameters $c_{\beta,1}$, $c_{\beta,2}$, and ξ_β can be defined as follows:

$$\xi_\beta := \frac{4}{\mu} \left(1 + \frac{v\beta}{\pi}\right), \quad c_{\beta,1} := e^{2/\xi_\beta} \left(\frac{24}{\pi} + \frac{12C}{v\beta}\right),$$

$$c_{\beta,2} := e^{2/\xi_\beta} \left(\frac{12+3C}{\pi} + \frac{3C}{v\beta}\right) [2 + \log(1+2g\beta)]. \quad (54)$$

The basic parameters are summarized in Table I.

Remark. The constant C_β depends on the inverse temperature β ; however, it increases, at most, logarithmically with β , that is, $C_\beta = \mathcal{O}(\log(\beta))$. By contrast, in the limit of $\beta \rightarrow +0$, the upper bound for $\text{QC}_{\rho_\beta}(O_A, O_B)$ apparently breaks down. However, the temperatures of $\beta \ll 1$ correspond to the high-temperature regime; hence, a significantly stronger statement (e.g., exponential decay of the mutual information, see Sec. IID) can be proven using the cluster expansion technique [27]. Therefore, the important temperature regime is $\beta \gg 1$, which cannot be captured by cluster expansion. Finally, it must be considered that the inequality (53) yields nontrivial upper bounds even for $\beta = \mathcal{O}(n^z)$ ($z > 0$).

A. Exponential entanglement clustering

The combination of Proposition 9 with Theorem 10 yields the following corollary:

Corollary 11. Let ρ_β be a quantum state given by a quantum Gibbs state with the short-range Hamiltonian (11). Then, for arbitrary subsystems A and B separated by a distance R (i.e., $d_{A,B} = R$), the PPT relative entanglement is upper bounded by

$$E_R^{\text{PPT}}(\rho_{\beta,AB}) \leq 8C_\beta^{1/2} e^{-R/(2\xi_\beta)+3\log(\mathcal{D}_{AB})} \quad (55)$$

with $\{C_\beta, \xi_\beta\}$ defined in Eq. (54), where we use $|\partial A| + |\partial B| \leq \mathcal{D}_{AB}$, $1 + \log|AB| \leq \mathcal{D}_{AB}$, and $\min(\mathcal{D}_A, \mathcal{D}_B) \leq \mathcal{D}_{AB}$ in applying inequality (53) to (52).

In the above upper bound, the bipartite entanglement decays exponentially beyond a distance $R \gtrsim \mathcal{O}(|A| + |B|)$. Hence, the inequality is meaningless when A and B depend on the system size (i.e., $\mathcal{D}_{AB} = e^{\mathcal{O}(n)}$). However, it cannot be improved using the decay of quantum correlations alone. To highlight this, consider a random state $|\psi_{\text{rand}}\rangle$ that has the same property as the infinite temperature states, provided the local regions are considered. As shown in Refs. [110,111], the state $|\psi_{\text{rand}}\rangle$ satisfies exponential clustering for the standard correlation functions (25), which clearly implies the exponential decay of quantum correlations from inequality (36). However, the state $|\psi_{\text{rand}}\rangle$ exhibits a large quantum entanglement between A and B , implying that the characteristics of the quantum Gibbs state must be exploited.

Further, using the quantum belief propagation technique [56,57], inequality (55) can be significantly improved for one-dimensional cases (see Appendix F for the proof):

Theorem 12. Let H be a 1D quantum Hamiltonian with a finite interaction length of k , at most. Thus, the PPT relative entanglement is upper bounded by

$$E_R^{\text{PPT}}(\rho_{\beta,AB}) \leq \bar{C}_\beta \log(\mathcal{D}_{AB}) e^{-R/[6\log(d_0)\xi_\beta^2]+7gk\beta}, \quad (56)$$

where d_0 is defined as the one-site Hilbert space dimension and $\bar{C}_\beta := 24(\bar{C}_\beta + 16d_0^4 C_\beta)^{1/2}$, with C_β defined in Eq. (54) and \bar{C}_β defined in Eq. (F6) as

$$\bar{C}_\beta := 1280 \left(\frac{5 + 2Ce^{\mu k}}{\pi^2} + \frac{2Ce^{\mu k}}{\pi v\beta} \right)^2. \quad (57)$$

Remark. The assumption of the finite interaction length in the statement is not essential. However, without this assumption, inequality (F35) in the proof becomes slightly more complicated.

Here, the PPT relative entanglement has been considered. In addition, the definition of $E_R^{\text{PPT}}(\rho_{\beta,AB})$ is significantly associated with that of entanglement negativity [50], which is another popular entanglement measure, particularly in the context of numerical calculations. Furthermore, part of the above results pertaining to PPT relative entanglement can be applied to entanglement negativity (Appendix G).

V. QUANTUM CORRELATIONS BASED ON THE SKEW INFORMATION

Herein, another type of quantum correlation based on the WYD skew information [112–114] is considered:

$$\mathcal{I}_\rho^{(\alpha)}(K) := \text{tr}(\rho K^2) - \text{tr}(\rho^{1-\alpha} K \rho^\alpha K) \quad (58)$$

for $0 < \alpha < 1$, where K is an arbitrary operator. The WYD skew information is considered as a measure of the non-commutability between ρ and K . However, as a representative application, it is utilized in formulating the Heisenberg uncertainty relation for mixed states [115–118]. More recently, the WYD skew information has garnered attention in the context of the quantum coherence theory [60,119–122].

In Refs. [58,59,123,124], the following quantity has been defined to characterize quantum correlations:

$$\bar{Q}_\rho(O_A, O_B) := \int_0^1 Q_\rho^{(\alpha)}(O_A, O_B) d\alpha$$

$$= \text{tr}(\rho O_A O_B) - \int_0^1 \text{tr}(\rho^{1-\alpha} O_A \rho^\alpha O_B) d\alpha \quad (59)$$

with

$$Q_\rho^{(\alpha)}(O_A, O_B) := \text{tr}(\rho O_A O_B) - \text{tr}(\rho^{1-\alpha} O_A \rho^\alpha O_B). \quad (60)$$

The quantity $Q_\rho^{(\alpha)}(O_A, O_B)$ is reduced to the standard correlation function $C_\rho(O_A, O_B)$ when ρ is a pure state.

The authors in Refs. [58,59] numerically verified that the quantum correlation defined by $\bar{Q}_\rho(O_A, O_B)$ decays exponentially with a finite correlation length, even at critical

points, in hard-core bosons and quantum rotors on a 2D square lattice. However, whether these observations hold universally at arbitrary temperatures remains unclear. This problem can be resolved through the following theorem (see Appendix C for the proof):

Theorem 13. The quantum correlation (60) is upper bounded for $0 \leq \alpha \leq 1$ as follows:

$$Q_{\rho\beta}^{(\alpha)}(O_A, O_B) \leq C'_\beta \min(|\partial A|, |\partial B|) e^{-R/\xi'_\beta}, \quad (61)$$

where C'_β and ξ'_β are characterized solely by the parameters in the Lieb-Robinson bound (15) as follows:

$$C'_\beta = \frac{12 + 2C}{\pi} + \frac{4C}{v\beta}, \quad \xi'_\beta{}^{-1} = \frac{\mu}{2 + (v\beta)/\pi}. \quad (62)$$

It is evident that the same upper bound trivially holds for $\tilde{Q}_\rho(O_A, O_B)$ in Eq. (59).

As shown in Appendix C, the proof technique employed here is similar to that in Refs. [125,126], where the clustering theorem for specific operators in fermion systems at arbitrary temperatures has been proven.

Thus, using Theorem 13, a general upper bound for the WYD skew information (see Appendix C 2 for the proof) can be obtained:

Corollary 14. Let K be an operator expressed as

$$K = \sum_{i \in \Lambda} O_i \quad (\|O_i\| \leq 1). \quad (63)$$

Then, the WYD skew information $\mathcal{I}_{\rho\beta}^{(\alpha)}(K)$ ($0 \leq \alpha \leq 1$) is upper bounded by

$$\begin{aligned} \mathcal{I}_{\rho\beta}^{(\alpha)}(K) &:= \text{tr}(\rho_\beta K^2) - \text{tr}(\rho_\beta^{1-\alpha} K \rho_\beta^\alpha K) \\ &\leq \tilde{C}'_\beta \xi_{\beta'}^D n = \mathcal{O}(\beta^D) n, \end{aligned} \quad (64)$$

where $\tilde{C}'_\beta := C'_\beta [(\mu/2)^D + \gamma e^{\mu/2} D!]$.

A. Quantum Fisher information

As a relevant quantity, the quantum Fisher information $\mathcal{F}_\rho(K)$, which is defined as follows [127], is considered:

$$\mathcal{F}_\rho(K) = \sum_{s,s'} \frac{2(\lambda_s - \lambda_{s'})^2}{\lambda_s + \lambda_{s'}} |\langle \lambda_s | K | \lambda_{s'} \rangle|^2, \quad (65)$$

where $K = \sum_{i \in \Lambda} O_i$ and $\rho = \sum_s \lambda_s |\lambda_s\rangle \langle \lambda_s|$ ($\lambda_s > 0$). Here, λ_s and $|\lambda_s\rangle$ are defined by the spectral decomposition $\rho = \sum_s \lambda_s |\lambda_s\rangle \langle \lambda_s|$. When considering the quantum Gibbs states (i.e., ρ_β), $\lambda_s = e^{-\beta E_s}$ and $|\lambda_s\rangle = |E_s\rangle$ are obtained, where $|E_s\rangle$ is the eigenstate of the Hamiltonian with the corresponding eigenenergy E_s . Subsequently, the quantum Fisher information is expressed as

$$\mathcal{F}_{\rho\beta}(K) = \sum_{s,s'=1}^{\mathcal{D}_\Lambda} \frac{2(e^{-\beta E_s} - e^{-\beta E_{s'}})^2}{e^{-\beta E_s} + e^{-\beta E_{s'}}} |\langle E_s | K | E_{s'} \rangle|^2,$$

where \mathcal{D}_Λ is the dimension of the total Hilbert space.

The quantum Fisher information was introduced in the field of quantum metrology [128–131]. As per the definition (65), the quantum Fisher information $\mathcal{F}_\rho(K)$ characterizes the sensitivity of the quantum state ρ to the unitary transformation $e^{-iK\theta}$. Specifically, the uncertainty in estimating the parameter θ is lower-bounded by the quantum Cramér-Rao bound [128,129]:

$$\Delta\theta \geq \frac{1}{\sqrt{m\mathcal{F}_\rho(K)}}, \quad (66)$$

where m is the number of independent measurements on $e^{-iK\theta} \rho e^{iK\theta}$. Thus, with an increase in the quantum Fisher information, the required number of measurements decreases. In the context of the entanglement theory, this is also regarded among the representative measures for macroscopic quantum entanglement [6,127,132–135]. In recent studies, the quantum Fisher information has garnered attention in the development of quantum technologies (see Refs. [6,136,137] for recent reviews).

The quantum Fisher information is associated with the WYD skew information through the inequality $(\mathcal{F}_{\rho\beta}(K)/4) \leq 2\mathcal{I}_{\rho\beta}^{(\alpha=1/2)}(K)$, which was proven in Theorem 2 of Ref. [138] (see also Ref. [139]). Hence, based on inequality (64), the upper bound can be obtained as

$$\mathcal{F}_{\rho\beta}(K) \leq 8\tilde{C}'_\beta \xi_{\beta'}^D n, \quad (67)$$

where \tilde{C}'_β and $\xi_{\beta'}$ are defined in Corollary 14. By contrast, a general lower bound for the quantum Fisher information is provided in Ref. [140]. Further, in Appendix H, several discussions related to the fundamental properties of the quantum Fisher information and quantum Fisher information matrix, which plays an important role in quantum correlation, are presented.

To discuss macroscopic entanglement using the quantum Fisher information, the scaling exponent $\mathcal{F}_{\rho\beta}(K) \propto n^p$ ($p \leq 2$) is considered. When $p = 2$, the state is composed of the superposition of macroscopically different quantum states; for example, the GHZ state has $p = 2$ [127,132]. By contrast, when $p = 1$, scaling is the same as the product states, and macroscopic superposition does not exist. Based on inequality (67), the scaling of the Fisher information is always given by $\mathcal{O}(n)$ (i.e., $p = 1$), provided $\beta = \text{poly-}\log(n)$. Thus, the results obtained offer rigorous proof for the absence of macroscopic superposition at finite temperatures.

At the quantum critical point (i.e., $\beta = \infty$), scaling of the quantum Fisher information typically behaves as $p > 1$ [see Eq. (22) of Ref. [140]; for example, $p = 7/4$ for the

critical transverse Ising model [141,142]. The obtained upper bound (67) characterizes the necessary temperature required when applying the many-body macroscopic entanglement to quantum metrology [61–65]; this has attracted considerable attention in recent studies.

VI. FURTHER DISCUSSION

A. Macroscopic quantum effect vs quantum entanglement

The entanglement properties have been discussed in the finite-temperature Gibbs state. This section shows that, in general, the observations on the entanglement properties for the finite-temperature mixed state are considerably different from those for pure states. Nevertheless, the typical unusual wave function at low temperatures in condensed matter physics is worth discussing, such as Bardeen-Cooper-Schrieffer states in a superconductor, which exhibit off-diagonal long-range orders (ODLRO [1]). In Refs. [143,144], Vedral discussed η -pairing states, which are eigenstates in the Hubbard and similar models, to explain high-temperature superconductivity. It was argued that such states have a vanishing entanglement between two sites as the distance diverges, whereas the classical correlations remain finite even in the thermodynamic limit. In addition, maximally mixed states with η -pairing states also exhibit this property. Consequently, this observation suggests that ODLRO is not directly associated with the quantum entanglement discussed in this study. The quantum entanglement properties in the finite-temperature Gibbs state have not been analytically scrutinized under a general framework thus far. However, recent large-scale numerical computations involving two-dimensional transverse field Ising models revealed that entanglement measured via the Rényi negativity is short-ranged, even at finite critical temperatures [54,55]. This observation is consistent with the general statement in the present study.

B. Relation to the quantum Markov property

In this subsection, a brief derivation of the relation between the clustering of quantum entanglement and the approximate quantum Markov property is presented.

For this purpose, the squashed entanglement [80,145,146], defined using the conditional mutual information $\mathcal{I}_{\rho_{ABE}}(A:B|E)$ for tripartite quantum systems, is considered:

$$\begin{aligned} \mathcal{I}_{\rho_{ABE}}(A:B|E) &:= S_{\rho_{ABE}}(AE) + S_{\rho_{ABE}}(BE) \\ &\quad - S_{\rho_{ABE}}(ABE) - S_{\rho_{ABE}}(E). \end{aligned} \quad (68)$$

Recall that $S_{\rho_{ABE}}(L)$ is the von Neumann entropy for the reduced density matrix on the subset $L \subseteq ABE$. Thus, the squashed entanglement is defined as follows:

$$E_{\text{sq}}(\rho_{AB}) := \inf_E \left\{ \frac{1}{2} \mathcal{I}_{\rho_{ABE}}(A:B|E) \mid \text{tr}_E(\rho_{ABE}) = \rho_{AB} \right\}, \quad (69)$$

where \inf_E is considered over all extensions of ρ_{AB} , such that $\text{tr}_E(\rho_{ABE}) = \rho_{AB}$. In contrast to the PPT relative entanglement (50), squashed entanglement is equal to zero if and only if the quantum state is not entangled [145].

In addition, squashed entanglement is strongly related to the quantum Markov property, which implies the following equation for the arbitrary tripartition of total systems ($\Lambda = A \sqcup C \sqcup B$):

$$\mathcal{I}_{\rho}(A:B|C) = 0 \quad \text{for } d_{A,B} \geq r_0, \quad (70)$$

where r_0 is a constant of $\mathcal{O}(1)$. When the Hamiltonian is short-ranged and commuting, the above Markov property strictly holds for quantum Gibbs states at arbitrary temperatures [147,148]. Further, the quantum Markov property has a useful operational meaning [149], and it is crucial to preparing the quantum Gibbs states on a quantum computer [27,150–152]. Thus, for noncommuting Hamiltonians with short-range interactions, it is conjectured that, in general, the quantum Markov property holds in an approximate sense:

Conjecture 15. (Quantum Markov conjecture) For arbitrary quantum Gibbs states, the conditional mutual information $\mathcal{I}_{\rho_{\beta}}(A:B|E)$ ($\Lambda = A \sqcup E \sqcup B$) exponentially decays with the distance between A and B :

$$\mathcal{I}_{\rho_{\beta}}(A:B|E) \leq \text{poly}(|A|, |B|) e^{-d_{A,B}/\xi_{\beta}} \quad (71)$$

with $\xi_{\beta} = \text{poly}(\beta)$.

If the inequality (71) holds, the exponential clustering for the squashed entanglement is obtained as

$$\begin{aligned} E_{\text{sq}}(\rho_{\beta,AB}) &\leq \frac{1}{2} \mathcal{I}_{\rho_{\beta}}(A:B|E) \\ &\leq \text{poly}(|A|, |B|) e^{-d_{A,B}/\xi_{\beta}}, \end{aligned} \quad (72)$$

where $E = \Lambda \setminus (AB)$ and $\rho_{ABE} = \rho_{\beta}$ are considered in Eq. (69). Thus far, the above conjecture has been proven only in high-temperature regimes, where thermal phase transition cannot occur, that is, $\beta \lesssim \log(n)$ in 1D cases [152] and $\beta < \beta_c$ ($\beta_c = \mathcal{O}(1)$) in high-dimensional cases [27]. Moreover, in these temperature regimes, regarding entanglement, considerably stronger statements than Eq. (72) (i.e., Corollary 4) have already been derived.

Finally, it is shown that inequality (72) cannot be used to prove the exponential clustering of other quantum entanglement measures [e.g., the relative entanglement (22) or the entanglement of formation (79)], in general.

To upper bound the other entanglement measures, it is necessary to upper bound the quantity $\delta_{\rho_{AB}}$, which is defined in Eq. (24) as $\delta_{\rho_{AB}} := \inf_{\sigma_{AB} \in \text{SEP}(A:B)} \|\rho_{AB} - \sigma_{AB}\|_1$. This characterizes the distance between the quantum ρ_{AB} and

nonentangled states. The squashed entanglement yields the following upper bound for $\delta_{\rho_{AB}}$ [145,146]:

$$\delta_{\rho_{AB}} \leq 42\sqrt{\mathcal{D}_{AB}E_{\text{sq}}(\rho_{AB})}, \quad (73)$$

where \mathcal{D}_{AB} is the dimension of the Hilbert space of AB . If $E_{\text{sq}}(\rho_{AB}) \ll 1/\mathcal{D}_{AB}$, it can be ensured that $\delta_{\rho_{AB}}$ is sufficiently small. However, \mathcal{D}_{AB} is exponentially large, with a size of $|AB|$. Hence, regardless of the quantum Markov Conjecture 15 being proven, the distance $\delta_{\rho_{AB}}$ for the quantum Gibbs state may still be considerably large when subsets A or B are as large as the system size n . Thus, a problem similar to that in inequality (52) of Proposition 9 is encountered. Therefore, the clustering problem of bipartite entanglement cannot be generalized to other entanglement measures by simply clarifying the quantum Markov property.

C. General upper bound on the quantum correlation

Here, it is shown that the entanglement formation [49,153] is a simple upper bound for the quantum correlation $\text{QC}_{\rho_{AB}}(O_A, O_B)$. The relation between the entanglement of formation and the quantum correlation $\text{QC}_{\rho_{AB}}(O_A, O_B)$ is derived from that between mutual information $\mathcal{I}_{\rho_{AB}}(A:B)$ and the standard correlation function $C_{\rho_{AB}}(O_A, O_B)$. The entanglement of formation is defined as follows:

$$\begin{aligned} E_F(\rho_{AB}) &:= \inf_{\{p_s, |\psi_{s,AB}\rangle\}} \sum_s \frac{p_s}{2} \mathcal{I}_{|\psi_{s,AB}\rangle}(A:B) \\ &= \inf_{\{p_s, |\psi_{s,AB}\rangle\}} \sum_s p_s S_{|\psi_{s,AB}\rangle}(A), \end{aligned} \quad (74)$$

where $\mathcal{I}_{|\psi_{s,AB}\rangle}(A:B)$ and $S_{|\psi_{s,AB}\rangle}(A)$ are the mutual information and the von Neumann entropy for the reduced density matrix on subset A , respectively. Furthermore, $\inf_{\{p_s, |\psi_{s,AB}\rangle\}}$ is considered for arbitrary decomposition $\rho = \sum_s p_s |\psi_{s,AB}\rangle\langle\psi_{s,AB}|$ with $p_s > 0$. In addition, $\mathcal{I}_{\rho_s}(A:B) = 2S_{\rho_s,AB}(A)$ when ρ_s is a pure state.

The mutual information $\mathcal{I}_{|\psi_{s,AB}\rangle}(A:B)$ captures the entire correlations between two subsystems [45]. Hence, it is quite plausible that the entanglement of formation provides an upper bound for quantum correlations. Indeed, the following lemma connects the quantum correlation $\text{QC}_{\rho_{AB}}(O_A, O_B)$ and the entanglement of formation:

Lemma 16. For arbitrary operators O_A and O_B , the quantum correlation $\text{QC}_{\rho_{AB}}(O_A, O_B)$ is upper bounded using the entanglement of formation $E_F(\rho_{AB})$ as follows:

$$\text{QC}_{\rho}(O_A, O_B) \leq 2\|O_A\| \cdot \|O_B\| \sqrt{E_F(\rho_{AB})}. \quad (75)$$

Proof.—First, we note that

$$\sum_s p_s |C_{\rho_{s,AB}}(O_A, O_B)|^2 \geq \left(\sum_s p_s |C_{\rho_{s,AB}}(O_A, O_B)| \right)^2, \quad (76)$$

which yields

$$\inf_{\{p_s, \rho_{s,AB}\}} \sum_s p_s |C_{\rho_{s,AB}}(O_A, O_B)|^2 \geq [\text{QC}_{\rho_{AB}}(O_A, O_B)]^2. \quad (77)$$

Hence, the aim is to provide an upper bound for the lhs in the above inequality.

