Exponential clustering of bipartite quantum entanglement at arbitrary temperatures

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Macroscopic quantum effects play central roles in the appearance of inexplicable phenomena in low-temperature quantum many-body physics. Such macroscopic quantumness is often evaluated using long-range entanglement, i.e., entanglement in the macroscopic length scale. The long-range entanglement not only characterizes the novel quantum phases but also serves as a critical resource for quantum computation. Thus, the problem that arises is under which conditions can the long-range entanglement be stable even at room temperatures. Here, we show that bi-partite long-range entanglement is unstable at arbitrary temperatures and exponentially decays with distance. Our results are consistent with the existing observations that long-range entanglement at non-zero temperatures can exist in topologically ordered phases, where tripartite correlations are dominant. In the derivation of our result, we introduce a quantum correlation defined by the convex roof of the standard correlation function. We establish an exponential clustering theorem for generic quantum many-body systems for such a quantum correlation at arbitrary temperatures, which yields our main result by relating quantum correlation to quantum entanglement. As a simple application of our analytical techniques, we derived a general limit on the Wigner-Yanase-Dyson skew information and the quantum Fisher information, which will attract significant attention in the field of quantum metrology. Our work reveals novel general aspects of low-temperature quantum physics and sheds light on the characterization of long-range entanglement.

I. INTRODUCTION

A. Background

In quantum many-body physics, the appearances of macroscopic quantum effects—for example, superconductivity, Bose-Einstein condensation, quantum spin liquid, and quantum topological order—are critical features in exotic quantum phenomena. In these phenomena, the length scale of the quantum effect is comparable to the one in the real world. The clarification of such macroscopic quantum effects has been a crucial problem in modern physics, and various types of characterization methods of the quantumness in macroscopic length scale have been proposed [1–4]. In particular, in the last two decades, quantum entanglement has become a representative measure for the quantumness [5, 6]. There is an enormous number of studies to investigate the entanglement behaviors in quantum many-body systems from various viewpoints [7–16]. These advancements in quantum entanglement not only deepen our understanding but also help establish efficient classical and quantum algorithms to simulate quantum many-body systems [17–21].

One of the most critical questions 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]. We notice that temperature plays an essential role in this question. Due to the fragility of quantumness, the thermal noise destroys the entanglement, making the length scale of the entanglement short range. Indeed, when the temperature is sufficiently high such that no thermal phase transition can occur, the quantum thermal state can be classified into the trivial phase [27] (i.e., generated by the finite depth quantum circuit [22]). In contrast, at zero temperature, various types of quantum systems are known to exhibit long-range entanglement [28–32]. At non-zero but low temperatures, where thermal phase transition can occur, the problem is highly elusive. Here, the effect of the thermal noise is sufficiently suppressed, and we suggest the possibility of observing long-range entanglement in this temperature regime. In such quantum systems, quantum phases protected by the topological order can exhibit long-range entanglement. Indeed, it