Second, the classical squashed (c-squashed) entanglement [94], which is obtained from the mixed convex roof of mutual information, is considered [154]:

$$E_{\text{sq}}^c(\rho_{AB}) := \inf_{\{p_s, \rho_{s,AB}\}} \sum_s \frac{p_s}{2} \mathcal{I}_{\rho_{s,AB}}(A:B), \quad (78)$$

where $\inf_{\{p_s, \rho_{s,AB}\}}$ is considered for all possible decompositions of ρ_{AB} such that $\rho_{AB} = \sum_s p_s \rho_{s,AB}$. The difference between $\mathcal{QI}_{\rho_{AB}}(A:B)$ and $E_F(\rho_{AB})$ is whether the decomposed quantum states of ρ are restricted to a pure state [156]. Trivially, the entanglement of formation $E_F(\rho_{AB})$ is lower-bounded as

$$E_F(\rho_{AB}) \geq E_{\text{sq}}^c(\rho_{AB}). \quad (79)$$

Finally, $E_{\text{sq}}^c(\rho_{AB})$ is compared with the lhs in Eq. (77). For this purpose, the following inequality reported in Eq. (5) of Ref. [45] is utilized:

$$\mathcal{I}_{\rho_{AB}}(A:B) \geq \frac{|C_{\rho_{AB}}(O_A, O_B)|^2}{2\|O_A\|^2 \cdot \|O_B\|^2}. \quad (80)$$

The application of the above inequality to definition (78) yields

$$\begin{aligned} E_{\text{sq}}^c(\rho_{AB}) &\geq \inf_{\{p_s, \rho_{s,AB}\}} \sum_s \frac{p_s}{2} \cdot \frac{|C_{\rho_{s,AB}}(O_A, O_B)|^2}{2\|O_A\|^2 \cdot \|O_B\|^2} \\ &\geq \frac{[\text{QC}_{\rho_{AB}}(O_A, O_B)]^2}{4\|O_A\|^2 \cdot \|O_B\|^2}, \end{aligned} \quad (81)$$

where Eq. (77) is used in the last inequality. Thus, by combining the above inequality with Eq. (79), the main inequality (75) is proven. This completes the proof. ■

D. Optimality of the obtained bounds

Herein, the optimality of the correlation length ξ_β or ξ'_β in Theorems 10 and 13 is discussed. The β dependence of the correlation length ξ_β (i.e., $\xi_\beta \propto \beta$) is shown to be qualitatively optimal, which cannot be improved, in general. This

point is ensured by the correspondence of the inverse temperatures and spectral gap as follows:

$$\beta \leftrightarrow 1/\Delta, \quad (82)$$

with Δ being the spectral gap between the ground and first excited states. Consequently, the correlation length of $\mathcal{O}(\Delta^{-1})$ in the gapped ground states [67,69,159] implies the correlation length of $\mathcal{O}(\beta)$ in the thermal states.

To elaborate, first, the following inequality for the number of energy eigenstates in an arbitrary energy shell $(E-1, E]$ [160–162] is assumed:

$$\mathcal{N}_{E,1} \leq n^{cE}, \quad (83)$$

where $\mathcal{N}_{E,1}$ is the number of eigenstates within the energy shell of $(E-1, E]$, and c is a constant of $\mathcal{O}(1)$. Furthermore, the energy origin is set such that the ground state's energy is equal to zero. Here, the above condition is satisfied in various types of quantum many-body systems [160].

Thus, under condition (83), the quantum Gibbs states ρ_β are close to the ground state ρ_∞ in the sense that

$$\|\rho_\beta - \rho_\infty\|_1 \leq \text{const} \times \frac{e^{-(\beta-c \log(n))\Delta}}{\beta - c \log(n)}. \quad (84)$$

Therefore, the properties of the thermal states and the ground state are approximately the same for $\beta \approx \log(n)/\Delta$ as follows:

$$\|\rho_\beta - \rho_\infty\|_1 = 1/\text{poly}(n). \quad (85)$$

When the ground state is nondegenerate and gapped, the correlation function $C_{\rho_\infty}(O_A, O_B)$ is expressed as [67,69]

$$C_{\rho_\infty}(O_A, O_B) = \text{QC}_{\rho_\infty}(O_A, O_B) = \text{const} \times e^{-\mathcal{O}(\Delta)R}, \quad (86)$$

where Eq. (34) is used for the pure state in the first equation. Subsequently, using the continuity bound (38),

$$\begin{aligned} \text{QC}_{\rho_\beta}(O_A, O_B) &= C_{\rho_\infty}(O_A, O_B) - 1/\text{poly}(n) \\ &= \text{const} \times e^{-\mathcal{O}(\Delta)R} - 1/\text{poly}(n) \\ &= \text{const} \times e^{-\mathcal{O}(R)/(\beta/\log(n))} - 1/\text{poly}(n), \end{aligned} \quad (87)$$

where the second equation results from the fact that $\beta \approx \log(n)/\Delta$ implies $\Delta \approx \log(n)/\beta$. Thus, the quantum correlation starts to decay for $R \gtrsim \beta/\log(n)$; hence, the correlation length is proportional to β at sufficiently low temperatures.

By contrast, for the WYD skew and quantum Fisher information, there is scope for improvement in the present β dependences, which have been assigned inequalities (64)

and (67), respectively. In the ground states, the WYD skew and quantum Fisher information reduce to the variance of the operator. For an arbitrary operator K expressed in Eq. (63), the variance $(\Delta K)^2 = \text{tr}(\rho_\infty K^2) - [\text{tr}(\rho_\infty K)]^2$ is upper bounded by [163,164]

$$\mathcal{I}_{\rho_\infty}^{(\alpha)}(K) = (\Delta K)^2 \leq \text{const} \times \Delta^{-1}n. \quad (88)$$

The above inequality holds in infinite-dimensional systems and long-range interacting systems; hence, the (β, Δ) correspondence (82) indicates an improvement in the current upper bounds as

$$\mathcal{I}_{\rho_\beta}^{(\alpha)}(K) \leq \mathcal{O}(\beta n) \quad \text{and} \quad \mathcal{F}_{\rho_\beta}(K) \leq \mathcal{O}(\beta n), \quad (89)$$

which affords better bounds in dimensions greater than 1 ($D \geq 2$).

E. Beyond quantum Gibbs states

Throughout the discussion, the equilibrium situation is considered at a finite temperature. However, when considering a nonequilibrium density matrix, the entanglement properties exhibit different properties, in general [165]. Consequently, a natural question arises as to whether the current results hold for more general quantum states. Based on definition (33) of the quantum correlation, concavity is satisfied, that is,

$$\text{QC}_\rho(O_A, O_B) \leq p_1 \text{QC}_{\rho_1}(O_A, O_B) + p_2 \text{QC}_{\rho_2}(O_A, O_B)$$

for an arbitrary decomposition of $\rho = p_1 \rho_1 + p_2 \rho_2$ ($p_1 > 0, p_2 > 0$). Hence, considering a quantum state in the form of

$$\rho = \int_0^\infty a(z) e^{-zH} dz \quad (90)$$

with $a(z)$ being a non-negative function, Theorem 10 can be applied to the state ρ . Subsequently, the state ρ has a finite quantum correlation length while the entanglement clustering is also satisfied. A similar discussion can also be applied to the WYD skew information $\mathcal{I}_\rho^{(\alpha)}(K)$ and the quantum Fisher information $\mathcal{F}_\rho(K)$ owing to their concavities [166]. Herein, if the state ρ includes extremely low-temperature states, for example, $\int_{\beta_0}^\infty a(z) \text{tr}(e^{-zH}) \approx 1$ with $\beta_0 \approx \mathcal{O}(n)$, the state ρ is similar to low-temperature Gibbs states; consequently, the quantum correlation length may become large.

As an important class of quantum states, the following density matrix is considered to be characterized by a monotonically decreasing function $F(x)$:

$$\rho = \frac{F(H)}{\text{tr}[F(H)]}, \quad (91)$$

where $F(x) \geq 0$. This class of the quantum state is referred to as the passive state [169,170], and it plays a crucial role in quantum thermodynamics [171–174]. Moreover, the quantum Gibbs state trivially corresponds to the case $F(x) = e^{-\beta x}$. Based on the Bernstein-Widder theorem [175–177], the passive state (91) can be represented in the form of Eq. (90) if and only if the function $F(x)$ is completely monotonic as follows:

$$(-1)^m \frac{d^m}{dx^m} F(x) \geq 0 \quad (92)$$

for arbitrary $m \geq 0$. Therefore, for every passive state with condition (92), structural restrictions similar to that for the quantum Gibbs state must be imposed [178].

VII. SUMMARY AND FUTURE WORKS

This study primarily addressed the conjecture of the exponential clustering of bipartite entanglement, which revealed the fundamental aspect of long-range entanglement. The entanglement was accessed via the introduction of a novel concept, referred to as the quantum correlation $\text{QC}_\rho(O_A, O_B)$, which is defined by the convex roof of the standard bipartite correlation function, as in Eq. (33). Consequently, as a fundamental theorem, the exponential clustering of the quantum correlation was derived, which holds at arbitrary temperatures, even at the critical point of thermal phase transition. Based on its definition and exploiting the fact that it uses the convex roof, quantum correlation exhibits properties similar to those of entanglement. Subsequently, several basic statements in Sec. III were derived, including the relationship between the quantum correlation and the PPT relative entanglement (Proposition 9). Further, based on the clustering theorem for the quantum correlation, entanglement clustering theorems (Corollary 11 and Theorem 12) for PPT relative entanglement (2) were presented. Moreover, using similar analytical techniques, the exponential clustering of another type of quantum correlation based on the WYD skew information (Theorem 13) was derived, which yielded the fundamental limitations of the WYD skew and quantum Fisher information (Corollary 14). Consequently, these serve as representative measures for quantum coherence and macroscopic entanglement.

Furthermore, this study expressed simple and general no-go theorems on the existence of long-range entanglement. On the other hand, there is still room for improvement of the present analytical techniques, and hence the obtained results may be further strengthened. Based on the results obtained, the strongest form of the bipartite entanglement clustering may be expressed as follows:

[the strongest conjecture]

$$E_R(\rho_{\beta,AB}) \leq \text{poly}(|A|, |B|) e^{-R/\tilde{\xi}_\beta} \quad (93)$$

for an arbitrary choice of A and B such that $d_{A,B} = R$, where $\tilde{\xi}_\beta = \text{poly}(\beta)$ and $\text{poly}(x)$ denote a finite degree polynomial. As shown in Sec. II C, from the continuity bounds, inequality (93) yields the same upper bound for other entanglement measures. However, the main theorems presented in this paper did not arrive at this form of entanglement clustering, and further investigations are required to refine the current results.

In conclusion, this study unveiled a fundamental limit on the characteristic length scale, such that certain types of quantum effects can exist. Moreover, the present results do not depend on system details, and they hold at arbitrary temperatures. The understanding of the universal structural constraints in low-temperature physics, which must be satisfied for every quantum many-body system, still remains limited. Consequently, identifying these constraints is a critical task for understanding the complicated quantum many-body phases as well as developing efficient algorithms for quantum many-body simulations. This study is expected to introduce a novel approach to address this profound problem.

Finally, the following topics are mentioned as specific open questions:

- (i) First, deriving a clustering theorem for the relative entanglement instead of the PPT relative entanglement. This may be addressed by resolving Conjecture 7. Subsequently, Proposition 9 can be improved; in other words, under the condition of (almost) zero quantum correlations [i.e., Eq. (51)], a similar inequality to Eq. (52) may hold for the relative entanglement $E_R(\rho_{AB})$ instead of $E_R^{\text{PPT}}(\rho_{AB})$. This improvement immediately yields the entanglement clustering for other popular measures, such as the entanglement of formations [see also the discussion after Eq. (24)].
- (ii) As a related problem, the $(|A|, |B|)$ dependence in Corollary 11 may be improved under dimensions greater than one. In the present form, the independence is in the exponential form, and hence, a meaningful bound for the case of $|A|$ and $|B|$ being as large as the system size cannot be obtained. To improve this, as has been discussed after Corollary 11, considering the operator correlations $\text{QC}_\rho(A, B)$ alone is not sufficient. Instead, the complete information between the two subsystems must be considered. However, at the current stage, the problem may be challenging as it should include an analogous difficulty to the data hiding problem in the context of the area law conjecture at zero temperature [110,111,160].
- (iii) Third, identifying the class of quantum coherence measures [180], which are always short range at nonzero temperatures, remains an intriguing problem. In this study, it was shown that bipartite entanglement cannot exist at long distances; however, as has been demonstrated in Sec. VI A, macroscopic quantum effects do not necessarily imply long-

distance entanglement. For example, quantum discord, a well-known measure for quantum correlation [181,182], only decays algebraically at thermal critical points [58]. Thus, the current results can still be expanded to include other coherence measures.

- (iv) Finally, the question remains as to whether entanglement clustering can be applied to more practical problems such as the efficient simulation of quantum Gibbs states. The clustering of entanglement imposes a strong constraint on the structure of quantum Gibbs states. Hence, it is likely that the property can be utilized to reduce computational complexity.

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APPENDIX A: SPECTRAL DECOMPOSITION OF OPERATORS

As a convenient notation, O_ω is defined for the arbitrary operator O as follows [56]:

$$O_\omega := \sum_{i,j} \langle E_i | O | E_j \rangle \delta(E_i - E_j - \omega) | E_i \rangle \langle E_j |, \quad (\text{A1})$$

where $\{|E_i\rangle\}$ and $\{E_i\}$ are the eigenstates and the corresponding eigenvalues of H , respectively. The operator O_ω yields terms such as $\langle E + \omega | O | E \rangle | E + \omega \rangle \langle E |$. Based on the above definition, the following can be obtained:

$$\int_{-\infty}^{\infty} O_\omega d\omega = O, \quad O_\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} O(t) e^{-i\omega t} dt, \quad (\text{A2})$$

and

$$\begin{aligned} \text{ad}_H(O_\omega) &= \omega O_\omega, & [\text{ad}_H(O_\omega)]^\dagger &= \omega O_\omega^\dagger, \\ [e^{-\beta H}, O_\omega] &= (1 - e^{\beta\omega}) e^{-\beta H} O_\omega, \end{aligned} \quad (\text{A3})$$

where $\text{ad}_H(\cdot) := [H, \cdot]$ is defined.

APPENDIX B: BEYOND SHORT-RANGE INTERACTING SPIN SYSTEMS

1. Long-range interacting cases

This section discusses the manner in which the current analyses can be generalized to systems with long-range interactions, where the decay of the function $J(x)$ in Eq. (10) is given in a polynomial form:

$$J(x) \leq \frac{g_0}{(x+1)^\alpha} \quad (\text{long-range interaction}). \quad (\text{B1})$$

When $\alpha > 2D$, the Lieb-Robinson bound (15) can be generalized to long-range interacting systems [183–189]. The Lieb-Robinson bound can be obtained in the following form:

$$\|[O_X(t), O_Y]\| \leq C' \min(|\partial X|, |\partial Y|) \frac{t(1+t)^{\eta_\alpha}}{R^{-\tilde{\alpha}}}, \quad (\text{B2})$$

where η_α and $\tilde{\alpha}$ depend on the spatial dimension D and the decay exponent α . For example, a loose estimation affords $\eta_\alpha = \alpha - D - 1$ and $\tilde{\alpha} = \alpha - 2D$ [187]. Nevertheless, a quantitatively optimal estimation of the parameters η_α and $\tilde{\alpha}$ remains unaddressed.

Using the Lieb-Robinson bound (B2), the main results can be generalized to long-range interacting systems. In this case, the exponential decay becomes the power-law decay. Analyses using the Lieb-Robinson bound can be summarized as follows:

- (1) For the proof of Theorem 13, the Lieb-Robinson bound is used in Eqs. (C23) or (C33).
- (2) For the proof of Theorem 10, the Lieb-Robinson bound is used in Eqs. (D65) and (D89).
- (3) For the proof of Theorem 12, the Lieb-Robinson bound is used in Eq. (F35).

2. Disordered systems

Other interesting systems include the disordered systems where randomness is added to the Hamiltonians. In such systems, the Lieb-Robinson bound can be proven to have improved as follows [190,191]:

$$\|[O_X(t), O_Y]\| \leq C \min(|\partial X|, |\partial Y|) t^\eta e^{-\mu R}, \quad (\text{B3})$$

where C, η, μ are constants of $\mathcal{O}(1)$, which depend on the system parameters. In this case, the norm $\|[O_X(t), O_Y]\|$ is exponentially small with respect to the distance R up to time $t \sim e^{\mathcal{O}(R)}$. This leads to the quantum correlation length of $\mathcal{O}(\text{polylog}(\beta))$ in the main theorem (i.e., Theorems 10, 12, and 13).

3. Quantum boson systems

Finally, in quantum boson systems, the Hamiltonian is locally unbounded (i.e., the parameter g is infinitely large, as shown in Fig. 1). In such systems, typically, the Lieb-Robinson bound is not obtained with a finite Lieb-Robinson velocity [192]. To extend the obtained results, the study may need to be restricted to particular classes of quantum many-body boson systems, such as free boson systems [193,194], spin-boson models [195,196], and Bose-Hubbard-type Hamiltonians [197–199]. The establishment of the Lieb-Robinson bound in boson systems is still an active area of research.

APPENDIX C: PROOFS OF THEOREM 13 AND COROLLARY 14

In this section, Theorem 13 is proven, followed by Theorem 10. The proof for Theorem 10 is considerably simpler than that for Theorem 13, although the essence for both is similar.

Theorem 13 and the resulting Corollary 14 provide the upper bounds for

$$Q_{\rho_\beta}^{(\alpha)}(O_A, O_B) := \text{tr}(\rho_\beta O_A O_B) - \text{tr}(\rho_\beta^{1-\alpha} O_A \rho_\beta^\alpha O_B) \quad (\text{C1})$$

and

$$\mathcal{I}_{\rho_\beta}^{(\alpha)}(K) := \text{tr}(\rho_\beta K^2) - \text{tr}(\rho_\beta^{1-\alpha} K \rho_\beta^\alpha K), \quad (\text{C2})$$

with $K = \sum_{i \in \Lambda} O_i (\|O_i\| \leq 1)$, respectively.

For the convenience of the readers, the rough forms of the statements are provided. In Theorem 13,

$$Q_{\rho_\beta}^{(\alpha)}(O_A, O_B) \leq C'_\beta \min(|\partial A|, |\partial B|) e^{-R/\xi'_\beta}, \quad (\text{C3})$$

where the parameters are $\mathcal{O}(1)$ constants that are expressed in Eq. (62). Furthermore, Corollary 14 provides the inequalities

$$\mathcal{I}_{\rho_\beta}^{(\alpha)}(K) \leq \tilde{C}'_\beta \xi_\beta^D n = \mathcal{O}(\beta^D) n, \quad (\text{C4})$$

for the WYD skew information.

1. Remark on the parameter regime $\alpha \notin [0, 1]$

As is evident, in general, obtaining the same results for the parameter regime $\alpha \notin [0, 1]$ is not possible. Mathematically, the proof in Appendix C 3 breaks down for $\alpha \notin [0, 1]$ because the function $g_{\alpha,\beta}(t)$ in Eq. (C20) no longer decays exponentially with t .

For example, when $\alpha = -1$, $\mathcal{I}_{\rho}^{(-1)}(K)$ is referred to as the purity of coherence [200]:

$$\begin{aligned} \mathcal{I}_{\rho}^{(-1)}(K) &= \text{tr}(\rho K^2) - \text{tr}(\rho^2 K \rho^{-1} K) \\ &= -\sum_{j,k} \frac{\lambda_k^2 - \lambda_j^2}{\lambda_j} |\langle \lambda_j | K | \lambda_k \rangle|^2, \end{aligned} \quad (\text{C5})$$

where $\rho = \sum_j \lambda_j |\lambda_j\rangle \langle \lambda_j|$ is the spectral decomposition of ρ . In general,

$$\begin{aligned} \mathcal{I}_{\rho}^{(\alpha)}(K) &= \text{tr}(\rho K^2) - \text{tr}(\rho_\beta^{1-\alpha} K \rho^\alpha K) \\ &= -\sum_{j,k} \frac{\lambda_k^{1-\alpha} - \lambda_j^{1-\alpha}}{\lambda_j^{-\alpha}} |\langle \lambda_j | K | \lambda_k \rangle|^2. \end{aligned} \quad (\text{C6})$$

For $\beta = \text{poly}[\log(n)]$, under the same assumption as for Eq. (83), the quantum Gibbs state ρ_β satisfies

$$\lambda_0 \approx 1, \quad \lambda_j = e^{-\beta E_j}. \quad (\text{C7})$$

Hence, the quantum Gibbs state is approximately given by the ground state. Thus, $\mathcal{I}_{\rho_\beta}^{(\alpha)}(K)$ in Eq. (C6) includes the following terms:

$$\begin{aligned} &\sum_j \left(\frac{\lambda_0^{1-\alpha}}{\lambda_j^{-\alpha}} + \frac{\lambda_j^{1-\alpha}}{\lambda_0^{-\alpha}} \right) |\langle \lambda_j | K | \lambda_0 \rangle|^2 \\ &\approx \sum_j (e^{-\alpha \beta E_j} + e^{(\alpha-1)\beta E_j}) |\langle \lambda_j | K | \lambda_0 \rangle|^2. \end{aligned} \quad (\text{C8})$$

For $\alpha \in [0, 1]$, both $e^{-\alpha \beta E_j}$ and $e^{(\alpha-1)\beta E_j}$ decay with E_j , whereas for $\alpha \notin [0, 1]$, either $e^{-\alpha \beta E_j}$ or $e^{(\alpha-1)\beta E_j}$ grows exponentially with E_j .

Typically, only $|\langle \lambda_j | K | \lambda_0 \rangle|^2 \lesssim e^{-\text{const} \times E_j}$ from Ref. [201] can be ensured. Hence, for $\alpha < 0$ ($\alpha > 1$), there exists a critical temperature $\beta_c \propto 1/(-\alpha)$ [$\beta_c \propto 1/(\alpha-1)$], such that Eq. (C8) exponentially grows with the system size n for $\beta > \beta_c$. Therefore, a meaningful upper bound $\mathcal{I}_{\rho_\beta}^{(\alpha)}(K)$ cannot be obtained without additional conditions (such as the high-temperature condition).

2. Proof of Corollary 14

First, Corollary 14 based on Theorem 13 is proven as follows:

$$\begin{aligned} \mathcal{I}_{\rho_\beta}^{(\alpha)}(K) &= \sum_{i,j} \text{tr}(\rho_\beta O_i O_j) - \text{tr}(\rho_\beta^{1-\alpha} O_i \rho_\beta^\alpha O_j) \\ &\leq \sum_{i,j} C'_\beta e^{-d_{i,j}/\xi'_\beta} \\ &\leq C'_\beta |\Lambda| \max_{i \in \Lambda} \sum_{j \in \Lambda} e^{-d_{i,j}/\xi'_\beta} = C'_\beta \zeta_{0,\xi'_\beta} n \end{aligned} \quad (\text{C9})$$

with $\zeta_{s,\xi} := \max_{i \in \Lambda} \sum_{j \in \Lambda} d_{i,j}^s e^{-d_{i,j}/\xi}$.

The parameter $\zeta_{s,\xi}$ is upper bounded by

$$\zeta_{s,\xi} \leq 1 + \gamma e^{1/\xi} \xi^{s+D} (s+D)!. \quad (\text{C10})$$

Using definition (7) for the parameter γ , the proof is straightforward as follows:

$$\begin{aligned} \sum_{j \in \Lambda} d_{i,j}^s e^{-d_{i,j}/\xi} &= 1 + \sum_{x=1}^{\infty} \sum_{j: d_{i,j}=x} x^s e^{-x/\xi} \\ &\leq 1 + \gamma \sum_{x=1}^{\infty} x^{s+D-1} e^{-x/\xi} \\ &\leq 1 + \gamma \int_0^{\infty} x^{s+D-1} e^{-(x-1)/\xi} dx \\ &= 1 + \gamma e^{1/\xi} \int_0^{\infty} \xi (\xi z)^{s+D-1} e^{-z} dz \\ &= 1 + \gamma e^{1/\xi} \xi^{s+D} (s+D)!. \end{aligned} \quad (\text{C11})$$

Using Eq. (C10) and $\xi'^{-1} \leq \mu/2$, ζ_{0,ξ'_β} can be reduced to the form

$$\begin{aligned}\zeta_{0,\xi'_\beta} &= 1 + \gamma e^{1/\xi'_\beta} \xi_\beta^D D! = \xi_\beta^D (\xi_\beta^{-D} + \gamma e^{1/\xi'_\beta} D!) \\ &\leq \xi_\beta^D [(\mu/2)^D + \gamma e^{\mu/2} D!].\end{aligned}\quad (\text{C12})$$

Thereafter, on applying the above inequality to Eq. (C9), the desired inequality (C4) can be obtained. This completes the proof. ■

3. Proof of Theorem 13

Herein, the upper bound of $Q_{\rho_\beta}^{(\alpha)}$ in Eq. (C1) is considered. Before beginning the proof, first, we consider the following trivial upper bound for $Q_\rho^{(\alpha)}(O_A, O_B)$ for arbitrary ρ as follows:

$$\begin{aligned}Q_\rho^{(\alpha)}(O_A, O_B) &\leq \text{tr}(\rho|O_A O_B|) + \frac{\text{tr}(\rho|O_A|^2) + \text{tr}(\rho|O_B|^2)}{2} \\ &\leq (\|O_A\| + \|O_B\|)^2/2 = 2,\end{aligned}\quad (\text{C13})$$

where $\|O_A\| = \|O_B\| = 1$. For the proof of inequality (C13), because $\text{tr}(\rho O_A O_B) \leq \text{tr}(\rho|O_A O_B|)$ is trivial, the following must be proven:

$$|\text{tr}(\rho^{1-\alpha} O_A \rho^\alpha O_B)| \leq \frac{\text{tr}(\rho|O_A|^2) + \text{tr}(\rho|O_B|^2)}{2}. \quad (\text{C14})$$

Using the spectral decomposition of $\rho = \sum_s \lambda_s |\lambda_s\rangle\langle\lambda_s|$,

$$\begin{aligned}&|\text{tr}(\rho^{1-\alpha} O_A \rho^\alpha O_B)| \\ &\leq \sum_{s,s'} \lambda_s^{1-\alpha} \lambda_{s'}^\alpha |\langle\lambda_s|O_A|\lambda_{s'}\rangle\langle\lambda_{s'}|O_B|\lambda_s\rangle| \\ &\leq \sum_{s,s'} \lambda_s^{1-\alpha} \lambda_{s'}^\alpha \frac{|\langle\lambda_s|O_A|\lambda_{s'}\rangle|^2 + |\langle\lambda_{s'}|O_B|\lambda_s\rangle|^2}{2}.\end{aligned}\quad (\text{C15})$$

Using the Hölder inequality,

$$\begin{aligned}&\sum_{s,s'} \lambda_s^{1-\alpha} \lambda_{s'}^\alpha |\langle\lambda_s|O_A|\lambda_{s'}\rangle|^2 \\ &= \sum_{s,s'} (\lambda_s |\langle\lambda_s|O_A|\lambda_{s'}\rangle|^2)^{1-\alpha} (\lambda_{s'} |\langle\lambda_{s'}|O_A|\lambda_s\rangle|^2)^\alpha \\ &\leq \left(\sum_{s,s'} \lambda_s |\langle\lambda_s|O_A|\lambda_{s'}\rangle|^2\right)^{1-\alpha} \left(\sum_{s,s'} \lambda_{s'} |\langle\lambda_{s'}|O_A|\lambda_s\rangle|^2\right)^\alpha \\ &= \sum_{s,s'} \lambda_s |\langle\lambda_s|O_A|\lambda_{s'}\rangle|^2 = \text{tr}(\rho|O_A|^2),\end{aligned}\quad (\text{C16})$$

where $O_A O_A^\dagger = |O_A|^2$ is used in the last equation. Thus, on applying inequality (C16) to (C15), inequality (C14) is proven. Therefore, inequality (C13) is proven.

Thereafter, we consider the nontrivial upper bound presented in Theorem 13, which utilizes the properties of quantum Gibbs states. When ρ is a Gibbs state (i.e., $\rho = \rho_\beta = e^{-\beta H}$), $\rho_\beta^{-\alpha} O_A \rho_\beta^\alpha$ is reduced to the imaginary time evolution. Therefore, at first glance, the quantity (C1) is not

upper bounded for low temperatures because the imaginary time evolution $e^{\beta\alpha H} O_A e^{-\beta\alpha H}$ is usually unbounded [202]. To prove Theorem 13, a direct treatment of the imaginary time evolution should necessarily be avoided. Instead, the condition $\alpha \in [0, 1]$ is utilized for this purpose. However, for $\alpha \notin [0, 1]$, the unboundedness of the norm of $e^{\beta\alpha H} O_A e^{-\beta\alpha H}$ cannot be avoided, which is reflected in the fact that the function $g_{\alpha,\beta}(t)$ in Eq. (C20) converges only for $\alpha \in [0, 1]$.

For this purpose, the imaginary time evolution is transformed in an appropriate manner. Using the notation of Eq. (A1),

$$\begin{aligned}&\text{tr}(\rho_\beta O_A O_B) - \text{tr}(\rho_\beta^{1-\alpha} O_A \rho_\beta^\alpha O_B) \\ &= \int_{-\infty}^{\infty} \text{tr}(\rho_\beta O_{A,\omega} O_B - \rho_\beta^{1-\alpha} O_{A,\omega} \rho_\beta^\alpha O_B) d\omega.\end{aligned}\quad (\text{C17})$$

Using $\rho_\beta = e^{-\beta H}$, we obtain

$$\begin{aligned}\rho_\beta O_{A,\omega} - \rho_\beta^{1-\alpha} O_{A,\omega} \rho_\beta^\alpha &= e^{-\beta H} (O_{A,\omega} - e^{\alpha\beta H} O_{A,\omega} e^{-\alpha\beta H}) \\ &= e^{-\beta H} (1 - e^{\alpha\beta\omega}) O_{A,\omega} \\ &= \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} [e^{-\beta H}, O_{A,\omega}],\end{aligned}$$

where Eq. (A3) is used in the last equation. Hence, using the identity $\text{tr}([O_A, O_B] O_3) = \text{tr}(O_A [O_B, O_3])$,

$$\begin{aligned}Q_{\rho_\beta}^{(\alpha)}(O_A, O_B) &= \int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} \text{tr}([e^{-\beta H}, O_{A,\omega}] O_B) d\omega \\ &= \int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} \text{tr}(e^{-\beta H} [O_{A,\omega}, O_B]) d\omega.\end{aligned}\quad (\text{C18})$$

From Eq. (A2),

$$\begin{aligned}&\int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} O_{A,\omega} d\omega \\ &= \int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} \frac{1}{2\pi} \int_{-\infty}^{\infty} O_A(t) e^{-i\omega t} dt d\omega \\ &= \int_{-\infty}^{\infty} g_{\alpha,\beta}(t) O_A(t) dt,\end{aligned}\quad (\text{C19})$$

where $g_{\alpha,\beta}(t)$ is defined by the Fourier transform of $(1 - e^{\alpha\beta\omega})/(1 - e^{\beta\omega})$ as

$$\begin{aligned}g_{\alpha,\beta}(t) &:= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega \\ &= -i\beta^{-1} \sum_{m=1}^{\infty} \text{sign}(t) e^{-2\pi m|t|/\beta} (-1 + e^{-2\pi i \alpha m \text{sign}(t)}),\end{aligned}\quad (\text{C20})$$

where the proof of the second equation is provided in Appendix C 3 a. Based on the above form, the following can be obtained:

$$\begin{aligned} |g_{\alpha,\beta}(t)| &\leq 2\beta^{-1} \sum_{m=1}^{\infty} e^{-2\pi m|t|/\beta} \\ &= 2\beta^{-1} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}}. \end{aligned} \quad (\text{C21})$$

Further, combining Eqs. (C18) and (C19) with inequality (C21) yields

$$\begin{aligned} |\mathcal{Q}_{\rho_\beta}^{(\alpha)}(O_A, O_B)| &= \left| \int_{-\infty}^{\infty} g_{\alpha,\beta}(t) \text{tr}(\rho_\beta[O_A(t), O_B]) dt \right| \\ &\leq 2\beta^{-1} \int_{-\infty}^{\infty} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt, \end{aligned} \quad (\text{C22})$$

where $\text{tr}(\rho_\beta[O_A(t), O_B]) \leq \|[O_A(t), O_B]\|$ are used.

Subsequently, using the Lieb-Robinson bound (15),

$$\begin{aligned} 2\beta^{-1} \int_{-\infty}^{\infty} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ \leq \min(|\partial A|, |\partial B|) \left[\frac{4}{\pi} \left(1 + \frac{\xi'_\beta}{R} \right) + 2C \left(\frac{2}{v\beta} + \frac{1}{\pi} \right) \right] e^{-R/\xi'_\beta}. \end{aligned} \quad (\text{C23})$$

The proof is provided in Appendix C 3 b. For $R \leq \xi'_\beta/2$, the rhs in Eq. (C23) is larger than the trivial upper bound (C13). Hence, $R \geq \xi'_\beta/2$ must be considered, which yields

$$\begin{aligned} 2\beta^{-1} \int_{-\infty}^{\infty} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ \leq \min(|\partial A|, |\partial B|) \left(\frac{12 + 2C}{\pi} + \frac{4C}{v\beta} \right) e^{-R/\xi'_\beta}. \end{aligned} \quad (\text{C24})$$

On applying the above inequality to Eq. (C22), Theorem 13 is proven. ■

a. Fourier transform of $(1 - e^{\alpha\beta\omega})/(1 - e^{\beta\omega})$

Herein, Eq. (C20) is proven. For this proof, the integral is rewritten as follows:

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega \\ = \begin{cases} \frac{1}{2\pi} \int_{C_-} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega & \text{for } t < 0, \\ \frac{1}{2\pi} \int_{C_+} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega & \text{for } t \geq 0, \end{cases} \end{aligned} \quad (\text{C25})$$

where the integral paths C_- and C_+ are described in Fig. 3.

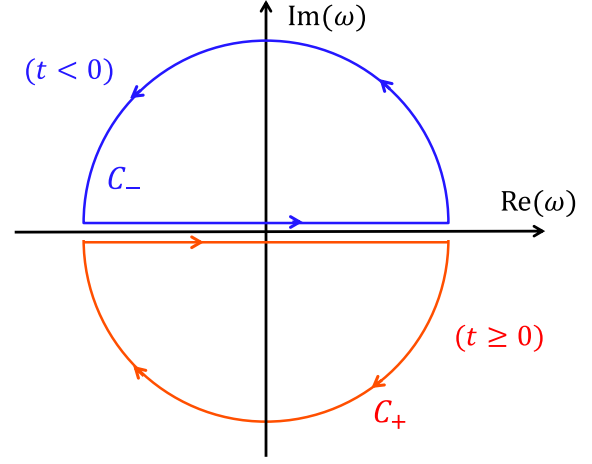


FIG. 3. Schematic of the integral paths in Eq. (C25).

First, the case of $t < 0$ is considered. Then, using the residue theorem,

$$\begin{aligned} \frac{1}{2\pi} \int_{C_-} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega \\ = i \sum_{m=1}^{\infty} \text{Res}_{\omega=(2\pi im)/\beta} \left(\frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} \right), \end{aligned} \quad (\text{C26})$$

where $\text{Res}_{\omega=(2\pi im)/\beta}$ is the residue at $\omega = (2\pi im)/\beta$. Owing to

$$\begin{aligned} i \text{Res}_{\omega=(2\pi im)/\beta} \left(\frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} \right) \\ = i\beta^{-1} e^{2\pi mt/\beta} (-1 + e^{2\pi i m \alpha}), \end{aligned} \quad (\text{C27})$$

Eq. (C26) can be reduced to

$$\begin{aligned} \frac{1}{2\pi} \int_{C_-} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega \\ = i\beta^{-1} \sum_{m=1}^{\infty} e^{2\pi mt/\beta} (-1 + e^{2\pi i m \alpha}). \end{aligned} \quad (\text{C28})$$

In the same manner, we obtain

$$\begin{aligned} \frac{1}{2\pi} \int_{C_+} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega \\ = -i \sum_{m=1}^{\infty} \text{Res}_{\omega=-(2\pi im)/\beta} \left(\frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} \right) \\ = -i\beta^{-1} \sum_{m=1}^{\infty} e^{-2\pi mt/\beta} (-1 + e^{-2\pi i m \alpha}). \end{aligned} \quad (\text{C29})$$

By combining the two cases (C28) and (C29),

$$\begin{aligned} & \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1 - e^{\alpha\beta\omega}}{1 - e^{\beta\omega}} e^{-i\omega t} d\omega \\ &= -i\beta^{-1} \sum_{m=1}^{\infty} \text{sign}(t) e^{-2\pi m|t|/\beta} (-1 + e^{-2\pi i\alpha m \text{sign}(t)}). \end{aligned}$$

This completes the proof of Eq. (C20). \blacksquare

b. Proof of the inequality (C23)

We first consider the decomposition

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ &= \int_{|t|>t_0} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ &+ \int_{|t|\leq t_0} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt, \end{aligned} \quad (\text{C30})$$

where $t_0 := \mu R/(2v)$ is chosen. For the first term in the rhs of Eq. (C30), from $1/(1 - e^{-|x|}) \leq 1 + 1/|x|$,

$$\frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \leq e^{-2\pi|t|/\beta} \left(1 + \frac{1}{2\pi|t|/\beta}\right), \quad (\text{C31})$$

which yields

$$\begin{aligned} & \int_{|t|>t_0} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ &\leq 2 \int_{|t|>t_0} e^{-2\pi|t|/\beta} \left(1 + \frac{1}{2\pi|t|/\beta}\right) dt \\ &\leq \frac{2\beta}{\pi} e^{-2\pi t_0/\beta} \left(1 + \frac{1}{2\pi t_0/\beta}\right) \\ &= \frac{2\beta}{\pi} e^{-\pi\mu R/(v\beta)} \left(1 + \frac{v\beta}{\pi\mu R}\right) \leq \frac{2\beta}{\pi} e^{-R/\xi'_\beta} \left(1 + \frac{\xi'_\beta}{R}\right), \end{aligned} \quad (\text{C32})$$

where $\|[O_A(t), O_B]\| \leq 2\|O_A\| \cdot \|O_B\| = 2$ and $\pi\mu/(v\beta) \geq \xi'^{-1}_\beta = \mu/[2 + (v\beta)/\pi]$ are used in the first and last inequalities, respectively. For the second term on the rhs of Eq. (C30), the Lieb-Robinson bound (15) is used as

$$\|[O_A(t), O_B]\| \leq C \min(|\partial A|, |\partial B|) (e^{v|t|} - 1) e^{-\mu R},$$

which yields

$$\begin{aligned} & \int_{|t|\leq t_0} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ &\leq C \min(|\partial A|, |\partial B|) e^{-\mu R} \\ &\times \int_{|t|\leq t_0} e^{-2\pi|t|/\beta} \left(1 + \frac{1}{2\pi|t|/\beta}\right) (e^{v|t|} - 1) dt. \end{aligned} \quad (\text{C33})$$

The integral for $|t| \leq t_0$ is upper bounded as follows:

$$\begin{aligned} & \int_{|t|\leq t_0} e^{-2\pi|t|/\beta} \left(1 + \frac{1}{2\pi|t|/\beta}\right) (e^{v|t|} - 1) dt \\ &\leq 2 \int_0^{t_0} e^{(v-2\pi/\beta)t} dt + \frac{v}{\pi/\beta} \int_0^1 \int_0^{t_0} e^{-2\pi t/\beta} e^{\lambda v t} dt d\lambda \\ &\leq \left(2 + \frac{v}{\pi/\beta}\right) \int_0^{t_0} e^{v t} dt \leq \left(\frac{2}{v} + \frac{1}{\pi/\beta}\right) e^{v t_0}, \end{aligned} \quad (\text{C34})$$

where $e^{v t} - 1 = v t \int_0^1 e^{\lambda v t} d\lambda$ is used in the first inequality. Further, the above inequality reduces inequality (C33) to

$$\begin{aligned} & \int_{|t|\leq t_0} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \\ &\leq C \min(|\partial A|, |\partial B|) \left(\frac{2}{v} + \frac{1}{\pi/\beta}\right) e^{v t_0 - \mu R} \\ &\leq \min(|\partial A|, |\partial B|) C \left(\frac{2}{v} + \frac{1}{\pi/\beta}\right) e^{-R/\xi'_\beta}, \end{aligned} \quad (\text{C35})$$

where we use $t_0 = \mu R/(2v)$ and $\mu/2 \geq \xi'^{-1}_\beta = \mu/[2 + (v\beta)/\pi]$.

Thereafter, applying inequalities (C32) and (C35) to Eq. (C30) yields

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt \leq \min(|\partial A|, |\partial B|) \\ &\times \left[\frac{2\beta}{\pi} \left(1 + \frac{\xi'_\beta}{R}\right) + C \left(\frac{2}{v} + \frac{1}{\pi/\beta}\right)\right] e^{-R/\xi'_\beta}, \end{aligned}$$

which, in turn, affords inequality (C23). This completes the proof. \blacksquare

APPENDIX D: PROOF OF THEOREM 10

This section presents the proof for one of the primary proposed theorems, which provides the exponential decay of the quantum correlation defined by

$$\text{QC}_\rho(O_A, O_B) := \inf_{\{P_s, \rho_s\}} \sum_s P_s |C_{\rho_s}(O_A, O_B)|. \quad (\text{D1})$$

In Theorem 10, the following inequality was proven:

$$\begin{aligned} & \text{QC}_\rho(O_A, O_B) \\ &\leq C_\beta (|\partial A| + |\partial B|) (1 + \log |AB|) e^{-R/\xi_\beta}, \end{aligned} \quad (\text{D2})$$

where ξ_β is a $\mathcal{O}(\beta)$ constant expressed as Eq. (54), and C_β is obtained from $c_{\beta,1} + c_{\beta,2}$, with $c_{\beta,1}$ and $c_{\beta,2}$ defined in Eq. (54).

Here, the logarithmic term $1 + \log |AB|$ originates from the norm of $\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}$ and $\rho^{-1/2} \mathcal{L}_{O_B} \rho^{1/2}$ in Eq. (D17). The explicit norm estimation is provided in Claim 22.

1. Proof of Theorem 10

For an arbitrary quantum state ρ , the spectral decomposition of ρ is denoted as

$$\rho = \sum_s \lambda_s |\lambda_s\rangle \langle \lambda_s|. \quad (\text{D3})$$

In the proof, the aim is to explicitly construct a set of ensembles $\{p_m, |\phi_m\rangle\}$ such that

$$\rho_\beta = \sum_m p_m |\phi_m\rangle \langle \phi_m|, \quad (\text{D4})$$

which satisfies inequality (D2). To prove the statements, the following steps are adopted. In the first and second lemmas (Lemmas 17 and 18), the generic quantum states are considered, and they provide general statements regarding the quantum correlations. Thereafter, in the third, fourth, and fifth lemmas (Lemmas 19–21), the property of quantum Gibbs states is utilized to provide an upper bound to the quantum correlations.

In the first step, the general upper bound for the quantum correlation is proven as follows:

Lemma 17. For an arbitrary operator O , \mathcal{L}_O is defined as follows:

$$\mathcal{L}_O := \sum_{s,s'} \frac{2\sqrt{\lambda_s \lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle \lambda_s | O | \lambda_{s'} \rangle |\lambda_s\rangle \langle \lambda_{s'}|. \quad (\text{D5})$$

Then, for the two operators O_A and O_B , if

$$[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0, \quad (\text{D6})$$

the quantum correlation is bound from above as follows:

$$\begin{aligned} & \text{QC}_\rho(O_A, O_B) \\ & \leq \frac{1}{4} \|[(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})]\|. \end{aligned} \quad (\text{D7})$$

Typically, condition (D6) is not satisfied. Further, in the second lemma, consider the case where Eq. (D6) holds only in an approximate sense. Thus, the lemma can be proven as follows:

Lemma 18. For two arbitrary operators O_A and O_B , if two operators $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$ can be determined such that

$$[\tilde{\mathcal{L}}_{O_A}, \tilde{\mathcal{L}}_{O_B}] = 0 \quad (\text{D8})$$

and

$$\|\mathcal{L}_{O_A} - \tilde{\mathcal{L}}_{O_A}\| \leq \delta_1, \quad \|\mathcal{L}_{O_B} - \tilde{\mathcal{L}}_{O_B}\| \leq \delta_2, \quad (\text{D9})$$

the quantum correlation $\text{QC}_\rho(O_A, O_B)$ is upper bounded as follows:

$$\begin{aligned} \text{QC}_\rho(O_A, O_B) & \leq 3\delta_1 + 3\delta_2 \\ & + \frac{1}{4} \|[(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})]\|. \end{aligned} \quad (\text{D10})$$

The final task is to provide an upper bound for the parameters $\{\delta_1, \delta_2\}$ and the norm of the commutator between $\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}$ and $\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2}$. Thus, we first consider an integral form of \mathcal{L}_O , which comprises the time evolution of $t \approx \beta$. The lemma on the basic properties of the operator \mathcal{L}_O is proven as follows:

Lemma 19. Let ρ be a quantum Gibbs state as $\rho = \rho_\beta = e^{-\beta H}$. Then, for an arbitrary operator O , the operator \mathcal{L}_O is given as follows:

$$\mathcal{L}_O = \int_{-\infty}^{\infty} f_\beta(t) O(t) dt, \quad (\text{D11})$$

where $f_\beta(t)$ is defined as

$$f_\beta(t) = \frac{1}{\beta \cosh(\pi t / \beta)}. \quad (\text{D12})$$

Furthermore, the norm of \mathcal{L}_O is upper bounded as follows:

$$\|\mathcal{L}_O\| \leq \|O\|. \quad (\text{D13})$$

Because the function $f_\beta(t)$ decays exponentially as $e^{-\mathcal{O}(|t|/\beta)}$, the operator \mathcal{L}_O is approximately constructed using the time-evolved operator $O(t)$ with $t \approx \beta$. Consequently, the Lieb-Robinson bound is applied to prove the quasilocality of \mathcal{L}_O and construct the operators $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$ in Lemma 18. From Lemma 19, the following lemma, which provides the upper bounds for δ_1 and δ_2 , is proven:

Lemma 20. When ρ is given by the quantum Gibbs state with a short-range Hamiltonian, as in Eq. (11), δ_1 and δ_2 are upper bounded as

$$\begin{aligned} \delta_1 & \leq e^{\mu/(2+2v\beta/\pi)} \left(\frac{8}{\pi} + \frac{4C}{v\beta} \right) |\partial A| e^{-\mu R/[4(1+v\beta/\pi)]}, \\ \delta_2 & \leq e^{\mu/(2+2v\beta/\pi)} \left(\frac{8}{\pi} + \frac{4C}{v\beta} \right) |\partial B| e^{-\mu R/[4(1+v\beta/\pi)]}. \end{aligned} \quad (\text{D14})$$

This lemma provides the upper bound for the first term of the rhs in inequality (D10) as follows:

$$3\delta_1 + 3\delta_2 \leq c_{\beta,1}(|\partial A| + |\partial B|)e^{-R/\xi_\beta}, \quad (\text{D15})$$

where the definition of $c_{\beta,1}$ and ξ_β is used in Eq. (54).