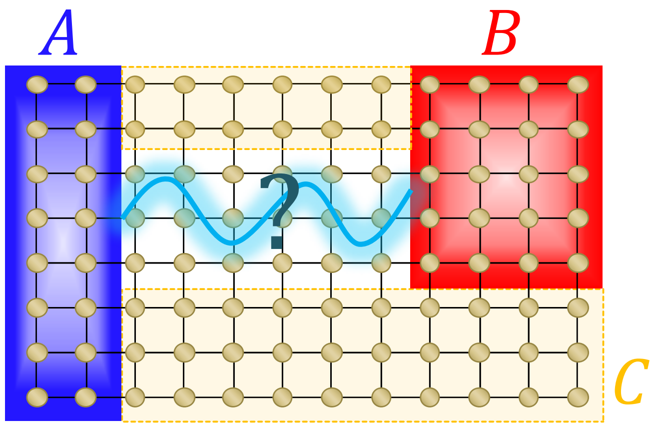

FIG. 1. (Entanglement between two separated subsystems A and B) If we consider the tripartite entanglement between subsystems A, B, and C, we can detect the long-range entanglement at non-zero temperatures. One can indeed observe it in topologically ordered quantum many-body systems. In this study, we elaborate the observation and aim to prove that (more than) tripartite entanglement is required for long-range entanglement. We show that at arbitrary non-zero temperatures, in any quantum Gibbs state with short-range interacting Hamiltonians, the quantum entanglement between two subsystems decays exponentially with distance, where the entanglement-length scale, at most, grows polynomially with inverse temperature β, as stated in the inequalities (1), (2) and (3).

has been shown that in the 4D Toric code model [33], entanglement can be long range even at room temperatures [34, 35] (see also [36, 37]).

The purpose of our study is to identify a limitation on the structure of the long-range entanglement at arbitrary non-zero temperatures. In the known example with long-range entanglement, protection by the topological order plays an essential role. Moreover, topological order is inherently a tripartite correlation [38–40]. These facts give rise to the following fundamental question: *"Can the long-range entanglement at non-zero temperatures only exist as (more than) tripartite correlations, or equivalently, does bi-partite entanglement necessarily decay to zero at long distances at arbitrary temperatures?"* We conjecture that the answer is yes (see Fig. 1). Whether the conjecture is true will provide crucial information for identifying the essence of long-range entanglement in the quantum phases at non-zero temperatures, which would become a guideline to search for candidate systems for quantum devices. The conjecture trivially holds for arbitrary commuting Hamiltonians [41], where all local interaction terms commute with each other. Hence, in the Toric code model, 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, our conjecture does not contradict the observations.

At present, rigorous and general studies on low-temperature phases are scarce. At low temperatures, unlike 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 computationally hard problems [42, 43]. In such situations, the thermal area law is known to be a representative characterization of low-temperature phases of many-body systems, which universally holds at arbitrary temperatures [11, 44, 45]. It states that entanglement between two adjacent subsystems is, at most, as large as the size of their boundaries. In other words, the area law implies that the entanglement should be localized around the boundary and indirectly supports our argument.

B. Brief description of our main results

Here, we provide an overview of the contributions of this study. We denote ρ_β as the quantum Gibbs state at inverse temperature β, where we consider a short-range interacting Hamiltonian (see Sec. II A for details). Then, let $\rho_{\beta,AB}$ be a reduced density matrix on the subsystems A and B, which are separated by a distance R. For arbitrary choice of A and B, we are now interested in the entanglement between A and B (see also Fig. 1).

First, the primary challenge faced during accessing the main problem is that the entanglement for the mixed state cannot be described in an analytically tractable form (see Eqs. (20) and (78) for example). On account of the computational hardness [46, 47], the entanglement cannot be computed even at numerical levels except for specific cases [48]. In free fermion and harmonic chains, analytical forms of entanglement negativity [49] [see Eq. (G1)] have been obtained [50–52] at finite temperatures. These studies have considered the entanglement negativity between adjacent subsystems A and B (i.e., $R = 0$) on one-dimensional chains and have analyzed how negativity is saturated as the sizes of A and B increase (e.g., setting $|A| = |B| = \ell$ and tuning the length ℓ). Thus, the saturation rate is roughly given by $e^{-\ell/\mathcal{O}(\beta)}$, and [52] concluded that the quantum coherence can only be maintained for length scales of $\mathcal{O}(\beta)$. Similar observations have been numerically obtained in a more general class of many-body systems [53, 54]. These results strongly support the clustering of bi-partite entanglement in specific models.