Before detailing the estimation for the second term of the rhs of Eq. (D10), it is shown that, for $R - 2 \leq \xi_\beta$, the upper bound (D15) results in a trivial upper bound for $\text{QC}_\rho(O_A, O_B)$. Indeed, for $R - 2 \leq \xi_\beta$,

$$\begin{aligned} c_{\beta,1}(|\partial A| + |\partial B|)e^{-R/\xi_\beta} &\geq c_{\beta,1}e^{-R/\xi_\beta} \\ &\geq e^{-(R-2)/\xi_\beta} \frac{24}{\pi} \geq \frac{24}{e\pi} \approx 2.8104, \end{aligned} \quad (\text{D16})$$

which is larger than the trivial upper bound $\|O_A\| \cdot \|O_B\| = 1$ [i.e., $\text{QC}_\rho(O_A, O_B) \leq 1$]. Therefore, we consider the regime of $R - 2 > \xi_\beta$ in the following.

The final task involves estimating the commutator,

$$\|[(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}), (\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2})]\|. \quad (\text{D17})$$

Herein, the quasilocality of $\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}$ must be characterized. For $\rho = e^{-\beta H}$, it is obtained from the imaginary time evolution of \mathcal{L}_{O_A} . For a large β , the unboundedness of the imaginary time evolution usually occurs [202]. Notably, owing to the speciality of \mathcal{L}_{O_A} , such an unboundedness can be avoided, and the following lemma can be proven:

Lemma 21. The norm of the commutator (D17) is upper bounded by

$$\begin{aligned} &|\partial A|(2 + \log(1 + \beta\|\text{ad}_H(O_B)\|)) + |\partial B|(2 + \log(1 + \beta\|\text{ad}_H(O_A)\|)) \\ &\leq (|\partial A| + |\partial B|)(2 + \log(1 + 2g\beta|AB|)) \\ &\leq (|\partial A| + |\partial B|) \left(\frac{2 + \log(1 + 2g\beta) + \log|AB|}{\log|AB| + 1} \right) (\log|AB| + 1) \\ &\leq (|\partial A| + |\partial B|)[2 + \log(1 + 2g\beta)](\log|AB| + 1). \end{aligned} \quad (\text{D20})$$

Thus, combining the above inequality with Eq. (D18), an upper bound is provided for the second term of the rhs in inequality (D10) by

$$\begin{aligned} &\frac{1}{4} \|[(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}), (\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2})]\| \\ &\leq c_{\beta,2}(|\partial A| + |\partial B|)(1 + \log|AB|)e^{-R/\xi_\beta}, \end{aligned} \quad (\text{D21})$$

where the definitions of $c_{\beta,2}$ in Eq. (54) are used.

Thus, by applying inequalities (D15) and (D21) to Lemma 18, the desired inequality (D2) can be obtained. This completes the proof of Theorem 10. ■

2. Proof of Lemma 17

In this proof, a technique similar to that outlined in Ref. [167] is employed. Let $\{|\psi_m\rangle\}$ be a set of orthonormal

$$\begin{aligned} &\|[(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}), (\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2})]\| \\ &\leq 3e^{2/\xi_\beta} \left[\frac{8}{\pi} \left(1 + \frac{\xi_\beta}{R-2} \right) + 4C \left(\frac{1}{\pi} + \frac{1}{v\beta} \right) \right] e^{-R/\xi_\beta} \\ &\quad \times \{ |\partial A|[2 + \log(1 + \beta\|\text{ad}_H(O_B)\|)] \\ &\quad + |\partial B|[2 + \log(1 + \beta\|\text{ad}_H(O_A)\|)] \} \\ &\leq e^{2/\xi_\beta} \left(\frac{48 + 12C}{\pi} + \frac{12C}{v\beta} \right) e^{-R/\xi_\beta} \\ &\quad \times \{ |\partial A|[2 + \log(1 + \beta\|\text{ad}_H(O_B)\|)] \\ &\quad + |\partial B|[2 + \log(1 + \beta\|\text{ad}_H(O_A)\|)] \}, \end{aligned} \quad (\text{D18})$$

where $R - 2 > \xi_\beta$ is used in the second inequality.

To estimate the upper bound of $\|\text{ad}_H(O_A)\|$ ($\|\text{ad}_H(O_B)\|$), consider the norm of a commutator $\text{ad}_H(O_X)$ ($\|O_X\| = 1$) for a general operator O_X , which is upper bounded using Eq. (8) as follows:

$$\begin{aligned} \|\text{ad}_H(O_X)\| &\leq \sum_{i \in X} \sum_{Z: Z \ni i} \|\text{ad}_{h_Z}(O_X)\| \\ &\leq 2 \sum_{i \in X} \sum_{Z: Z \ni i} \|h_Z\| \cdot \|O_X\| \leq 2g|X|. \end{aligned} \quad (\text{D19})$$

Hence, using $\log(1 + xy) \leq \log(1 + y) + \log(x)$ for $x \geq 1$ and $y \geq 0$,

quantum states. Define the unitary matrix U , which provides the quantum states: $\{|\psi_m\rangle\}$ in the base of $\{|\lambda_s\rangle\}_s$,

$$|\psi_m\rangle = \sum_s U_{m,s} |\lambda_s\rangle. \quad (\text{D22})$$

Then, by defining the ensemble $\{p_m, |\phi_m\rangle\}$ as

$$|\phi_m\rangle = \frac{1}{\sqrt{p_m}} \sqrt{\rho} |\psi_m\rangle, \quad p_m = \langle \psi_m | \rho | \psi_m \rangle, \quad (\text{D23})$$

the density operator ρ is rewritten as

$$\rho = \sum_m p_m |\phi_m\rangle \langle \phi_m|. \quad (\text{D24})$$

In general, $\{|\phi_m\rangle\}$ are not orthogonal to each other (i.e., $\langle \phi_m | \phi_{m'} \rangle \neq 0$). For this decomposition, the quantum correlation $\text{QC}_\rho(O_A, O_B)$ is upper bounded by

$$\text{QC}_\rho(O_A, O_B) \leq \sum_m p_m |\text{C}_{|\phi_m\rangle}(O_A, O_B)|, \quad (\text{D25})$$

where $\text{C}_{|\phi_m\rangle}(O_A, O_B)$ has been defined as a standard correlation function, that is, $\text{C}_{|\phi_m\rangle}(O_A, O_B) = \langle \phi_m | O_A O_B | \phi_m \rangle - \langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle$. Our task is to identify a good set $\{|\psi_m\rangle\}$ such that $\{|\phi_m\rangle\}$ has a weak correlation with O_A and O_B .

For an arbitrary operator O ,

$$\begin{aligned} \langle \phi_m | O | \phi_m \rangle &= \sum_{s,s'} \frac{U_{m,s'} U_{m,s}^*}{p_m} \sqrt{\lambda_s \lambda_{s'}} \langle \lambda_s | O | \lambda_{s'} \rangle \\ &= \sum_{s,s'} \frac{U_{m,s'} U_{m,s}^*}{p_m} \frac{\lambda_s + \lambda_{s'}}{2} \langle \lambda_s | \mathcal{L}_O | \lambda_{s'} \rangle \\ &= \sum_{s,s'} \frac{U_{m,s'} U_{m,s}^*}{p_m} \frac{1}{2} \langle \lambda_s | \{\rho, \mathcal{L}_O\} | \lambda_{s'} \rangle \\ &= \frac{1}{2p_m} \langle \psi_m | \{\rho, \mathcal{L}_O\} | \psi_m \rangle, \end{aligned} \quad (\text{D26})$$

where definition (D5) is used for \mathcal{L}_O from the second to third equations. Here, the definition is shown again for the convenience of the reader:

$$\mathcal{L}_O := \sum_{s,s'} \frac{2\sqrt{\lambda_s \lambda_{s'}}}{\lambda_s + \lambda_{s'}} \langle \lambda_s | O | \lambda_{s'} \rangle | \lambda_s \rangle \langle \lambda_{s'}|. \quad (\text{D27})$$

Herein, $\{|\psi_m\rangle\}$ are chosen as the simultaneous eigenstates of \mathcal{L}_{O_A} and \mathcal{L}_{O_B} . Note that such a choice is possible because of condition (D6), that is, $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$. We then obtain, from Eq. (D26),

$$\begin{aligned} \langle \phi_m | O_A | \phi_m \rangle &= \frac{1}{2p_m} \langle \psi_m | \{\rho, \mathcal{L}_{O_A}\} | \psi_m \rangle \\ &= \frac{\alpha_{1,m}}{p_m} \langle \psi_m | \rho | \psi_m \rangle = \alpha_{1,m} \end{aligned} \quad (\text{D28})$$

and $\langle \phi_m | O_B | \phi_m \rangle = \alpha_{2,m}$, where $\alpha_{1,m}$ and $\alpha_{2,m}$ are defined as the m th eigenvalues of \mathcal{L}_{O_A} and \mathcal{L}_{O_B} , respectively. Therefore, we obtain

$$\langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle = \alpha_{1,m} \alpha_{2,m} \quad (\text{D29})$$

for an arbitrary m .

We next consider $\langle \phi_m | O_A O_B | \phi_m \rangle$. Then, from Eq. (D26),

$$\langle \phi_m | O_A O_B | \phi_m \rangle = \frac{1}{2p_m} \langle \psi_m | \{\rho, \mathcal{L}_{O_A O_B}\} | \psi_m \rangle. \quad (\text{D30})$$

Further, based on the equation, if $\mathcal{L}_{O_A O_B} = \mathcal{L}_{O_A} \mathcal{L}_{O_B}$ can be obtained, $\langle \phi_m | O_A O_B | \phi_m \rangle = \alpha_{1,m} \alpha_{2,m}$ can also be easily proven in the same manner as for Eq. (D28). However, the difficulty lies in the fact that, in general, $\mathcal{L}_{O_A O_B} \neq \mathcal{L}_{O_A} \mathcal{L}_{O_B}$; hence, a different approach is required.

For this purpose, first consider

$$\begin{aligned} \langle \phi_m | O | \psi_{m'} \rangle &= \sum_{s,s'} \frac{U_{m',s'} U_{m,s}^*}{\sqrt{p_m}} \sqrt{\lambda_s} \langle \lambda_s | O | \lambda_{s'} \rangle \\ &= \sum_{s,s'} \frac{U_{m',s'} U_{m,s}^*}{\sqrt{p_m}} \sqrt{\lambda_s \lambda_{s'}} \langle \lambda_s | O \rho^{-1/2} | \lambda_{s'} \rangle \\ &= \sum_{s,s'} \frac{U_{m',s'} U_{m,s}^*}{\sqrt{p_m}} \frac{\lambda_s + \lambda_{s'}}{2} \langle \lambda_s | \mathcal{L}_{O \rho^{-1/2}} | \lambda_{s'} \rangle \\ &= \frac{1}{2\sqrt{p_m}} \langle \psi_{m'} | \{\rho, \mathcal{L}_{O \rho^{-1/2}}\} | \psi_{m'} \rangle, \end{aligned} \quad (\text{D31})$$

where $\mathcal{L}_{O \rho^{-1/2}} = \mathcal{L}_O \rho^{-1/2}$ is used from definition (D27). Subsequently,

$$\begin{aligned} \langle \phi_m | O_A O_B | \phi_m \rangle &= \sum_{m'} \langle \phi_m | O_A | \psi_{m'} \rangle \langle \psi_{m'} | O_B | \phi_m \rangle \\ &= \frac{1}{4p_m} \sum_{m'} \langle \psi_m | \{\rho, \mathcal{L}_{O_A} \rho^{-1/2}\} | \psi_{m'} \rangle \langle \psi_{m'} | \{\rho, \rho^{-1/2} \mathcal{L}_{O_B}\} | \psi_m \rangle \\ &= \frac{1}{4p_m} \langle \psi_m | \{\rho, \mathcal{L}_{O_A} \rho^{-1/2}\} \{\rho, \rho^{-1/2} \mathcal{L}_{O_B}\} | \psi_m \rangle, \end{aligned} \quad (\text{D32})$$

where $\sum_{m'} |\psi_{m'}\rangle \langle \psi_{m'}| = 1$ is used. Thus, Eq. (D32) is further reduced to

$$\begin{aligned} \langle \phi_m | O_A O_B | \phi_m \rangle &= \frac{1}{4p_m} \langle \psi_m | (\rho \mathcal{L}_{O_A} \rho^{-1/2} + \mathcal{L}_{O_A} \rho^{1/2}) (\rho^{1/2} \mathcal{L}_{O_B} + \rho^{-1/2} \mathcal{L}_{O_B} \rho) | \psi_m \rangle \\ &= \frac{1}{4p_m} \langle \psi_m | (\rho \mathcal{L}_{O_A} \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \rho \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \mathcal{L}_{O_B} \rho + \rho \mathcal{L}_{O_A} \rho^{-1} \mathcal{L}_{O_B} \rho) | \psi_m \rangle. \end{aligned} \quad (\text{D33})$$

Using $\mathcal{L}_{O_A}|\psi_m\rangle = \alpha_{1,m}|\psi_m\rangle$ and $\mathcal{L}_{O_B}|\psi_m\rangle = \alpha_{2,m}|\psi_m\rangle$, the above equation can be reduced to

$$\begin{aligned}\langle\phi_m|O_A O_B|\phi_m\rangle &= \frac{1}{4p_m}\langle\psi_m|(\rho\alpha_{1,m}\alpha_{2,m} + \alpha_{1,m}\rho\alpha_{2,m} + \alpha_{1,m}\alpha_{2,m}\rho + \rho\mathcal{L}_{O_A}\rho^{-1}\mathcal{L}_{O_B}\rho)|\psi_m\rangle \\ &= \frac{3}{4}\alpha_{1,m}\alpha_{2,m} + \frac{1}{4p_m}\langle\psi_m|\rho\mathcal{L}_{O_A}\rho^{-1}\mathcal{L}_{O_B}\rho|\psi_m\rangle,\end{aligned}\quad (\text{D34})$$

where $\langle\psi_m|\rho|\psi_m\rangle = p_m$.

The remaining task entails estimating the error as

$$\langle\psi_m|\rho\mathcal{L}_{O_A}\rho^{-1}\mathcal{L}_{O_B}\rho|\psi_m\rangle - p_m\alpha_{1,m}\alpha_{2,m}.\quad (\text{D35})$$

To obtain this, consider

$$\begin{aligned}\langle\psi_m|\rho\mathcal{L}_{O_A}\rho^{-1}\mathcal{L}_{O_B}\rho|\psi_m\rangle &= \langle\psi_m|\rho^{1/2}(\rho^{1/2}\mathcal{L}_{O_A}\rho^{-1/2})(\rho^{-1/2}\mathcal{L}_{O_B}\rho^{1/2})\rho^{1/2}|\psi_m\rangle \\ &= \langle\psi_m|\rho^{1/2}(\rho^{-1/2}\mathcal{L}_{O_B}\rho^{1/2})(\rho^{1/2}\mathcal{L}_{O_A}\rho^{-1/2})\rho^{1/2}|\psi_m\rangle \\ &\quad + \langle\psi_m|\rho^{1/2}[(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}), (\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2})]\rho^{1/2}|\psi_m\rangle \\ &= p_m\alpha_{1,m}\alpha_{2,m} + p_m\langle\phi_m|[(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}), (\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2})]|\phi_m\rangle,\end{aligned}\quad (\text{D36})$$

where $\mathcal{L}_{O_A}|\psi_m\rangle = \alpha_{1,m}|\psi_m\rangle$ and $\mathcal{L}_{O_B}|\psi_m\rangle = \alpha_{2,m}|\psi_m\rangle$ are used from the second to third equations. Thus, by applying Eq. (D36) to Eq. (D34),

$$|\langle\phi_m|O_A O_B|\phi_m\rangle - \alpha_{1,m}\alpha_{2,m}| \leq \frac{1}{4}\|[(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}), (\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2})]\|. \quad (\text{D37})$$

Therefore, by combining the above inequality and Eq. (D29) with (D25), inequality (D7) is proven. This completes the proof. ■

3. Proof of Lemma 18

The approach used in this proof is similar to that for the proof of Lemma 17. Herein, $\{|\psi_m\rangle\}$ are chosen as the simultaneous eigenstates of $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$, instead of \mathcal{L}_{O_A} and \mathcal{L}_{O_B} :

$$\tilde{\mathcal{L}}_{O_A}|\psi_m\rangle = \tilde{\alpha}_{1,m}|\psi_m\rangle, \quad \tilde{\mathcal{L}}_{O_B}|\psi_m\rangle = \tilde{\alpha}_{2,m}|\psi_m\rangle. \quad (\text{D38})$$

Then, the same inequality as in Eq. (D25) is obtained:

$$\text{QC}_\rho(O_A, O_B) \leq \sum_m p_m |\text{C}_{|\phi_m\rangle}(O_A, O_B)|. \quad (\text{D39})$$

We begin by estimating $\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle$. Using Eq. (D26),

$$\begin{aligned}\langle\phi_m|O_A|\phi_m\rangle &= \frac{1}{2p_m}\langle\psi_m|\{\rho, \mathcal{L}_{O_A}\}|\psi_m\rangle \\ &= \tilde{\alpha}_{1,m} + \frac{1}{2p_m}\langle\psi_m|\{\rho, \delta\mathcal{L}_{O_A}\}|\psi_m\rangle,\end{aligned}\quad (\text{D40})$$

where $\delta\mathcal{L}_{O_A} := \mathcal{L}_{O_A} - \tilde{\mathcal{L}}_{O_A}$. In the same manner, $\langle\phi_m|O_B|\phi_m\rangle = \tilde{\alpha}_{2,m} + [1/(2p_m)]\langle\psi_m|\{\rho, \delta\mathcal{L}_{O_B}\}|\psi_m\rangle$. Thus,

$$\begin{aligned}|\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle - \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m}| \\ \leq \frac{1}{2p_m}|\langle\psi_m|\{\rho, \delta\mathcal{L}_{O_A} + \delta\mathcal{L}_{O_B}\}|\psi_m\rangle|,\end{aligned}\quad (\text{D41})$$

which yields

$$\begin{aligned}\sum_m p_m |\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle - \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m}| \\ \leq \frac{1}{2}\sum_m |\langle\psi_m|\{\rho, \delta\mathcal{L}_{O_A} + \delta\mathcal{L}_{O_B}\}|\psi_m\rangle|.\end{aligned}\quad (\text{D42})$$

For an arbitrary operator O , $|\langle\psi_m|O|\psi_m\rangle| \leq \langle\psi_m|O|\psi_m\rangle$; hence,

$$\begin{aligned}\sum_m |\langle\psi_m|\{\rho, \delta\mathcal{L}_{O_A} + \delta\mathcal{L}_{O_B}\}|\psi_m\rangle| \\ \leq \sum_m \langle\psi_m|\{\rho, \delta\mathcal{L}_{O_A} + \delta\mathcal{L}_{O_B}\}|\psi_m\rangle \\ \leq \|\{\rho, \delta\mathcal{L}_{O_A}\}\|_1 + \|\{\rho, \delta\mathcal{L}_{O_B}\}\|_1 \\ \leq 2\|\rho\|_1 \cdot (\|\delta\mathcal{L}_{O_A}\| + \|\delta\mathcal{L}_{O_B}\|) \leq 2(\delta_1 + \delta_2),\end{aligned}\quad (\text{D43})$$

where $\text{tr}(|O|) = \|O\|_1$, $\|O + O'\|_1 \leq \|O\|_1 + \|O'\|_1$ and $\|OO'\|_1 \leq \|O\|_1 \cdot \|O'\|_1$ are used for the arbitrary operators O and O' , respectively. Further, applying inequality (D43) to (D41) yields

$$\sum_m p_m |\langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle - \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m}| \leq \delta_1 + \delta_2. \quad (\text{D44})$$

Next, the error that originates from $\langle \phi_m | O_A O_B | \phi_m \rangle$ is estimated. Consider the same equation as Eq. (D34):

$$\begin{aligned} \langle \phi_m | O_A O_B | \phi_m \rangle &= \frac{1}{4p_m} \langle \psi_m | (\rho \mathcal{L}_{O_A} \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \rho \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \mathcal{L}_{O_B} \rho + \rho \mathcal{L}_{O_A} \rho^{-1} \mathcal{L}_{O_B} \rho) | \psi_m \rangle \\ &= \frac{1}{4p_m} \langle \psi_m | (\rho \mathcal{L}_{O_A} \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \rho \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \mathcal{L}_{O_B} \rho + \mathcal{L}_{O_B} \rho \mathcal{L}_{O_A}) | \psi_m \rangle \\ &\quad + \frac{1}{4} \langle \phi_m | [(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})] | \phi_m \rangle, \end{aligned} \quad (\text{D45})$$

where, in the second equation, Eq. (D36) is used as follows:

$$\begin{aligned} \langle \psi_m | \rho \mathcal{L}_{O_A} \rho^{-1} \mathcal{L}_{O_B} \rho | \psi_m \rangle &= \langle \psi_m | \rho^{1/2} (\rho^{-1/2} \mathcal{L}_{O_B} \rho^{1/2}) (\rho^{1/2} \mathcal{L}_{O_A} \rho^{-1/2}) \rho^{1/2} | \psi_m \rangle \\ &\quad + \langle \psi_m | \rho^{1/2} [(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})] \rho^{1/2} | \psi_m \rangle \\ &= \langle \psi_m | \mathcal{L}_{O_B} \rho \mathcal{L}_{O_A} | \psi_m \rangle + p_m \langle \phi_m | [(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})] | \phi_m \rangle. \end{aligned} \quad (\text{D46})$$

Further, in Eq. (D45),

$$\begin{aligned} \langle \psi_m | \rho \mathcal{L}_{O_A} \mathcal{L}_{O_B} | \psi_m \rangle &= \langle \psi_m | \rho \mathcal{L}_{O_A} (\tilde{\alpha}_{2,m} + \delta \mathcal{L}_{O_B}) | \psi_m \rangle \\ &= \langle \psi_m | \rho (\tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m} + \delta \mathcal{L}_{O_A} \tilde{\alpha}_{2,m} + \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B}) | \psi_m \rangle \\ &= \langle \psi_m | \rho \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m} + \rho \delta \mathcal{L}_{O_A} \mathcal{L}_{O_B} + \rho \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} - \rho \delta \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} | \psi_m \rangle. \end{aligned} \quad (\text{D47})$$

In a similar manner,

$$\begin{aligned} \langle \psi_m | \mathcal{L}_{O_A} \rho \mathcal{L}_{O_B} | \psi_m \rangle &= \langle \psi_m | \tilde{\alpha}_{1,m} \rho \tilde{\alpha}_{2,m} + \delta \mathcal{L}_{O_A} \rho \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \rho \delta \mathcal{L}_{O_B} - \delta \mathcal{L}_{O_A} \rho \delta \mathcal{L}_{O_B} | \psi_m \rangle, \\ \langle \psi_m | \mathcal{L}_{O_A} \mathcal{L}_{O_B} \rho | \psi_m \rangle &= \langle \psi_m | \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m} \rho + \delta \mathcal{L}_{O_A} \mathcal{L}_{O_B} \rho + \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} \rho - \delta \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} \rho | \psi_m \rangle, \\ \langle \psi_m | \mathcal{L}_{O_B} \rho \mathcal{L}_{O_A} | \psi_m \rangle &= \langle \psi_m | \tilde{\alpha}_{1,m} \rho \tilde{\alpha}_{2,m} + \mathcal{L}_{O_B} \rho \delta \mathcal{L}_{O_A} + \delta \mathcal{L}_{O_B} \rho \mathcal{L}_{O_A} - \delta \mathcal{L}_{O_B} \rho \delta \mathcal{L}_{O_A} | \psi_m \rangle. \end{aligned} \quad (\text{D48})$$

Using the above equations, Eq. (D45) is reduced to

$$\begin{aligned} \langle \phi_m | O_A O_B | \phi_m \rangle &= \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m} + \frac{1}{4p_m} \langle \psi_m | (\rho \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} + \delta \mathcal{L}_{O_A} \rho \mathcal{L}_{O_B} + \delta \mathcal{L}_{O_A} \mathcal{L}_{O_B} \rho + \mathcal{L}_{O_B} \rho \delta \mathcal{L}_{O_A}) | \psi_m \rangle \\ &\quad + \frac{1}{4p_m} \langle \psi_m | (\rho \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \rho \delta \mathcal{L}_{O_B} + \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} \rho + \delta \mathcal{L}_{O_B} \rho \mathcal{L}_{O_A}) | \psi_m \rangle \\ &\quad - \frac{1}{4p_m} \langle \psi_m | (\rho \delta \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} + \delta \mathcal{L}_{O_A} \rho \delta \mathcal{L}_{O_B} + \delta \mathcal{L}_{O_A} \delta \mathcal{L}_{O_B} \rho + \delta \mathcal{L}_{O_B} \rho \delta \mathcal{L}_{O_A}) | \psi_m \rangle \\ &\quad + \frac{1}{4} \langle \phi_m | [(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})] | \phi_m \rangle, \end{aligned} \quad (\text{D49})$$

where $\langle \psi_m | \rho | \psi_m \rangle = p_m$. Thus,

$$\begin{aligned} &\sum_m p_m |\langle \phi_m | O_A O_B | \phi_m \rangle - \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m}| \\ &\leq (\|\delta \mathcal{L}_{O_A}\| \cdot \|\mathcal{L}_{O_B}\| + \|\mathcal{L}_{O_A}\| \cdot \|\delta \mathcal{L}_{O_B}\| + \|\delta \mathcal{L}_{O_A}\| \cdot \|\delta \mathcal{L}_{O_B}\|) + \frac{1}{4} \| [(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})] \|, \end{aligned} \quad (\text{D50})$$

where analyses similar to those for inequality (D43) are used. Using condition (D9) and $\|\mathcal{L}_{O_A}\| \leq \|O_A\| = 1$, which is proven as inequality (D13) in Lemma 19, the inequality of

$$\sum_m p_m |\langle \phi_m | O_A O_B | \phi_m \rangle - \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m}| \leq \delta_1 + \delta_2 + \delta_1 \delta_2 + \frac{1}{4} \|[(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})]\| \quad (\text{D51})$$

is obtained. Further, by combining inequalities (D44) and (D51),

$$\begin{aligned} & \sum_m p_m |\langle \phi_m | O_A O_B | \phi_m \rangle - \langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle| \\ &= \sum_m p_m |\langle \phi_m | O_A O_B | \phi_m \rangle - \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m} - \langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle + \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m}| \\ &\leq \sum_m p_m (|\langle \phi_m | O_A O_B | \phi_m \rangle - \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m}| + p_m |\langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle - \tilde{\alpha}_{1,m} \tilde{\alpha}_{2,m}|) \\ &\leq 2\delta_1 + 2\delta_2 + \delta_1 \delta_2 + \frac{1}{4} \|[(\rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2}), (\rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2})]\|. \end{aligned} \quad (\text{D52})$$

When $\delta_1 \geq 1/2$ or $\delta_2 \geq 1/2$, the upper bound is worse than the trivial bound 1, and hence, the inequality is meaningful only for $\delta_1 \leq 1/2$ and $\delta_2 \leq 1/2$, which yields $\delta_1 \delta_2 \leq \delta_1 + \delta_2$. Thus, by applying the above inequality to Eq. (D39), the main inequality (D10) is proven. This completes the proof. ■

4. Proof of Lemma 19

First, the eigenvalues $\{\lambda_s\}$ and the eigenstates $\{|\lambda_s\rangle\}$ are rewritten as

$$\lambda_s = e^{-\beta E_s}, \quad |\lambda_s\rangle = |E_s\rangle, \quad (\text{D53})$$

where $H|E_s\rangle = E_s|E_s\rangle$. Then, for an arbitrary operator O , definition (D5) provides

$$\begin{aligned} \mathcal{L}_O &= \sum_{s,s'} \frac{2\sqrt{e^{-\beta(E_s - E_{s'})}}}{1 + e^{-\beta(E_s - E_{s'})}} \langle E_s | O | E_{s'} \rangle |E_s\rangle \langle E_{s'}| \\ &= \int_{-\infty}^{\infty} \frac{2\sqrt{e^{-\beta\omega}}}{1 + e^{-\beta\omega}} O_\omega d\omega, \end{aligned} \quad (\text{D54})$$

where the notation of Eq. (A1) is used.

Using Eq. (A2), the above form is reduced to

$$\begin{aligned} \mathcal{L}_O &= \int_{-\infty}^{\infty} \frac{2\sqrt{e^{-\beta\omega}}}{1 + e^{-\beta\omega}} \frac{1}{2\pi} \int_{-\infty}^{\infty} O(t) e^{-i\omega t} dt d\omega \\ &= \int_{-\infty}^{\infty} f_\beta(t) O(t) dt, \end{aligned} \quad (\text{D55})$$

with

$$f_\beta(t) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{2\sqrt{e^{-\beta\omega}}}{1 + e^{-\beta\omega}} e^{-i\omega t} d\omega. \quad (\text{D56})$$

Further, by following the same analysis as in Appendix C 3 a, it can be proven that $f_\beta(t)$ is given by

$$\begin{aligned} & \overline{f_\beta(t)} \\ &= \begin{cases} i \sum_{m=1}^{\infty} \text{Res}_{\omega=(2\pi im - i\pi)/\beta} \left(\frac{2\sqrt{e^{-\beta\omega}}}{1 + e^{-\beta\omega}} e^{-i\omega t} \right) & \text{for } t < 0, \\ -i \sum_{m=1}^{\infty} \text{Res}_{\omega=(-2\pi im + i\pi)/\beta} \left(\frac{2\sqrt{e^{-\beta\omega}}}{1 + e^{-\beta\omega}} e^{-i\omega t} \right) & \text{for } t \geq 0, \end{cases} \\ &= \begin{cases} -\sum_{m=1}^{\infty} \frac{2(-1)^m}{\beta} e^{\pi(2m-1)t/\beta} & \text{for } t < 0, \\ -\sum_{m=1}^{\infty} \frac{2(-1)^m}{\beta} e^{-\pi(2m-1)t/\beta} & \text{for } t \geq 0, \end{cases} \\ &= \sum_{m=1}^{\infty} \frac{2(-1)^m}{\beta} e^{-\pi(2m-1)|t|/\beta} = \frac{1}{\beta \cosh(\pi|t|/\beta)}. \end{aligned}$$

This completes the proof of Eq. (D11).

The proof of inequality (D13) is simply given as follows. Owing to $f_\beta(t) \geq 0$,

$$\|\mathcal{L}_O\| \leq \int_{-\infty}^{\infty} f_\beta(t) \|O(t)\| dt \leq \|O\| \int_{-\infty}^{\infty} f_\beta(t) dt. \quad (\text{D57})$$

Using the inverse Fourier transform

$$\int_{-\infty}^{\infty} f_\beta(t) e^{i\omega t} dt = \frac{2\sqrt{e^{-\beta\omega}}}{1 + e^{-\beta\omega}} \quad (\text{D58})$$

with $\omega = 0$, the inequality (D57) is reduced to Eq. (D13). This completes the proof. ■

5. Proof of Lemma 20

First, consider the explicit construction of $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$, such that $[\tilde{\mathcal{L}}_{O_A}, \tilde{\mathcal{L}}_{O_B}] = 0$. For this purpose, Eq. (D11) is used in Lemma 19, and the time-evolved operator $O_A(t)$ is approximated on $A[r_1]$ (see Fig. 4), which yields

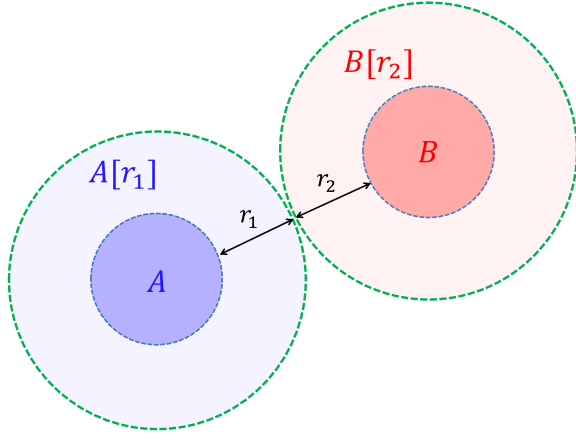


FIG. 4. Approximations of \mathcal{L}_{O_A} and \mathcal{L}_{O_B} . To obtain the approximations $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$, which commute with each other, \mathcal{L}_{O_A} and \mathcal{L}_{O_B} are approximated onto the extended regions $A[r_1]$ and $B[r_2]$ ($r_1 + r_2 < R$), respectively. In Eqs. (D59) and (D60), the explicit forms of \mathcal{L}_{O_A} and \mathcal{L}_{O_B} are presented.

$$\tilde{\mathcal{L}}_{O_A} = \int_{-\infty}^{\infty} f_{\beta}(t) O_A(t, A[r_1]) dt, \quad (\text{D59})$$

where the notation of $O_A(t, A[r_1])$ has been provided in Eq. (16), and r_1 is chosen appropriately. Note that $\tilde{\mathcal{L}}_{O_A}$ is now supported on the subset $A[r_1]$. In the same manner, $\tilde{\mathcal{L}}_{O_B}$ is defined as

$$\tilde{\mathcal{L}}_{O_B} = \int_{-\infty}^{\infty} f_{\beta}(t) O_B(t, B[r_2]) dt. \quad (\text{D60})$$

Thus, if we set $r_1 + r_2 < d_{A,B} = R$, $[\tilde{\mathcal{L}}_{O_A}, \tilde{\mathcal{L}}_{O_B}] = 0$ is obtained. Therefore, in the following discussions, $r_1 = r_2 = \lceil R/2 \rceil - 1$ is chosen.

Using Eq. (D59), δ_1 can be estimated as

$$\delta_1 \leq \int_{-\infty}^{\infty} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt. \quad (\text{D61})$$

For the estimation of the integral, an approach similar to that in Appendix C 3 b is used. First,

$$\begin{aligned} & \int_{-\infty}^{\infty} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt \\ &= \int_{|t| > t_0} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt \\ &+ \int_{|t| \leq t_0} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt, \end{aligned} \quad (\text{D62})$$

where $t_0 := \mu r_1 / (2v)$. Owing to

$$\begin{aligned} f_{\beta}(t) &= \frac{1}{\beta \cosh(\pi|t|/\beta)} \leq \frac{2}{\beta} e^{-\pi|t|/\beta}, \\ \|O_A(t) - O_A(t, A[r_1])\| &\leq 2\|O_A\| = 2, \end{aligned} \quad (\text{D63})$$

the first term is upper bounded as

$$\begin{aligned} & \int_{|t| > t_0} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt \\ &\leq \frac{4}{\beta} \int_{|t| > t_0} e^{-\pi|t|/\beta} dt \leq \frac{8}{\pi} e^{-\pi \mu r_1 / (2v\beta)}. \end{aligned} \quad (\text{D64})$$

The quantity $\|O_A(t) - O_A(t, A[r_1])\|$ is upper bounded using the Lieb-Robinson bound (18), and hence, the second term is upper bounded as

$$\begin{aligned} & \int_{|t| \leq t_0} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt \\ &\leq \frac{2}{\beta} \int_{|t| \leq t_0} e^{-\pi|t|/\beta} C |\partial A| (e^{v|t|} - 1) e^{-\mu r_1} dt \\ &\leq \frac{4C}{\beta} |\partial A| \int_0^{t_0} e^{v|t|} e^{-\mu r_1} dt \\ &\leq \frac{4C}{v\beta} |\partial A| e^{-\mu r_1 + vt_0} = \frac{4C}{v\beta} |\partial A| e^{-\mu r_1 / 2}. \end{aligned} \quad (\text{D65})$$

Further, applying inequalities (D64) and (D65), Eq. (D62) is reduced to

$$\begin{aligned} \delta_1 &\leq \int_{-\infty}^{\infty} f_{\beta}(t) \|O_A(t) - O_A(t, A[r_1])\| dt \\ &\leq \left(\frac{8}{\pi} + \frac{4C}{v\beta} \right) |\partial A| e^{-\min[\mu r_1 / 2, \pi \mu r_1 / (2v\beta)]} \\ &\leq \left(\frac{8}{\pi} + \frac{4C}{v\beta} \right) |\partial A| e^{-\mu r_1 / (2 + 2v\beta/\pi)}, \end{aligned} \quad (\text{D66})$$

where $|\partial A| \geq 1$ is used in the second inequality. In the same manner,

$$\begin{aligned} \delta_2 &\leq \int_{-\infty}^{\infty} f_{\beta}(t) \|O_B(t) - O_B(t, B[r_2])\| dt \\ &\leq \left(\frac{8}{\pi} + \frac{4C}{v\beta} \right) |\partial B| e^{-\mu r_2 / (2 + 2v\beta/\pi)}. \end{aligned} \quad (\text{D67})$$

Thus, applying $r_1 = r_2 = \lceil R/2 \rceil - 1$, inequality (D14) is proven. This completes the proof. ■

6. Proof of Lemma 21

First, consider the integral expression of $\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2}$ for an arbitrary operator O . Using

$$e^{\pm \beta H / 2} O_{\omega} e^{\mp \beta H / 2} = e^{\pm \beta \omega / 2} O_{\omega}, \quad (\text{D68})$$

based on Eq. (D54), we obtain

$$\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2} = \int_{-\infty}^{\infty} \frac{2\sqrt{e^{-\beta\omega}}}{1+e^{-\beta\omega}} e^{\pm\beta\omega/2} O_{\omega} d\omega. \quad (\text{D69})$$

Using Eq. (A2), the above equation is reduced to

$$\begin{aligned} & \rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2} \\ &= \int_{-\infty}^{\infty} \frac{2\sqrt{e^{-\beta\omega}}}{1+e^{-\beta\omega}} e^{\pm\beta\omega/2} \frac{1}{2\pi} \int_{-\infty}^{\infty} O(t) e^{-i\omega t} dt d\omega \\ &= \int_{-\infty}^{\infty} g_{\beta,\pm}(t) O(t) dt, \end{aligned} \quad (\text{D70})$$

where $g_{\beta}(t)$ is defined as

$$g_{\beta,\pm}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{2\sqrt{e^{-\beta\omega}}}{1+e^{-\beta\omega}} e^{\pm\beta\omega/2} e^{-i\omega t} d\omega. \quad (\text{D71})$$

Further,

$$\begin{aligned} g_{\beta,\pm}(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} [\pm \tanh(\beta\omega/2) + 1] e^{-i\omega t} d\omega \\ &= \delta(t) \pm g_{\beta}(t), \end{aligned} \quad (\text{D72})$$

where $\delta(t)$ is the delta function and $g_{\beta}(t)$ is the Fourier transform of $\tanh(\beta\omega/2)$.

As in Appendix C 3 a, herein,

$$\begin{aligned} & g_{\beta}(t) \\ &= \begin{cases} i \sum_{m=1}^{\infty} \text{Res}_{\omega=(2\pi im - i\pi)/\beta} (\tanh(\beta\omega/2) e^{-i\omega t}) & \text{for } t < 0, \\ -i \sum_{m=1}^{\infty} \text{Res}_{\omega=(-2\pi im + i\pi)/\beta} (\tanh(\beta\omega/2) e^{-i\omega t}) & \text{for } t \geq 0, \end{cases} \\ &= \begin{cases} i \sum_{m=1}^{\infty} \frac{2}{\beta} e^{\pi(2m-1)t/\beta} & \text{for } t < 0, \\ -i \sum_{m=1}^{\infty} \frac{2}{\beta} e^{-\pi(2m-1)t/\beta} & \text{for } t \geq 0, \end{cases} \\ &= \frac{-2i}{\beta} \text{sign}(t) \sum_{m=1}^{\infty} e^{-\pi(2m-1)|t|/\beta} \\ &= -i \frac{\text{sign}(t)}{\beta \sinh(\pi|t|/\beta)} = \frac{-i}{\beta \sinh(\pi t/\beta)}. \end{aligned} \quad (\text{D73})$$

Consequently,

$$\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2} = O \pm \int_{-\infty}^{\infty} g_{\beta}(t) O(t) dt. \quad (\text{D74})$$

For the proof of the lemma, the following two claims must be proven:

Claim 22. Let O be an arbitrary operator supported on a subset $X \subset \Lambda$. Then, the norm of $\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2}$ is upper bounded as

$$\|\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2}\| \leq \|O\| \log \left(1 + \frac{\beta \|\text{ad}_H(O)\|}{\|O\|} \right) + 2\|O\|. \quad (\text{D75})$$

Claim 23. Let O be the operator defined in Claim 22. Then, for $\|O\| = 1$, the operator $\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2}$ is approximated on $X[r]$ with an error of

$$\begin{aligned} & \|\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2} - (\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2})_{X[r]}\| \\ & \leq |\partial X| \left[\frac{8}{\pi} \left(1 + \frac{\xi_{\beta}}{2r} \right) + 4C \left(\frac{1}{\pi} + \frac{1}{v\beta} \right) \right] e^{-2r/\xi_{\beta}}, \end{aligned} \quad (\text{D76})$$

where $(\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2})_{X[r]}$ is supported on $X[r]$ and chosen appropriately.