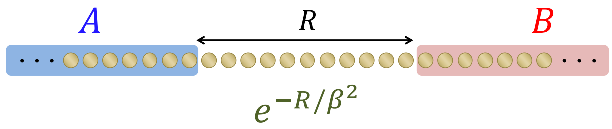

FIG. 2. (Schematic diagram of 1D entanglement clustering) In the obtained bound (2), the subset dependence $e^{\mathcal{O}(|A|+|B|)}$ prohibits us from applying it to upper bound the entanglement between two large blocks. In one-dimensional systems, we can resolve this problem and obtain better subset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

To overcome the difficulties in the analysis of the entanglement, we first introduce a quantum correlation $\mathrm{QC}_\rho(O_A, O_B)$, which is defined on the basis of the analogy of the entanglement measure and is given by the convex roof of the standard correlation function $\mathrm{C}_\rho(O_A, O_B) = \mathrm{tr}(\rho O_A O_B) - \mathrm{tr}(\rho O_A)\mathrm{tr}(\rho O_B)$, as in Eq. (33). The quantum correlation $\mathrm{QC}_\rho(O_A, O_B)$ is strongly associated with the 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 particular, we can generally prove exponential clustering of the quantum correlation at arbitrary temperatures of arbitrary dimensions (see Theorem 10):

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

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

Based on the upper bound (1), we prove the following statement on the entanglement clustering (see Corollary 11):

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

where $E_R^{\mathrm{PPT}}(\rho_{AB})$ is the PPT relative entanglement (50). At the present stage, two points might 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., $\mathrm{poly}(|A|, |B|)$]. To improve the first point, we must relate the zero quantum correlation to the separable condition instead of the PPT condition

(Lemma 8). However, this point remains to be open (Conjecture 7). On the second point, by refining the analyses based on the belief propagation [55, 56], we can improve the inequality (2) in one-dimensional systems (Theorem 12, Fig. 2):

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

Thus, we can obtain a much better clustering theorem for the bipartite entanglement measure in one-dimensional systems.

Finally, as a related quantity, we also consider another type of quantum correlation that is based on the Wigner-Yanase-Dyson (WYD) skew information [57, 58]: $\bar{Q}_\rho(O_A,O_B) := \int_0^1 Q_\rho^{(\alpha)}(O_A,O_B)d\alpha$ with $Q_\rho^{(\alpha)}(O_A,O_B) := \mathrm{tr}(\rho O_A O_B) - \mathrm{tr}\left(\rho^{1-\alpha} O_A \rho^\alpha O_B\right)$. In a previous study [57], it was numerically verified that the quantity $\bar{Q}_\rho(O_A,O_B)$ shows an exponential decay with distance even at the critical point. Because the WYD skew information is considered as a measure of quantum coherence [59], the decay rate of $\bar{Q}_\rho(O_A,O_B)$ has been dubbed as the 'quantum coherence length' [57]. Using a similar analysis to the proof of Ineq. (1), we also prove that the numerical observations in Ref. [57, 58] universally hold (Theorem 13):

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

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

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

with K being an arbitrary operator in the form of $K = \sum_{i\in\Lambda} O_i$ (Λ: total set of the sites), where $\mathcal{I}_{\rho_\beta}^{(\alpha)}(K)$ and $\mathcal{F}_{\rho_\beta}(K)$ are the WYD skew information (58) and the quantum Fisher information (65), respectively. These general limits provide useful information for applying the quantum many-body systems to quantum metrology [60–64].

The rest of this paper is organized as follows. In Sec. II, we formulate the precise setting and notations used throughout the paper and provide some preliminaries such as the Lieb-Robinson bound and the entanglement measure. In Sec. III, we introduce the quantum correlation $\mathrm{QC}_{\rho_\beta}(O_A,O_B)$ as the convex roof of the standard correlation function. We also provide several rigorous results on the relationships between the quantum correlation and quantum entanglement. In Sec. IV, our main results on the clustering theorem on the quantum correlation [Ineq. (1)] and the PPT relative entanglement [Ineqs. (2) and (3)] are provided. In Sec. V, we show our results on the WYD skew information and the quantum Fisher information [Ineqs. (4) and (5)]. In Sec. VI, we discuss the following several topics relevant to the present results: i) relationship between the macroscopic quantum effect and quantum entanglement (Sec. VI A), ii) relationship between entanglement clustering and quantum Markov property (Sec. VI A), iii) relationship between the quantum correlation and entanglement of formation (Sec. VI C), iv) the optimality of our main theorems (Sec. VI D), and v) extension of our results to more general quantum states based on the Bernstein-Widder theorem (Sec. VI E). Finally, in Sec. VII, we summarize the paper, along with a discussion regarding the scope for future work.