Using these claims, an upper bound for the norm of Eq. (D17) can be provided. Let us approximate

$$\begin{aligned} \mathfrak{D}_1 &:= \rho^{-1/2} \mathcal{L}_{O_A} \rho^{1/2} \approx \mathfrak{D}_{1,A[r_1]}, \\ \mathfrak{D}_2 &:= \rho^{1/2} \mathcal{L}_{O_B} \rho^{-1/2} \approx \mathfrak{D}_{2,B[r_2]}, \end{aligned} \quad (\text{D77})$$

where $r_1 + r_2 < R$. Then, from $[\mathfrak{D}_{1,A[r_1]}, \mathfrak{D}_{2,B[r_2]}] = 0$,

$$\begin{aligned} \|\mathfrak{D}_1, \mathfrak{D}_2\| &= \|[\mathfrak{D}_1 - \mathfrak{D}_{1,A[r_1]}, \mathfrak{D}_2] \\ & \quad + [\mathfrak{D}_{1,A[r_1]}, \mathfrak{D}_2 - \mathfrak{D}_{2,B[r_2]}]\| \\ & \leq 2\|\delta\mathfrak{D}_1\| \cdot \|\mathfrak{D}_2\| + 2\|\delta\mathfrak{D}_2\| \cdot \|\mathfrak{D}_1\| \\ & \quad + 2\|\delta\mathfrak{D}_1\| \cdot \|\delta\mathfrak{D}_2\|, \end{aligned} \quad (\text{D78})$$

where $\delta\mathfrak{D}_1 := \mathfrak{D}_1 - \mathfrak{D}_{1,A[r_1]}$ and $\delta\mathfrak{D}_2 := \mathfrak{D}_2 - \mathfrak{D}_{2,B[r_2]}$ are defined, and $\|\mathfrak{D}_{1,A[r_1]}\| \leq \|\mathfrak{D}_1\| + \|\delta\mathfrak{D}_1\|$ is used in the inequality. For $\|\delta\mathfrak{D}_s\| > \|\mathfrak{D}_s\|$ ($s = 1, 2$), the above inequality is worse than the trivial inequality, that is, $\|[\mathfrak{D}_1, \mathfrak{D}_2]\| \leq 2\|\mathfrak{D}_1\| \cdot \|\mathfrak{D}_2\|$. Hence, only $\|\delta\mathfrak{D}_s\| \leq \|\mathfrak{D}_s\|$ is considered, which yields

$$\|\mathfrak{D}_1, \mathfrak{D}_2\| \leq 3(\|\delta\mathfrak{D}_1\| \cdot \|\mathfrak{D}_2\| + \|\delta\mathfrak{D}_2\| \cdot \|\mathfrak{D}_1\|). \quad (\text{D79})$$

By choosing $r_1 = r_2 = \lceil R/2 \rceil - 1$ and applying Claims 22 and 23, the main inequality (D18) is obtained as follows:

$$\begin{aligned} \|\mathfrak{D}_1, \mathfrak{D}_2\| & \leq 3e^{2/\xi_{\beta}} \left[\frac{8}{\pi} \left(1 + \frac{\xi_{\beta}}{R-2} \right) + 4C \left(\frac{1}{\pi} + \frac{1}{v\beta} \right) \right] e^{-R/\xi_{\beta}} \\ & \quad \times \{ |\partial A| [2 + \log(1 + \beta \|\text{ad}_H(O_B)\|)] \\ & \quad + |\partial B| [2 + \log(1 + \beta \|\text{ad}_H(O_A)\|)] \}, \end{aligned} \quad (\text{D80})$$

where $\|O_A\| = \|O_B\| = 1$. This completes the proof of Lemma 21.

a. Proof of Claim 22

From the integral expression (D74),

$$\|\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2}\| \leq \|O\| + \left\| \int_{-\infty}^{\infty} g_{\beta}(t) O(t) dt \right\|. \quad (\text{D81})$$

In a standard approach, the following is used:

$$\left\| \int_{-\infty}^{\infty} g_{\beta}(t) O(t) dt \right\| \leq \|O\| \int_{-\infty}^{\infty} |g_{\beta}(t)| dt. \quad (\text{D82})$$

$$\begin{aligned} \left\| \int_{-\infty}^{\infty} g_{\beta}(t) O(t) dt \right\| &\leq \left\| \int_{|t|>\delta t} g_{\beta}(t) O(t) dt \right\| + \left\| \int_{|t|\leq\delta t} g_{\beta}(t) O(t) dt + \int_{|t|\leq\delta t} it \int_0^1 g_{\beta}(t) \text{ad}_H(O)(\lambda) d\lambda dt \right\| \\ &\leq 2\|O\| \int_{t>\delta t} \frac{1}{\beta \sinh(\pi t/\beta)} dt + 2\|\text{ad}_H(O)\| \int_0^{\delta t} \frac{t}{\beta \sinh(\pi t/\beta)} dt \\ &\leq \frac{2\|O\|}{\pi} \log \left[\tanh \left(\frac{\pi \delta t}{2\beta} \right) \right] + \frac{2\|\text{ad}_H(O)\|}{\pi} \delta t \leq \frac{2\|O\|}{\pi} \log \left(1 + \frac{2\beta}{\pi \delta t} \right) + \frac{2\|\text{ad}_H(O)\|}{\pi} \delta t, \end{aligned} \quad (\text{D84})$$

where $\int_{|t|\leq\delta t} g_{\beta}(t) dt = 0$, $1/\sinh(x) \leq 1/x$, and $-\log[\tanh(x)] \leq \log(1+1/x)$ are used in the second, third, and fourth inequalities, respectively. Note that $g_{\beta}(-t) = -g_{\beta}(t)$. Thus, by choosing $\delta t = \|O\|/\|\text{ad}_H(O)\|$,

$$\left\| \int_{-\infty}^{\infty} g_{\beta}(t) O(t) dt \right\| \leq \frac{2\|O\|}{\pi} \log \left(1 + \frac{2\beta \|\text{ad}_H(O)\|}{\pi \|O\|} \right) + \frac{2\|O\|}{\pi}. \quad (\text{D85})$$

Therefore, by combining inequalities (D81) and (D85) with $2/\pi \leq 1$, inequality (D75) is proven. ■

b. Proof of Claim 23

As in the proof of Lemma 20, we consider a similar approximation to the one in Eq. (D59). Using the integral expression (D74), we obtain

$$(\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2})_{X[r]} := O \pm \int_{-\infty}^{\infty} g_{\beta}(t) O(t, X[r]) dt, \quad (\text{D86})$$

which yields

$$\begin{aligned} &\|\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2} - (\rho^{\pm 1/2} \mathcal{L}_O \rho^{\mp 1/2})_{X[r]}\| \\ &\leq \int_{-\infty}^{\infty} |g_{\beta}(t)| \cdot \|O(t, X[r]) - O(t)\| dt. \end{aligned} \quad (\text{D87})$$

Using $1/\sinh(x) \leq 2e^{-x}(1+1/x)$ ($x \geq 0$),

$$|g_{\beta}(t)| = \frac{1}{\beta \sinh(\pi|t|/\beta)} \leq \frac{2e^{-\pi|t|/\beta}}{\beta} \left(1 + \frac{1}{\pi|t|/\beta} \right). \quad (\text{D88})$$

In addition, as per the Lieb-Robinson bound (18),

However, the integral of $|g_{\beta}(t)|$ does not converge because $|g_{\beta}(t)| \propto 1/t$ for $t \ll 1$.

Thus, to obtain a refined bound, $O(t)$ is parametrized as $O(\lambda t)$ using the parameter λ . Subsequently,

$$O(t) = O + \int_0^1 \frac{d}{d\lambda} O(\lambda t) d\lambda = O + it \int_0^1 \text{ad}_H(O)(\lambda) d\lambda, \quad (\text{D83})$$

which yields

$$\|O(t) - O_X(t, X[r])\| \leq \min(C|\partial X|(e^{v|t|} - 1)e^{-\mu r}, 2). \quad (\text{D89})$$

Subsequently, analyses similar to those for Eqs. (C32), (C33), and (C35) can be applied. For $t_0 = \mu r/(2v)$, we obtain

$$\begin{aligned} &\int_{-\infty}^{\infty} |g_{\beta}(t)| \cdot \|O(t, X[r]) - O(t)\| dt \\ &\leq \int_{|t|>t_0} \frac{2e^{-\pi|t|/\beta}}{\beta} \left(1 + \frac{1}{\pi|t|/\beta} \right) \cdot 2dt \\ &\quad + \int_{|t|\leq t_0} \frac{2e^{-\pi|t|/\beta}}{\beta} \left(1 + \frac{1}{\pi|t|/\beta} \right) \cdot C|\partial X|(e^{v|t|} - 1)e^{-\mu r} dt \\ &\leq \frac{8e^{-\pi t_0/\beta}}{\pi} \left(1 + \frac{1}{\pi t_0/\beta} \right) + \frac{4C}{\beta} |\partial X| \left(\frac{1}{v} + \frac{1}{\pi/\beta} \right) e^{-\mu r + v t_0} \\ &\leq |\partial X| \left[\frac{8}{\pi} \left(1 + \frac{2v\beta}{\pi\mu r} \right) e^{-\pi\mu r/(2v\beta)} + 4C \left(\frac{1}{\pi} + \frac{1}{v\beta} \right) e^{-\mu r/2} \right] \\ &\leq |\partial X| \left[\frac{8}{\pi} \left(1 + \frac{\xi_{\beta}}{2r} \right) + 4C \left(\frac{1}{\pi} + \frac{1}{v\beta} \right) \right] e^{-2r/\xi_{\beta}}, \end{aligned}$$

where the definition of $\xi_{\beta} := 4/\mu(1+v\beta/\pi)$ is used in the last inequality. This completes the proof of Claim 23. ■

APPENDIX E: PROOF OF PROPOSITION 9

Herein, the proof of Proposition 9, which connects the PPT relative entanglement and quantum correlation, is presented. When the quantum correlation satisfies

$$\text{QC}_{\rho_{AB}}(O_A, O_B) \leq \epsilon \|O_A\| \cdot \|O_B\| \quad (\text{E1})$$

for two arbitrary operators O_A and O_B , Proposition 9 yields

$$E_R^{\text{PPT}}(\rho_{AB}) \leq 4\mathcal{D}_{AB}\bar{\delta}\log(1/\bar{\delta}) \leq 4\mathcal{D}_{AB}\bar{\delta}^{1/2}, \quad (\text{E2})$$

where $\bar{\delta} := 4\epsilon \min(\mathcal{D}_A, \mathcal{D}_B)$.

1. Proof

In inequality (E2), if $\bar{\delta} > 1/\mathcal{D}_{AB}$, the upper bound is worse than the trivial bound, i.e., $E_R^{\text{PPT}}(\rho_{AB}) \leq \log[\min(\mathcal{D}_A, \mathcal{D}_B)] \leq (1/2)\log(\mathcal{D}_{AB})$. Hence, only the case of $\bar{\delta} \leq 1/\mathcal{D}_{AB}$ is considered.

The eigenstates of $\rho_{AB}^{T_A}$ with negative eigenvalues are defined as $\{|\eta_i\rangle\}_{i=1}^{M_0}$. Then, the proof of Proposition 9 is immediately obtained via the following lemma:

Lemma 24. For the quantum state ρ_{AB} given in Proposition 9, the minimum negative eigenvalue of $\rho_{AB}^{T_A}$ satisfies

$$\delta := -\min_{i \in [M_0]} \langle \eta_i | \rho_{AB}^{T_A} | \eta_i \rangle \leq 4\epsilon \min(\mathcal{D}_A, \mathcal{D}_B) = \bar{\delta}, \quad (\text{E3})$$

where the parameter ϵ has been defined in Eq. (E1).

To prove inequality (52), a quantum state $\tilde{\sigma}_{AB}$ is defined as follows:

$$\tilde{\sigma}_{AB} = (1 - \mathcal{D}_{AB}\bar{\delta})\rho_{AB} + \bar{\delta} \cdot \hat{1}_{AB}, \quad (\text{E4})$$

where $\text{tr}(\tilde{\sigma}_{AB}) = 1$ since $\text{tr}(\bar{\delta} \cdot \hat{1}_{AB}) = \mathcal{D}_{AB}\bar{\delta}$. Because of the definition of δ in Eq. (E3), we have $\tilde{\sigma}_{AB}^{T_A} \geq 0$ (i.e., $\tilde{\sigma}_{AB} \in \text{PPT}$). We then obtain

$$E_R^{\text{PPT}}(\rho_{AB}) \leq S(\rho_{AB} || \tilde{\sigma}_{AB}). \quad (\text{E5})$$

Subsequently, using the continuity bound on the relative entropy (Theorem 196 of Ref. [203], or Ref. [79]),

$$S(\rho_{AB} || \tilde{\sigma}_{AB}) \leq \delta_{AB} \log(\mathcal{D}_{AB}) - \delta_{AB} \log(\delta_{AB}) - \delta_{AB} \log[\lambda_{\min}(\tilde{\sigma}_{AB})] \quad (\text{E6})$$

under the assumption of $\delta_{AB} \leq 1/e$, where $\delta_{AB} := \|\rho_{AB} - \tilde{\sigma}_{AB}\|_1$ and $\lambda_{\min}(\tilde{\sigma}_{AB})$ are defined as the minimum eigenvalues of $\tilde{\sigma}_{AB}$. Based on definition (E4), $\lambda_{\min}(\tilde{\sigma}_{AB}) \geq \bar{\delta}$ and

$$\delta_{AB} \leq 2\mathcal{D}_{AB}\bar{\delta}. \quad (\text{E7})$$

First, the case of $2\mathcal{D}_{AB}\bar{\delta} \leq 1/e$, that is, $\bar{\delta} \leq 1/(2e\mathcal{D}_{AB})$, is considered. Then, $-\delta_{AB} \log(\delta_{AB}) \leq -2\mathcal{D}_{AB}\bar{\delta} \log(2\mathcal{D}_{AB}\bar{\delta})$, and hence, inequality (E6) reduces to

$$S(\rho_{AB} || \tilde{\sigma}_{AB}) \leq -2\mathcal{D}_{AB}\bar{\delta} \log(2\bar{\delta}^2) \leq -4\mathcal{D}_{AB}\bar{\delta} \log(\bar{\delta}). \quad (\text{E8})$$

In the case of $\bar{\delta} > 1/(2e\mathcal{D}_{AB})$, the rhs of the above inequality is larger than the trivial upper bound

$(1/2)\log(\mathcal{D}_{AB})$. Therefore, by combining inequality (E8) with (E5), the main inequality (52) is proven. This completes the proof. ■

2. Proof of Lemma 24

The next task is to estimate

$$\min_i \langle \eta_i | \rho_{AB}^{T_A} | \eta_i \rangle = \inf_{|\eta\rangle} \text{tr}(\rho_{AB}^{T_A} P_\eta) \quad (\text{E9})$$

under the assumption of Eq. (E1), where $P_\eta := |\eta\rangle\langle\eta|$. Therefore, first,

$$\begin{aligned} \text{tr}(\rho_{AB}^{T_A} P_\eta) &= \text{tr}(\rho_{AB} P_\eta^{T_A}) \\ &= \text{tr}(\rho_{AB} P_\eta) + \text{tr}[\rho_{AB}(P_\eta^{T_A} - P_\eta)] \end{aligned}$$

is rewritten, and the second term is subsequently proven to be approximately equal to zero for an arbitrary quantum state $|\eta\rangle$. Because the eigenvalues of $\rho_{AB}^{T_A}$ do not depend on the choice of basis [95], the basis that yields the Schmidt decomposition of $|\eta\rangle$ is selected as follows:

$$|\eta\rangle = \sum_{s=1}^{\mathcal{D}_A} \nu_s |s_A, s_B\rangle, \quad \sum_s |\nu_s|^2 = 1, \quad (\text{E10})$$

where we assume $\mathcal{D}_A < \mathcal{D}_B$ without loss of generality.

To verify this point, we first consider the qubit case, that is, $\mathcal{D}_A = \mathcal{D}_B = 2$. Consider the proof of the following lemma:

Lemma 25. When $\mathcal{D}_A = \mathcal{D}_B = 2$, we have

$$|\text{tr}[\rho_{AB}(P_\eta^{T_A} - P_\eta)]| \leq 2\epsilon, \quad (\text{E11})$$

where the parameter ϵ is given in Eq. (E1).

To generalize the results of two qubits to two-qudit systems, consider

$$P_\eta^{T_A} - P_\eta = \sum_{s,s':s \neq s'}^{\mathcal{D}_A} \nu_s \nu_{s'} (-|s_A, s_B\rangle\langle s'_A, s'_B| + |s'_A, s_B\rangle\langle s_A, s'_B|)$$

and

$$\begin{aligned} &\nu_s \nu_{s'} (-|s_A, s_B\rangle\langle s'_A, s'_B| + |s'_A, s_B\rangle\langle s_A, s'_B|) + \text{H.c.} \\ &= (\nu_s^2 + \nu_{s'}^2)(|\eta_{s,s'}\rangle\langle\eta_{s,s'}|^{T_A} - |\eta_{s,s'}\rangle\langle\eta_{s,s'}|), \end{aligned} \quad (\text{E12})$$

where $|\eta_{s,s'}\rangle := (\nu_s^2 + \nu_{s'}^2)^{-1/2}(\nu_s |s_A, s_B\rangle + \nu_{s'} |s'_A, s'_B\rangle)$. Now, the quantum state $|\eta_{s,s'}\rangle$ is reduced to a quantum state with two qubits. Thus, from Lemma 25,

$$|\text{tr}[\rho_{AB}(|\eta_{s,s'}\rangle\langle\eta_{s,s'}|^{T_A} - |\eta_{s,s'}\rangle\langle\eta_{s,s'}|)]| \leq 2\epsilon, \quad (\text{E13})$$

which yields

$$\begin{aligned}
& |\text{tr}[\rho_{AB}(P_\eta^{T_A} - P_\eta)]| \\
&= \sum_{1 \leq s < s' \leq \mathcal{D}_A} (\nu_s^2 + \nu_{s'}^2) |\text{tr}[\rho_{AB}(|\eta_{s,s'}\rangle\langle\eta_{s,s'}|^{T_A} - |\eta_{s,s'}\rangle\langle\eta_{s,s'}|)]| \\
&\leq 2\epsilon \sum_{1 \leq s < s' \leq \mathcal{D}_A} (\nu_s^2 + \nu_{s'}^2) \leq 4\epsilon \mathcal{D}_A. \quad (\text{E14})
\end{aligned}$$

Consequently,

$$\text{tr}(\rho_{AB} P_\eta^{T_A}) \geq \text{tr}(\rho_{AB} P_\eta) - 4\epsilon \mathcal{D}_A \geq -4\epsilon \mathcal{D}_A, \quad (\text{E15})$$

where $\text{tr}(\rho_{AB} P_\eta) \geq 0$ is used in the second inequality. Further, using the above inequality,

$$\inf_{|\eta\rangle} \text{tr}(\rho_{AB}^{T_A} P_\eta) \geq -4\epsilon \mathcal{D}_A. \quad (\text{E16})$$

When $\mathcal{D}_B \leq \mathcal{D}_A$, the above lower bound is replaced by $\inf_{|\eta\rangle} \text{tr}(\rho_{AB}^{T_A} P_\eta) \geq -4\epsilon \mathcal{D}_B$. Therefore, the parameter δ ($= -\min_i \langle \eta_i | \rho_{AB}^{T_A} | \eta_i \rangle$) is upper bounded by

$$\delta \leq 4\epsilon \min(\mathcal{D}_A, \mathcal{D}_B). \quad (\text{E17})$$

Using this, inequality (G4) is reduced to the main inequality (52). This completes the proof. ■

a. Proof of Lemma 25

When $\mathcal{D}_A = \mathcal{D}_B = 2$, an arbitrary operator O_{AB} is described in the form of

$$O_{AB} = \sum_{P=x,y,z} (J_P \hat{\sigma}_{1,P} \hat{\sigma}_{2,P} + h_{1,P} \hat{\sigma}_{1,P} + h_{2,P} \hat{\sigma}_{2,P}) \quad (\text{E18})$$

by appropriately choosing the bases (see Lemma 1 of Ref. [204] for an example), where $A = \{1\}$ and $B = \{2\}$ and $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ are the Pauli matrices. Then, the partial transpose T_A only changes $\hat{\sigma}_{1,y} \rightarrow -\hat{\sigma}_{1,y}$, and hence,

$$\begin{aligned}
O_{AB} - O_{AB}^{T_A} &= 2(J_y \hat{\sigma}_{1,y} \hat{\sigma}_{2,y} + h_{1,y} \hat{\sigma}_{1,y}) \\
&= 2\hat{\sigma}_{1,y} \otimes (J_y \hat{\sigma}_{2,y} + h_{1,y}). \quad (\text{E19})
\end{aligned}$$

In this manner, the following can be expressed:

$$P_\eta^{T_A} - P_\eta = \Phi_A \otimes \Phi_B, \quad (\text{E20})$$

where $\|\Phi_A\| \leq 2$ and $\|\Phi_B\| = 1$ can be realized owing to $\|P_\eta^{T_A} - P_\eta\| \leq 2$. Subsequently, based on condition (E1) and inequality (37) in Lemma 5,

$$\text{QC}_{\rho_{AB}}(\Phi_A, \Phi_B) \leq \text{QC}_\rho(\Phi_A, \Phi_B) \leq \epsilon \|\Phi_A\| \cdot \|\Phi_B\|,$$

which yields

$$\begin{aligned}
& |\text{tr}[\rho_{AB}(P_\eta^{T_A} - P_\eta)]| \\
&= |\text{tr}(\rho_{AB} \Phi_A \otimes \Phi_B)| \\
&\leq \left| \sum_s p_s \text{tr}(\rho_{s,A} \Phi_A) \text{tr}(\rho_{s,B} \Phi_B) \right| \\
&\quad + \left| \sum_s p_s (\text{tr}(\rho_{s,AB} \Phi_A \Phi_B)) - \text{tr}(\rho_{s,A} \Phi_A) \text{tr}(\rho_{s,B} \Phi_B) \right| \\
&\leq \sum_s p_s |\text{tr}(\rho_{s,A} \otimes \rho_{s,B} \Phi_A \otimes \Phi_B)| + \text{QC}_{\rho_{AB}}(\Phi_A, \Phi_B) \\
&\leq \sum_s p_s |\text{tr}[\rho_{s,A} \otimes \rho_{s,B} (P_\eta^{T_A} - P_\eta)]| + 2\epsilon, \quad (\text{E21})
\end{aligned}$$

where $\{\rho_{s,A}\}_s$ and $\{\rho_{s,B}\}_s$ are the reduced density matrices of $\{\rho_{s,AB}\}_s$, which are appropriately chosen such that they yield $\text{QC}_{\rho_{AB}}(\Phi_A, \Phi_B)$.

The aim is to prove

$$\text{tr}[\rho_A \otimes \rho_B (P_\eta^{T_A} - P_\eta)] = 0 \quad (\text{E22})$$

for arbitrary ρ_A and ρ_B . Let u_A and u_B be unitary matrices that diagonalize ρ_A and ρ_B , respectively. Then,

$$\begin{aligned}
& \text{tr}[\rho_A \otimes \rho_B (P_\eta^{T_A} - P_\eta)] \\
&= \text{tr}[\tilde{\rho}_A \otimes \tilde{\rho}_B (u_A \otimes u_B) (P_\eta^{T_A} - P_\eta) (u_A \otimes u_B)^\dagger] \\
&= \text{tr}[\tilde{\rho}_A \otimes \tilde{\rho}_B (\tilde{P}_\eta^{\dagger_A} - \tilde{P}_\eta)], \quad (\text{E23})
\end{aligned}$$

where $\tilde{\rho}_A := u_A \rho_A u_A^\dagger$, $\tilde{\rho}_B := u_B \rho_B u_B^\dagger$, $\tilde{P}_\eta := (u_A \otimes u_B) P_\eta (u_A \otimes u_B)^\dagger$. Note that, by using the form (E10), $P_\eta^{T_A} = P_\eta^{\dagger_A}$ is true, with \dagger_A being the partial conjugate transpose. This yields

$$(u_A \otimes u_B) P_\eta^{\dagger_A} (u_A \otimes u_B)^\dagger = \tilde{P}_\eta^{\dagger_A}. \quad (\text{E24})$$

In Eq. (E23), only the diagonal terms of $(\tilde{P}_\eta^{\dagger_A} - \tilde{P}_\eta)$ contribute to the value, as $\tilde{\rho}_A \otimes \tilde{\rho}_B$ is a diagonal matrix. It is evident that all the diagonal terms in $(\tilde{P}_\eta^{\dagger_A} - \tilde{P}_\eta)$ are equal to zero, and hence, it can be concluded that Eq. (E23) reduces to Eq. (E22). Thus, by applying Eq. (E22) to inequality (E21), the main inequality (E11) is obtained. This completes the proof. ■

APPENDIX F: PROOF OF THEOREM 12

This section presents the proof of Theorem 12, where the following inequality has been obtained for one-dimensional quantum Gibbs states:

$$E_R^{\text{PPT}}(\rho_{\beta,AB}) \leq \bar{C}_\beta \log(\mathcal{D}_{AB}) e^{-R/[6 \log(d_0) \bar{C}_\beta^2] + 7gk\beta}, \quad (\text{F1})$$

where $\bar{C}_\beta := 24(\bar{C}_\beta + 16d_0^4 C_\beta)^{1/2}$, with C_β and \bar{C}_β defined in Eqs. (54) and (57), respectively. Here, the assumption of a finite interaction length has been imposed for Hamiltonian H .

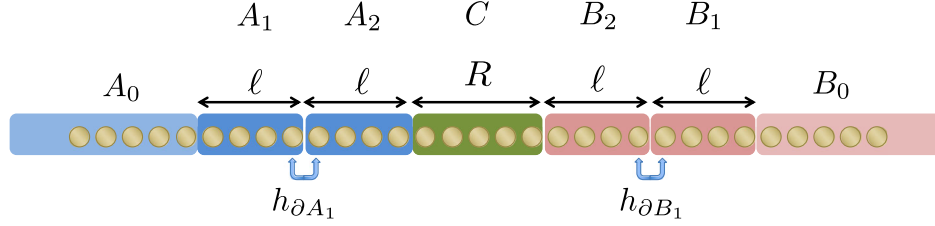


FIG. 5. For the proof, subsets A and B are decomposed into three pieces. The decomposed subsets, i.e., A_1 , A_2 , B_2 , and B_1 , are considered such that they have the same cardinality, that is, $|A_1| = |A_2| = |B_2| = |B_1| = \ell$. The interactions between the subsystems A_1 and A_2 (B_1 and B_2) are denoted as $h_{\partial A_1}$ ($h_{\partial B_1}$). Then, in the Hamiltonian $H - h_{\partial A_1} - h_{\partial B_1}$, the regions A_0A_1 , A_2CB_2 , and B_1B_0 are decoupled. Consequently, using the quantum belief propagation, it is proven that regions A_0 and B_0 do not influence the entanglement value. Then, the entanglement between A and B is characterized by the entanglement between A_1A_2 and B_1B_2 . Further, because the size of these regions is 2ℓ , the dependence on the Hilbert space dimension in Eq. (55) is significantly improved.

1. Proof

For the proof, first, the subsystems A and B are decomposed as follows (Fig. 5):

$$A = A_0 \sqcup A_1 \sqcup A_2, \quad B = B_0 \sqcup B_1 \sqcup B_2, \quad (\text{F2})$$

where $|A_1| = |A_2| = |B_0| = |B_1| = \ell$. Let $h_{\partial A_1}$ ($h_{\partial B_1}$) denote the interactions between A_1 and A_2 (B_1 and B_2):

$$\begin{aligned} h_{\partial A_1} &= \sum_{Z: Z \cap A_1 \neq \emptyset, Z \cap A_2 \neq \emptyset} h_Z, \\ h_{\partial B_1} &= \sum_{Z: Z \cap B_1 \neq \emptyset, Z \cap B_2 \neq \emptyset} h_Z. \end{aligned} \quad (\text{F3})$$

Then, the quantum Gibbs state ρ_β can be described as

$$\rho_\beta = \Phi e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})} \Phi^\dagger, \quad (\text{F4})$$

where Φ is an appropriate operator. It can be proven that Φ is afforded by a quasilocal operator and approximated by $\Phi_{A_1, A_2} \otimes \Phi_{B_1, B_2}$, which is formulated by the following lemma:

Lemma 26. The operator Φ in Eq. (F4) is approximated as follows:

$$\begin{aligned} \tilde{\Phi} &= \Phi_{A_1, A_2} \otimes \Phi_{B_1, B_2} \text{ s.t. } \|\rho_\beta - (\tilde{\Phi} e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})} \tilde{\Phi}^\dagger)\|_1 \\ &\leq \tilde{C}_\beta e^{-2\ell/\xi_\beta + 14gk\beta} =: \delta_{1, \ell}, \end{aligned} \quad (\text{F5})$$

where the correlation length ξ_β has been defined in Eq. (54), and

$$\tilde{C}_\beta := 1280 \left(\frac{5 + 2Ce^{\mu k}}{\pi^2} + \frac{2Ce^{\mu k}}{\pi v \beta} \right)^2. \quad (\text{F6})$$

Further,

$$\|\tilde{\Phi}\| \leq e^{2gk\beta}. \quad (\text{F7})$$

In the following, the main inequality (F1) is proven based on the above lemma. For this purpose, $\tilde{\rho}_\beta$ and \tilde{Z} are defined as follows:

$$\begin{aligned} \tilde{\rho}_\beta &= \frac{e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}}{\tilde{Z}}, \\ \tilde{Z} &:= \text{tr}(e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}). \end{aligned} \quad (\text{F8})$$

Because

$$e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})} = e^{-\beta(H_{A_0A_1} + H_{A_2CB_2} + H_{B_1B_0})}, \quad (\text{F9})$$

we obtain $\tilde{\rho}_{\beta, AB}$ in the form of

$$\tilde{\rho}_{\beta, AB} = \tilde{\rho}_{A_0A_1} \otimes \tilde{\rho}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1}, \quad (\text{F10})$$

where $\tilde{\rho}_{A_0A_1}$, $\tilde{\rho}_{A_2B_2}$, and $\tilde{\rho}_{B_0B_1}$ are normalized, respectively. Here, $\tilde{\delta}$ for $\tilde{\rho}_{A_2B_2}$ is defined in the same manner as for Eq. (E3), whereas $\tilde{\sigma}_{A_2B_2}$ is defined as

$$\tilde{\sigma}_{A_2B_2} = \tilde{\rho}_{A_2B_2} + \tilde{\delta} \cdot \hat{1}_{A_2B_2}. \quad (\text{F11})$$

Using the above $\tilde{\sigma}_{A_2B_2}$, $\tilde{\sigma}_{AB}$ is defined as

$$\begin{aligned} \tilde{\sigma}_{AB} &:= \frac{\tilde{Z}}{Z_{\tilde{\sigma}}} \tilde{\Phi} \tilde{\rho}_{A_0A_1} \otimes \tilde{\sigma}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} \tilde{\Phi}^\dagger \\ &= \frac{\tilde{Z}}{Z_{\tilde{\sigma}}} (\tilde{\Phi} \tilde{\rho}_{\beta, AB} \tilde{\Phi}^\dagger + \tilde{\delta} \cdot \tilde{\Phi} \tilde{\rho}_{A_0A_1} \otimes \hat{1}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} \tilde{\Phi}^\dagger), \end{aligned} \quad (\text{F12})$$

where $Z_{\tilde{\sigma}}$ is the normalization factor used to realize $\text{tr}(\tilde{\sigma}_{AB}) = 1$.

Note that $\tilde{\sigma}_{AB}^{T_A} \geq 0$ can be proven as follows. Because $\tilde{\sigma}_{A_2B_2}^{T_A} \geq 0$, we obtain

$$(\tilde{\rho}_{A_0A_1} \otimes \tilde{\sigma}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1})^{T_A} \geq 0. \quad (\text{F13})$$

Hence, by representing the spectral decomposition of the above operator as

$$\tilde{\rho}_{A_0A_1} \otimes \tilde{\sigma}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} = \sum_i \tilde{\lambda}_i |\tilde{\lambda}_i\rangle \langle \tilde{\lambda}_i| \quad (\text{F14})$$

with $\tilde{\lambda}_i \geq 0$, the following is obtained:

$$\begin{aligned} & (\tilde{\Phi} \tilde{\rho}_{A_0A_1} \otimes \tilde{\sigma}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} \tilde{\Phi}^\dagger)^{T_A} \\ &= \sum_i \tilde{\lambda}_i (\Phi_{A_1A_2}^* \otimes \Phi_{B_1B_2}) |\tilde{\lambda}_i\rangle \langle \tilde{\lambda}_i| (\Phi_{A_1A_2}^T \otimes \Phi_{B_1B_2}^\dagger) \\ &\geq 0, \end{aligned} \quad (\text{F15})$$

which yields the inequality $\tilde{\sigma}_{AB}^{T_A} \geq 0$ from definition (F12).

In the following calculations, the aim is to estimate the upper bound of $\|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1$. We have

$$\begin{aligned} & \|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1 \\ &\leq \|\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \rho_{\beta,AB}\|_1 + \|\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \tilde{\sigma}_{AB}\|_1. \end{aligned} \quad (\text{F16})$$

For the first term, because $\tilde{\Phi}$ is supported on $A_1A_2 \cup B_1B_2$,

$$\begin{aligned} \|\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \rho_{\beta,AB}\|_1 &= \|\text{tr}_C(\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \rho_{\beta,AB})\|_1 \\ &\leq \|\rho_{\beta,AB} - (\tilde{\Phi} e^{-\beta(H-h_{\partial A_1} - h_{\partial B_1})} \tilde{\Phi}^\dagger)\|_1 \\ &\leq \delta_{1,\ell}, \end{aligned} \quad (\text{F17})$$

where $\delta_{1,\ell}$ has been defined in Lemma 26. For the second term, based on definition (F12),

$$\begin{aligned} \|\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \tilde{\sigma}_{AB}\|_1 &\leq \left\| \left(1 - \frac{1}{Z_{\tilde{\sigma}}}\right) \tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger \right\|_1 \\ &\quad + \frac{\tilde{\delta} \tilde{Z}}{Z_{\tilde{\sigma}}} \|\tilde{\Phi} \tilde{\rho}_{A_0A_1} \otimes \hat{1}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} \tilde{\Phi}^\dagger\|_1 \\ &\leq \left|1 - \frac{1}{Z_{\tilde{\sigma}}}\right| (1 + \delta_{1,\ell}) + \frac{\tilde{\delta} \tilde{Z}}{Z_{\tilde{\sigma}}} \|\tilde{\Phi}\|^2, \end{aligned} \quad (\text{F18})$$

where inequality (F17) is used with $\|\rho_{\beta,AB}\|_1 = 1$ for deriving the first term of the rhs.

The remaining task entails estimating the parameters \tilde{Z} , $\tilde{\delta}$, and $Z_{\tilde{\sigma}}$. Consider the proof of the following inequalities:

$$\begin{aligned} \tilde{Z} &\leq e^{4gk\beta}, \quad \tilde{\delta} \leq \delta_{2,R}, \quad \delta_{2,R} := 16C_\beta e^{-R/\xi_\beta + 2\ell \log(d_0)}, \\ \frac{1}{Z_{\tilde{\sigma}}} &\leq 1 + 2\tilde{\delta}_{\ell,R}, \quad \tilde{\delta}_{\ell,R} := \delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}, \end{aligned} \quad (\text{F19})$$

where the case of $\tilde{\delta}_{\ell,R} \leq 1/2$ is considered. In the case of $\tilde{\delta}_{\ell,R} > 1/2$, the desired inequality (F24) below is trivially true because, in this case, it becomes worse than the trivial bound $\|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1 \leq 2$.

Proof of inequalities in Eq. (F19).—The first inequality in Eq. (F19) for the partition function \tilde{Z} can be immediately derived using the Golden-Thompson inequality:

$$\begin{aligned} \tilde{Z} &= \text{tr}(e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})}) \\ &\leq \text{tr}(e^{-\beta H} e^{\beta(h_{\partial A_1}+h_{\partial B_1})}) \\ &\leq \text{tr}(e^{-\beta H}) e^{\beta(\|h_{\partial A_1}\|+\|h_{\partial B_1}\|)} \leq e^{4gk\beta}, \end{aligned} \quad (\text{F20})$$

where we use $\text{tr}(e^{-\beta H}) = 1$, and the norm of $\|h_{\partial A_1}\| + \|h_{\partial B_1}\|$ is upper bounded in Eq. (F39).

In addition, for $\tilde{\delta}$, Lemma 24 is applied with Theorem 10 to $\tilde{\rho}_{A_2B_2}$, which yields the second inequality in Eq. (F19):

$$\begin{aligned} \tilde{\delta} &\leq 4 \min(\mathcal{D}_{A_2}, \mathcal{D}_{B_2}) \times C_\beta (|\partial A_2| + |\partial B_2|) \\ &\quad \times (1 + \log |A_2 B_2|) e^{-R/\xi_\beta} \\ &\leq 16C_\beta e^{-R/\xi_\beta + 2\ell \log(d_0)} = \delta_{2,R}, \end{aligned} \quad (\text{F21})$$

where we use $|A_2| = |B_2| = \ell$, $|\partial A_2| = |\partial B_2| = 2$, and $1 + \log |A_2 B_2| = 1 + \log(2\ell) \leq d_0^\ell$ for $d_0 \geq 2$.

Finally, from Eq. (F12),

$$\begin{aligned} Z_{\tilde{\sigma}} &= \text{tr}(\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger + \tilde{\delta} \cdot \tilde{Z} \cdot \tilde{\Phi} \tilde{\rho}_{A_0A_1} \otimes \hat{1}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} \tilde{\Phi}^\dagger) \\ &\geq \|\rho_{\beta,AB}\|_1 - \|\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \rho_{\beta,AB}\|_1 \\ &\quad - \tilde{\delta} \cdot \tilde{Z} \cdot \|\tilde{\Phi}\|^2 \mathcal{D}_{A_2 B_2} \\ &\geq 1 - \delta_{1,\ell} - \delta_{2,R} d_0^{2\ell} e^{8gk\beta} = 1 - \tilde{\delta}_{\ell,R}, \end{aligned} \quad (\text{F22})$$

where, in the last inequality, $\mathcal{D}_{A_2 B_2} = d_0^{2\ell}$, $\tilde{Z} \leq e^{4gk\beta}$, and $\|\tilde{\Phi}\| \leq e^{2gk\beta}$ are used in Eq. (F7). Further, using $1/(1-x) \leq 1+2x$ for $0 \leq x \leq 1/2$, the third inequality in Eq. (F19) can be proven from the above inequality. This completes the proof of the inequalities in Eq. (F19). ■

Combining inequalities (F18) and (F19) yields

$$\begin{aligned} \|\tilde{Z} \tilde{\Phi} \tilde{\rho}_{\beta,AB} \tilde{\Phi}^\dagger - \tilde{\sigma}_{AB}\|_1 &\leq 2\tilde{\delta}_{\ell,R} (1 + \delta_{1,\ell}) + \delta_{2,R} e^{8gk\beta} (1 + 2\tilde{\delta}_{\ell,R}). \end{aligned} \quad (\text{F23})$$

Then, on applying inequalities (F17) and (F23) to (F16), we obtain

$$\|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1 \leq 2\tilde{\delta}_{\ell,R}^2 + 3\tilde{\delta}_{\ell,R} \leq 4\tilde{\delta}_{\ell,R}, \quad (\text{F24})$$

where $\tilde{\delta}_{\ell,R} \leq 1/2$ is used for the second inequality. Subsequently, on choosing $\ell = \lceil R/(6 \log(d_0) \xi_\beta) \rceil$,

$$\begin{aligned} \tilde{\delta}_{\ell,R} &= \delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta} \\ &= \tilde{C}_\beta e^{-2\ell/\xi_\beta + 14gk\beta} + 16C_\beta e^{-R/\xi_\beta + 4\ell \log(d_0) + 8gk\beta} \\ &\leq (\tilde{C}_\beta + 16d_0^4 C_\beta) e^{-R/[3 \log(d_0) \xi_\beta^2] + 14gk\beta} =: \bar{\delta}_{AB}. \end{aligned} \quad (\text{F25})$$

Finally, to apply the continuity bound (E6), $\lambda_{\min}(\tilde{\sigma}_{AB})$ must be controlled. For this purpose, we consider

$$\tilde{\sigma}_{AB}' = (1 - \bar{\delta}_{AB}) \tilde{\sigma}_{AB} + \bar{\delta}_{AB} \mathcal{D}_{AB}^{-1} \hat{1}_{AB}, \quad (\text{F26})$$

which yields $\lambda_{\min}(\tilde{\sigma}_{AB}') \geq \bar{\delta}_{AB} \mathcal{D}_{AB}^{-1}$. Note that $\tilde{\sigma}_{AB}' \in \text{PPT}$. Then,

$$\|\tilde{\sigma}_{AB}' - \rho_{\beta,AB}\|_1 \leq 4\bar{\delta}_{AB} + \|\tilde{\sigma}_{AB}' - \tilde{\sigma}_{AB}\|_1 \leq 6\bar{\delta}_{AB}. \quad (\text{F27})$$

Inequality (E6) on relative entropy yields

$$\begin{aligned} S(\rho_{\beta,AB} \|\tilde{\sigma}_{AB}') &\leq 6\bar{\delta}_{AB} \log(\mathcal{D}_{AB}) - 6\bar{\delta}_{AB} \log(6\bar{\delta}_{AB}) \\ &\quad - 6\bar{\delta}_{AB} \log[\lambda_{\min}(\tilde{\sigma}_{AB}')] \\ &\leq 12\bar{\delta}_{AB} \log(\mathcal{D}_{AB} \bar{\delta}_{AB}^{-1}) \\ &\leq 24\sqrt{\bar{\delta}_{AB}} \log(\mathcal{D}_{AB}), \end{aligned} \quad (\text{F28})$$

where $x \log(z/x) \leq 2\sqrt{x} \log(z)$ is used for $0 \leq x \leq 2$ and $z \geq 2$. Because $E_R^{\text{PPT}}(\rho_{AB}) \leq S(\rho_{\beta,AB} \|\tilde{\sigma}_{AB}')$, the main inequality (F1) is proven by applying the definition of $\bar{\delta}_{AB}$ in Eq. (F25) to Eq. (F28). This completes the proof. ■

a. Proof of Lemma 26

Using the quantum belief propagation [57], Φ is described as follows:

$$\begin{aligned} \Phi &:= \mathcal{T} e^{\int_0^1 \phi(\tau) d\tau}, \\ \phi(\tau) &:= -\frac{\beta}{2} \int_{-\infty}^{\infty} F_{\beta}(t) [h_{\partial A_1}(H_{\tau}, t) + h_{\partial B_1}(H_{\tau}, t)] dt, \\ H_{\tau} &:= H - (1-\tau)h_{\partial A_1} - (1-\tau)h_{\partial B_1}, \end{aligned} \quad (\text{F29})$$

where \mathcal{T} is the time ordering operator, $h_{\partial A_1}(H_{\tau}, t) = e^{iH_{\tau}t} h_{\partial A_1} e^{-iH_{\tau}t}$. Here, $F_{\beta}(t)$ is defined as

$$F_{\beta}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{F}_{\beta}(\omega) e^{-i\omega t} d\omega, \quad \tilde{F}_{\beta}(\omega) := \frac{\tanh(\beta\omega/2)}{\beta\omega/2}.$$

The explicit form of $F_{\beta}(t)$ can be calculated as follows [see Eq. (103) in Supplementary Information of Ref. [205]:]

$$\begin{aligned} F_{\beta}(t) &= \frac{2}{\beta\pi} \log\left(\frac{e^{\pi|t|/\beta} + 1}{e^{\pi|t|/\beta} - 1}\right) \leq \frac{4/(\beta\pi)}{e^{\pi|t|/\beta} - 1} \\ &\leq \frac{4}{\beta\pi} e^{-\pi|t|/\beta} \left(1 + \frac{1}{\pi|t|/\beta}\right), \end{aligned} \quad (\text{F30})$$

where $\log[(e^x + 1)/(e^x - 1)] \leq 2/(e^x - 1)$ and $1/(e^x - 1) \leq e^{-x}(1 + x^{-1})$ are used for $x \geq 0$.

Herein, an approximation is adopted as follows:

$$\begin{aligned} \tilde{\Phi} &:= \mathcal{T} e^{\int_0^1 \tilde{\phi}(\tau) d\tau}, \\ \tilde{\phi}(\tau) &:= -\frac{\beta}{2} \int_{-\infty}^{\infty} F_{\beta}(t) [h_{\partial A_1}(H_{\tau}, t, A_1 A_2) \\ &\quad + h_{\partial B_1}(H_{\tau}, t, B_1 B_2)] dt, \end{aligned} \quad (\text{F31})$$

where the notations of Eq. (16) are used. Here, $h_{\partial A_1}(H_{\tau}, t, A_1 A_2)$ and $h_{\partial B_1}(H_{\tau}, t, B_1 B_2)$ are supported on $A_1 A_2$ and $B_1 B_2$, respectively. Because $[h_{\partial A_1}(H_{\tau}, t, A_1 A_2), h_{\partial B_1}(H_{\tau}, t, B_1 B_2)] = 0$, $\tilde{\Phi}$ is given in the form of

$$\tilde{\Phi} = \Phi_{A_1 A_2} \otimes \Phi_{B_1 B_2}. \quad (\text{F32})$$

Consider the norm of $\Phi - \tilde{\Phi}$, which is upper bounded as

$$\|\Phi - \tilde{\Phi}\| \leq e^{\int_0^1 (\|\phi(\tau)\| + \|\tilde{\phi}(\tau)\|) d\tau} \int_0^1 \|\phi(\tau) - \tilde{\phi}(\tau)\| d\tau, \quad (\text{F33})$$

where the analysis in Claim 25 of Ref. [46] is used. To estimate the rhs of Eq. (F33), first consider

$$\begin{aligned} &\int_0^1 (\|\phi(\tau)\| + \|\tilde{\phi}(\tau)\|) d\tau \\ &\leq \beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|) \int_{-\infty}^{\infty} F_{\beta}(t) dt \\ &= \beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|), \end{aligned} \quad (\text{F34})$$

where $\|h_{\partial A_1}(H_{\tau}, t, A_1 A_2)\| \leq \|h_{\partial A_1}(H_{\tau}, t)\| = \|h_{\partial A_1}\|$ and $\int_{-\infty}^{\infty} F_{\beta}(t) dt = \tilde{F}(0) = 1$ are used. Second, using the Lieb-Robinson bound (18),

$$\begin{aligned} &\|h_{\partial A_1}(H_{\tau}, t) - h_{\partial A_1}(H_{\tau}, t, A_1 A_2)\| \\ &\leq \|h_{\partial A_1}\| \min(2, 2C(e^{v|t|} - 1)e^{-\mu(\ell-k)}), \end{aligned} \quad (\text{F35})$$

where $|\partial \text{Supp}(h_{\partial A_1})| = 2$ is used on a 1D chain, and it is assumed that $h_{\partial A_1}$ has the interaction length k [i.e., $|\text{Supp}(h_{\partial A_1})| \leq 2k$]. Note that $\|h_{\partial A_1}(H_{\tau}, t) - h_{\partial A_1}(H_{\tau}, t, A_1 A_2)\|$ is trivially smaller than $2\|h_{\partial A_1}\|$.