II. SET UP AND PRELIMINARIES

We consider a quantum system on a D-dimensional lattice with n sites. On each of the site, the Hilbert space with dimension d_0 is assigned. We let Λ be the set of total sites, and for an arbitrary partial set $X \subseteq \Lambda$, we denote the cardinality (the number of sites contained in X) as $|X|$. We also denote the complementary subset of X by $X^{\mathrm{c}} := \Lambda \setminus X$. For an arbitrary subset $X \subseteq \Lambda$, we define $\mathcal{D}_X$ as the dimension of the Hilbert space on X, i.e., $\mathcal{D}_X = d_0^{|X|}$. Finally, we give $X \cup Y$ simply by XY.

For arbitrary subsets $X, Y \subseteq \Lambda$, we define $d_{X,Y}$ as the shortest path length on the graph that connects X and Y; that is, if $X \cap Y \neq \emptyset$, $d_{X,Y} = 0$. When X comprises only one element (i.e., $X = \{i\}$), we denote $d_{\{i\},Y}$ by $d_{i,Y}$ for simplicity. We also denote the surface subset of X by $\partial X := \{i \in X | d_{i,X^{\mathrm{c}}} = 1\}$.

For a subset $X \subseteq \Lambda$, we define the extended subset $X[r]$ as

$$X[r] := \{i \in \Lambda | d_{X,i} \le r\}, \tag{6}$$

where $X[0] = X$, and r is an arbitrary positive number (i.e., $r \in \mathbb{R}^+$). From the notation, for $i \in \Lambda$, the subset $i[r]$ is a ball region with radius r centered at the site i. We introduce a geometric parameter γ which is determined only by the lattice structure. We define $\gamma \ge 1$ as a constant of $\mathcal{O}(1)$ that satisfies the following inequalities:

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

where $r \ge 1$.

A. Hamiltonian and quantum Gibbs state

Throughout the study, we consider generic Hamiltonians with few-body interactions. Here, the Hamiltonian is given by the following k-local form:

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

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

$$H_L = \sum_{Z:Z\subset L} h_Z, \tag{9}$$

To characterize the interaction strength of the Hamiltonian, we impose the following assumption for the Hamiltonian:

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

where $J(x)$ is a function that monotonically decreases with $x \geq 0$. Here, we mainly consider the short-range interaction, where the decay of the function $J(x)$ is faster than exponential decay, i.e.,

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

with $g_0 = \mathcal{O}(1)$ and $\mu_0 = \mathcal{O}(1)$. Our results are generalized to more broader classes of interactions, as is discussed in Appendix B.

Using the Hamiltonian, we define the quantum Gibbs state as follows:

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

where β is the inverse temperature. Throughout the paper, by appropriately choosing the energy origin, we let $Z = 1$, i.e.,

$$\rho_\beta = e^{-\beta H}. \tag{13}$$

When we consider a reduced density matrix on a region L ($L \subset \Lambda$), we denote it by $\rho_{\beta,L}$:

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

where $\mathrm{tr}_{L^{\mathrm{c}}}$ is the partial trace for subset L^{c}.