Consequently, on combining the above inequality with Eqs. (F29) and (F31), we obtain

$$\begin{aligned} &\|\phi(\tau) - \tilde{\phi}(\tau)\| \\ &\leq \frac{\beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|)}{2} \\ &\quad \times \int_{-\infty}^{\infty} F_{\beta}(t) \min(2, 2C(e^{v|t|} - 1)e^{-\mu(\ell-k)}) dt. \end{aligned} \quad (\text{F36})$$

Given the form of $F_{\beta}(t)$ in Eq. (F30), the same calculations as in Appendix C3b can be applied. Thus, for $t_0 = \mu\ell/(2v)$,

$$\begin{aligned}
\frac{\|\phi(\tau) - \tilde{\phi}(\tau)\|}{\beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|)} &\leq \int_{t_0}^{\infty} \frac{4}{\beta\pi} e^{-\pi t/\beta} \left(1 + \frac{1}{\pi t/\beta}\right) \cdot 2dt + \int_0^{t_0} \frac{4}{\beta\pi} e^{-\pi t/\beta} \left(1 + \frac{1}{\pi t/\beta}\right) \cdot 2C(e^{vt} - 1)e^{-\mu(\ell-k)} dt \\
&\leq \frac{8}{\pi^2} \left(1 + \frac{1}{\pi t_0/\beta}\right) e^{-\pi t_0/\beta} + \frac{8Ce^{\mu k}}{\beta\pi} e^{-\mu\ell} \int_0^{t_0} \left(1 + \frac{1}{\pi t/\beta}\right) (e^{vt} - 1) dt \\
&\leq \frac{8}{\pi^2} \left(1 + \frac{1}{\pi t_0/\beta}\right) e^{-\pi t_0/\beta} + \frac{8Ce^{\mu k}}{\beta\pi} e^{-\mu\ell} \left(\frac{e^{vt_0}}{v} + \frac{e^{vt_0}}{\pi/\beta}\right) \\
&= \frac{8}{\pi^2} \left(1 + \frac{2\beta v}{\pi\mu\ell}\right) e^{-\pi\mu\ell/(2\beta v)} + \frac{8Ce^{\mu k}}{\beta\pi} \left(\frac{1}{v} + \frac{\beta}{\pi}\right) e^{-\mu\ell/2} \\
&\leq \left[\frac{8}{\pi^2} \left(1 + \frac{\xi_\beta}{2\ell}\right) + \frac{8Ce^{\mu k}}{\pi} \left(\frac{1}{\pi} + \frac{1}{v\beta}\right)\right] e^{-2\ell/\xi_\beta}, \tag{F37}
\end{aligned}$$

where the definition of $\xi_\beta := \frac{4}{\mu} \{1 + [(v\beta)/\pi]\}$ is used.

Owing to inequality (F34), the lhs of Eq. (F37) is trivially smaller than 1. By contrast, for $\ell \leq \xi_\beta/3$, the rhs of Eq. (F37) is larger than $20e^{-2/3}/\pi^2$, which is worse than the trivial upper bound. Hence, only the case of $\ell \geq \xi_\beta/3$ is considered, which reduces Eq. (F37) to

$$\begin{aligned}
\frac{\|\phi(\tau) - \tilde{\phi}(\tau)\|}{\beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|)} &\leq \left(\frac{20 + 8Ce^{\mu k}}{\pi^2} + \frac{8Ce^{\mu k}}{\pi v\beta}\right) e^{-2\ell/\xi_\beta}. \tag{F38}
\end{aligned}$$

From Eq. (8), the upper bound can be obtained as

$$\|h_{\partial A_1}\| \leq \sum_{i \in \text{Supp}(h_{\partial A_1})} \sum_{Z: Z \ni i} \|h_Z\| \leq |\text{Supp}(h_{\partial A_1})| g \leq 2gk, \tag{F39}$$

which reduces inequalities (F34) and (F38) to

$$\begin{aligned}
\int_0^1 (\|\phi(\tau)\| + \|\tilde{\phi}(\tau)\|) d\tau &\leq 4gk\beta, \\
\|\phi(\tau) - \tilde{\phi}(\tau)\| &\leq 4gk\beta \left(\frac{20 + 8Ce^{\mu k}}{\pi^2} + \frac{8Ce^{\mu k}}{\pi v\beta}\right) e^{-2\ell/\xi_\beta}, \tag{F40}
\end{aligned}$$

respectively. Further, by applying the above inequalities to Eq. (F33), the following is obtained:

$$\|\Phi - \tilde{\Phi}\| \leq 16gk\beta e^{4gk\beta} \left(\frac{5 + 2Ce^{\mu k}}{\pi^2} + \frac{2Ce^{\mu k}}{\pi v\beta}\right) e^{-2\ell/\xi_\beta}. \tag{F41}$$

Finally, consider the norm of

$$\begin{aligned}
\rho_\beta - \tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}^\dagger &= \rho_\beta - \tilde{\Phi} \Phi^{-1} \rho_\beta (\tilde{\Phi} \Phi^{-1})^\dagger \\
&= (1 - \tilde{\Phi} \Phi^{-1}) \rho_\beta [1 - (\tilde{\Phi} \Phi^{-1})^\dagger] + \tilde{\Phi} \Phi^{-1} \rho_\beta [1 - (\tilde{\Phi} \Phi^{-1})^\dagger] \\
&\quad + (1 - \tilde{\Phi} \Phi^{-1}) \rho_\beta (\tilde{\Phi} \Phi^{-1})^\dagger,
\end{aligned}$$

where Eq. (F4), that is, $e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} = \Phi^{-1} \rho_\beta (\Phi^\dagger)^{-1}$, is used. Subsequently, using the above equation,

$$\begin{aligned}
\|\rho_\beta - (\tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}^\dagger)\|_1 &\leq \|\rho_\beta\|_1 \|1 - \tilde{\Phi} \Phi^{-1}\| (\|1 - \tilde{\Phi} \Phi^{-1}\| + 2\|\tilde{\Phi} \Phi^{-1}\|) \\
&\leq 3\|1 - \tilde{\Phi} \Phi^{-1}\|^2 + 2\|1 - \tilde{\Phi} \Phi^{-1}\|, \tag{F42}
\end{aligned}$$

where the triangle inequality is employed to obtain $\|\tilde{\Phi} \Phi^{-1}\| \leq \|1 - \tilde{\Phi} \Phi^{-1}\| + 1$. Based on the inequality of $\|\Phi^{-1}\| \leq e^{2gk\beta}$, which is derived in the same manner as Eq. (F34), we obtain

$$\begin{aligned}
\|1 - \tilde{\Phi} \Phi^{-1}\| &\leq \|\Phi^{-1}\| \cdot \|\Phi - \tilde{\Phi}\| \\
&\leq 16gk\beta e^{6gk\beta} \left(\frac{5 + 2Ce^{\mu k}}{\pi^2} + \frac{2Ce^{\mu k}}{\pi v\beta}\right) e^{-2\ell/\xi_\beta} \\
&\leq 16e^{7gk\beta} \left(\frac{5 + 2Ce^{\mu k}}{\pi^2} + \frac{2Ce^{\mu k}}{\pi v\beta}\right) e^{-2\ell/\xi_\beta} \tag{F43}
\end{aligned}$$

from inequality (F41), where $xe^{6x} \leq e^{7x}$ is used for $x \geq 0$.

Therefore, by combining inequalities (F42) and (F43), inequality (F5) can be obtained as follows:

$$\begin{aligned} \|\rho_\beta - (\tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}^\dagger)\|_1 & \rho_\beta \approx \tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}. \quad (\text{G6}) \\ & \leq 1280 \left(\frac{5 + 2Ce^{\mu k}}{\pi^2} + \frac{2Ce^{\mu k}}{\pi v \beta} \right)^2 e^{-2\ell/\xi_\beta + 14gk\beta}. \end{aligned}$$

Finally, on the norm $\|\tilde{\Phi}\|$, considering Eq. (F34),

$$\|\tilde{\Phi}\| \leq e^{\int_0^1 \|\tilde{\phi}(\tau)\| d\tau} \leq e^{\frac{\ell}{2}(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|)} \leq e^{2gk\beta},$$

which yields inequality (F7). This completes the proof. ■

APPENDIX G: REMARK ON ENTANGLEMENT NEGATIVITY

The PPT relative entanglement in Eq. (50) is relevant to another definition of quantum entanglement. Herein, consider entanglement negativity, which is given by [50]

$$E_N(\rho_{AB}) := \log \|\rho_{AB}^{T_A}\|_1. \quad (\text{G1})$$

Using Proposition 9, the following corollary is obtained:

Corollary 27. Let ρ be an arbitrary quantum state such that

$$\text{QC}_\rho(O_A, O_B) \leq \epsilon \|O_A\| \cdot \|O_B\| \quad (\text{G2})$$

for two arbitrary operators O_A and O_B ; then,

$$E_N(\rho_{AB}) \leq \|\rho_{AB}^{T_A}\|_1 - 1 \leq 8\epsilon \min(\mathcal{D}_A, \mathcal{D}_B) \mathcal{D}_{AB}, \quad (\text{G3})$$

where the first inequality is trivially derived from $\log(1+x) \leq x$ for $x \geq 0$. Recall that \mathcal{D}_{AB} is the Hilbert space dimension in the region AB . Thus, by applying Theorem 10 to inequality (G3), an inequality similar to Eq. (55) can be derived.

Proof of Corollary 27.—First, because $\text{tr}(\rho_{AB}^{T_A}) = 1$,

$$\begin{aligned} \|\rho_{AB}^{T_A}\|_1 &= 1 + \sum_{i=1}^{M_0} 2|\langle \eta_i | \rho_{AB}^{T_A} | \eta_i \rangle| \leq 1 + 2M_0 \cdot \delta \\ &\leq 1 + 2\mathcal{D}_{AB} \cdot \delta \quad (\text{G4}) \end{aligned}$$

with $\delta := -\min_i \langle \eta_i | \rho_{AB}^{T_A} | \eta_i \rangle$, where $M_0 \leq \mathcal{D}_{AB}$. Here, the value M_0 can be as large as $(\mathcal{D}_A - 1)(\mathcal{D}_B - 1)$, in general (see Ref. [206]). Thus, using the upper bound on δ in Lemma 24, inequality (G3) is proven. This completes the proof. ■

By contrast, an inequality similar to Eq. (F1) cannot be derived for 1D quantum Gibbs states if entanglement negativity is considered. This is explained as follows. As shown in Lemma 26, the following was derived:

$$\|\rho_\beta - \tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}\|_1 \leq e^{-\ell/\mathcal{O}(\beta) + \mathcal{O}(\beta)}, \quad (\text{G5})$$

where $\tilde{\Phi}$ has been supported on $A_1 A_2 \cup B_1 B_2$. Thus, it is concluded that, for $\ell \gtrsim \beta^2$,

The primary difficulty is that entanglement negativity cannot satisfy a convenient continuity inequality. In Eq. (16) of Ref. [90], it has been proven that, for arbitrary quantum states ρ_{AB} and ρ'_{AB} ,

$$\begin{aligned} |E_N(\rho_{AB}) - E_N(\rho'_{AB})| & \leq \log(1 + \sqrt{\mathcal{D}_{AB}} \|\rho_{AB} - \rho'_{AB}\|_2) \\ & \leq \log(1 + \sqrt{\mathcal{D}_{AB}} \|\rho_{AB} - \rho'_{AB}\|_1). \quad (\text{G7}) \end{aligned}$$

Hence, even for $\|\rho - \rho'\|_1 = e^{-\mathcal{O}(n^z)}$ ($0 < z < 1$), the difference in entanglement negativity can be significantly large [207]. Therefore, error estimation (G5) cannot be utilized for this purpose.

Adopting the same steps as those for Appendix F,

$$\|(\rho_\beta - \tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}^\dagger)^{T_A}\|_1$$

needs to be calculated instead of

$$\|\rho_\beta - \tilde{\Phi} e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} \tilde{\Phi}\|_1$$

to obtain a meaningful upper bound for entanglement negativity. However, in general, the partial-transpose operation can significantly increase the operator norm, that is, $\|O^{T_A}\|_1 \leq \min(\mathcal{D}_A, \mathcal{D}_A^c) \|O\|_1$, as shown in Refs. [209,210]. Owing to this difficulty, the possibility of deriving a statement similar to Theorem 12 for entanglement negativity (G1) remains unclear. However, it is expected to be proven for entanglement negativity by employing an analysis similar to that in Ref. [211].

APPENDIX H: QUANTUM FISHER INFORMATION MATRIX

Here, the definition (33) for the quantum correlation $\text{QC}_\rho(O_A, O_B)$ proposed is compared with the quantum Fisher information matrix. First, it should be noted that the quantum Fisher information can be defined in the form of the convex roof of the variance. If ρ is a pure state, the quantum Fisher information $\mathcal{F}_\rho(K)$ simply reduces to the variance of K :

$$\mathcal{F}_\rho(K) = 4(\langle \psi | K^2 | \psi \rangle - \langle \psi | K | \psi \rangle^2), \quad (\text{H1})$$

where $\rho = |\psi\rangle\langle\psi|$. For the general state ρ , the quantum Fisher information is known to be equal to the convex roof of the variance [167,168]:

$$\mathcal{F}_\rho(K) = 4 \inf_{\{p_s, |\psi_s\rangle\}} \sum_s p_s (\langle \psi_s | K^2 | \psi_s \rangle - \langle \psi_s | K | \psi_s \rangle^2), \quad (\text{H2})$$

where minimization is considered for all possible decompositions of ρ , such that $\rho = \sum_s p_s |\psi_s\rangle\langle\psi_s|$ with $p_s > 0$. Thus, the quantum Fisher information shows a certain similarity to the quantum correlation $\text{QC}_\rho(O_A, O_B)$.

To view this similarity in more detail, consider the following quantum Fisher information matrix [136]:

$$\mathcal{F}_\rho(O_i, O_j) = \sum_{s,s'} \frac{2(\lambda_s - \lambda_{s'})^2}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O_i|\lambda_{s'}\rangle\langle\lambda_{s'}|O_j|\lambda_s\rangle. \quad (\text{H3})$$

Herein,

$$\mathcal{F}_\rho(K) = \sum_{i,j} \mathcal{F}_\rho(O_i, O_j). \quad (\text{H4})$$

The quantum Fisher information matrix has been used in the multiparameter quantum estimation theory [136,212–214]. Then, the question remains as to whether it can be associated with the convex roof of certain observables in the analogy of Eq. (H2).

The partial answer to this question is yes. The quantum Fisher information matrix is relevant to the following quantity $\text{QC}_\rho^*(O_A, O_B)$, which is weaker than Eq. (33):

$$\text{QC}_\rho^*(O_A, O_B) := \inf_{\{p_s, \rho_s\}} \left| \sum_s p_s \text{C}_{\rho_s}(O_A, O_B) \right|, \quad (\text{H5})$$

which is the minimization of the absolute value of the average correlation. Based on the above quantity, the following statement can be proven, which is similar to Lemma 17:

Lemma 28. For two arbitrary operators O_A and O_B , if

$$[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0, \quad (\text{H6})$$

the quantity $\text{QC}_\rho^*(O_A, O_B)$ is upper bounded in Eq. (H5) as follows:

$$\text{QC}_\rho^*(O_A, O_B) \leq \frac{1}{4} |\mathcal{F}_\rho(O_A, O_B)|. \quad (\text{H7})$$

Here, the operator \mathcal{L}_O has been defined in Eq. (D5). If condition (H6) holds only approximately (i.e., $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] \approx 0$), a similar modification to Lemma 18 is required.

Remark. For the quantity $\text{QC}_\rho^*(O_A, O_B)$ in Eq. (H5), at first glance, no meaningful constraints on the entanglement structure can be observed, as $\text{C}_{\rho_s}(O_A, O_B)$ can have a negative value. In other words, even if $\text{QC}_\rho^*(O_A, O_B)$ is equal to zero, $\text{QC}_\rho(O_A, O_B)$ may still be large. However, the same statement as Lemma 8 can be proven for $\text{QC}_\rho^*(O_A, O_B)$ on the Peres-Horodecki separability criterion (i.e., the PPT condition):

Lemma 29. Consider the proof for the following statement:

$$\begin{aligned} \text{QC}_{\rho_{AB}}^*(O_A, O_B) = 0 \quad \text{for arbitrary pairs of } O_A, O_B \\ \rightarrow \rho_{AB} \text{ satisfies the PPT condition.} \end{aligned} \quad (\text{H8})$$

From statement (H8) and inequality (H7), it is evident that the quantum Fisher information matrix also plays a role in quantum correlation measures.

1. Proof of Lemma 28

Herein, consider the proof of Lemma 17. Consider the decomposition of ρ as follows:

$$\begin{aligned} \rho &= \sum_m p_m |\phi_m\rangle\langle\phi_m|, \\ |\phi_m\rangle &= \frac{1}{\sqrt{p_m}} \sqrt{\rho} |\psi_m\rangle, \quad p_m = \langle\psi_m|\rho|\psi_m\rangle, \end{aligned} \quad (\text{H9})$$

where $|\psi_m\rangle$ is chosen as the simultaneous eigenstates of \mathcal{L}_{O_A} and \mathcal{L}_{O_B} with the corresponding eigenvalues $\alpha_{1,m}$ and $\alpha_{2,m}$, respectively. Then, an equation identical to Eq. (D29) is obtained:

$$\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle = \alpha_{1,m}\alpha_{2,m}. \quad (\text{H10})$$

Next, consider the proof

$$\sum_m p_m \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle = \frac{1}{2} \text{tr}(\{\rho, \mathcal{L}_{O_A} \mathcal{L}_{O_B}\}), \quad (\text{H11})$$

where $\{\cdot, \cdot\}$ is the anticommutator. By expanding the rhs of Eq. (H11),

$$\begin{aligned} \frac{1}{2} \text{tr}(\{\rho, \mathcal{L}_{O_A} \mathcal{L}_{O_B}\}) &= \frac{1}{2} \sum_m \langle\psi_m|\{\rho, \mathcal{L}_{O_A} \mathcal{L}_{O_B}\}|\psi_m\rangle \\ &= \sum_m \langle\psi_m|\rho|\psi_m\rangle \alpha_{1,m} \alpha_{2,m}, \end{aligned} \quad (\text{H12})$$

which reduces to the lhs of Eq. (H11) from $p_m = \langle\psi_m|\rho|\psi_m\rangle$ and Eq. (H10).

By contrast, using the spectral decomposition of $\rho = \sum_s \lambda_s |\lambda_s\rangle\langle\lambda_s|$,

$$\begin{aligned} \frac{1}{2} \text{tr}(\{\rho, \mathcal{L}_{O_A} \mathcal{L}_{O_B}\}) \\ = \sum_{s,s'} \frac{2\lambda_s \lambda_{s'}}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O_A|\lambda_{s'}\rangle\langle\lambda_{s'}|O_B|\lambda_s\rangle, \end{aligned} \quad (\text{H13})$$

where the form of \mathcal{L}_O in Eq. (D5) is used. Further, by combining Eqs. (H11) and (H13),

$$\begin{aligned} & \sum_m P_m \langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle \\ &= \sum_{s,s'} \frac{2\lambda_s \lambda_{s'}}{\lambda_s + \lambda_{s'}} \langle \lambda_s | O_A | \lambda_{s'} \rangle \langle \lambda_{s'} | O_B | \lambda_s \rangle. \end{aligned} \quad (\text{H14})$$

Finally,

$$\begin{aligned} & \sum_m P_m \langle \phi_m | O_A O_B | \phi_m \rangle = \text{tr}(\rho O_A O_B) \\ &= \sum_{s,s'} \frac{\lambda_s + \lambda_{s'}}{2} \langle \lambda_s | O_A | \lambda_{s'} \rangle \langle \lambda_{s'} | O_B | \lambda_s \rangle, \end{aligned} \quad (\text{H15})$$

where $[O_A, O_B] = 0$. Thus, by subtracting Eq. (H14) from Eq. (H15),

$$\begin{aligned} & \sum_m P_m (\langle \phi_m | O_A O_B | \phi_m \rangle - \langle \phi_m | O_A | \phi_m \rangle \langle \phi_m | O_B | \phi_m \rangle) \\ &= \sum_{s,s'} \frac{(\lambda_s - \lambda_{s'})^2}{2(\lambda_s + \lambda_{s'})} \langle \lambda_s | O_A | \lambda_{s'} \rangle \langle \lambda_{s'} | O_B | \lambda_s \rangle \\ &= \frac{1}{4} \mathcal{F}_\rho(O_A, O_B) \end{aligned} \quad (\text{H16})$$

is obtained. Therefore, on applying the above equation to Eq. (H5), inequality (H7) is proven. This completes the proof. ■

2. Proof of Lemma 29

Consider the proof of the statement

$$\begin{aligned} \text{QC}_{\rho_{AB}}^*(O_A, O_B) = 0 \text{ for arbitrary pairs of } O_A, O_B \\ \rightarrow \rho_{AB} \text{ satisfies the PPT condition.} \end{aligned} \quad (\text{H17})$$

This statement can be easily evaluated via the following discussion.

First, if inequality (52) in Proposition 9 can be proven by assuming inequality (51) for $\text{QC}_\rho^*(O_A, O_B)$ instead of $\text{QC}_\rho(O_A, O_B)$, the statement (H17) is obtained. Second, in the proof of Proposition 9, inequality (51) is used only for deriving the upper bound (E21) for the proof of Lemma 25. From the second to the third lines in Eq. (E21), $\text{QC}_\rho(O_A, O_B)$ is used as an upper bound for

$$\left| \sum_s p_s (\text{tr}(\rho_{s,A} \Phi_A \Phi_B)) - \text{tr}(\rho_{s,A} \Phi_A) \text{tr}(\rho_{s,B} \Phi_B) \right|;$$

however, $\text{QC}_\rho^*(O_A, O_B)$ also serves as the upper bound for the above quantity. Consequently, inequality (52) can be proven using the constraint on $\text{QC}_\rho^*(O_A, O_B)$ alone. This completes the proof. ■

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