B. Lieb-Robinson bound

We here show the Lieb-Robinson bound that characterizes the quasi-locality by time evolution [65–68]. The Lieb-Robinson bound plays essential roles in deriving most of our main results and is formulated as follows:

Lemma 1 (Lieb-Robinson bound [69])**.** *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:*

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

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

Using the Lieb-Robinson bound (15), we also obtain the approximation of $O_X(t)$ onto a local region $Y \supset X$. We define $O_X(t, Y)$

$$O_X(t, Y) := \frac{1}{\mathrm{tr}_{Y^{\mathrm{c}}}(\hat{1})} \mathrm{tr}_{Y^{\mathrm{c}}}\left[O_X(t)\right] \otimes \hat{1}_{Y^{\mathrm{c}}}, \tag{16}$$

where $\mathrm{tr}_{Y^{\mathrm{c}}}(\cdots)$ means the partial transpose for the Hilbert space on the 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. [70], for arbitrary subsets $Y \supseteq X$, we have

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

where $\inf_{U_{Y^{\mathrm{c}}}}$ takes all unitary operators $U_{Y^{\mathrm{c}}}$ which are supported on Y^{c}. By choosing $Y = X[R]$ with $R \in \mathbb{N}$, we can obtain the following inequality by using the Lieb-Robinson bound (15):

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

where we apply the inequality (15) to $[O_X(t), U_{X[R]^{\mathrm{c}}}]$ with $U_{X[R]^{\mathrm{c}}}$, an arbitrary unitary operator. From the above inequality, we can ensure $O_X(t) \approx O_X(t, X[R])$ for $R \gtrsim (v/\mu)t$. We often refer to (v/μ) as the "Lieb-Robinson velocity:" $v_{\mathrm{LR}} = v/\mu$. In Table I, we summarize the fundamental parameters we use.

As long as the Lieb-Robinson bound holds, we can extend our main results to more general quantum systems such as the long-range interacting systems with power-law decaying interactions (see also Appendix B).

C. Quantum entanglement

Here, we show the basic definition of the quantum entanglement [5, 71]. We first define $\mathrm{SEP}(A:B)$ as a set of separable quantum states on the subset AB. For an arbitrary quantum state ρ, the reduced density matrix ρ_{AB} satisfies $\rho_{AB} \in \mathrm{SEP}(A:B)$ if and only if the following decomposition exists:

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

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

In quantifying the entanglement, we adopt the relative entanglement [72–74] as follows:

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

where $\mathcal{X}$ is the arbitrary class of quantum states we are interested in, and $S(\rho_{AB}||\sigma_{AB})$ is the relative entropy, i.e.,

$$\begin{aligned} &S(\rho_{AB}||\sigma_{AB}) \\ &:= \mathrm{tr}\left[\rho_{AB} \log(\rho_{AB})\right] - \mathrm{tr}\left[\rho_{AB} \log(\sigma_{AB})\right]. \end{aligned} \tag{21}$$

In particular, if we choose $\mathcal{X} = \mathrm{SEP}(A:B)$, we denote

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

for simplicity.

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

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

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

$$\begin{aligned} \delta_{\rho_{AB}} &:= \inf_{\sigma_{AB} \in \mathrm{SEP}(A:B)} \|\rho_{AB} - \sigma_{AB}\|_1 \\ &\leq \sqrt{2E_R(\rho_{AB})}. \end{aligned} \tag{24}$$

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 Ineq. (15))	C, v, μ

The quantity $\delta_{\rho_{AB}}$ yields meaningful upper bounds for various entanglement measures. Using the continuity of the information measures [75, 76], most of the entanglement measures are upper-bounded by $\mathcal{O}(\delta_{\rho_{AB}}) \times \log(\mathcal{D}_{AB})$: for example, the entanglement of formation [77], the entanglement of purification [76], the relative entanglement [78], and the squashed entanglement [75, 79].

D. Clustering theorem at high-temperatures: known results

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

For an arbitrary quantum state ρ, we first define the standard correlation function $\mathrm{C}_\rho(O_A, O_B)$ between observables O_A and O_B as

$$\mathrm{C}_\rho(O_A, O_B) := \mathrm{tr}(\rho O_A O_B) - \mathrm{tr}(\rho O_A) \cdot \mathrm{tr}(\rho O_B). \quad (25)$$

As a stronger concept of the bi-partite correlation, we define the mutual information $\mathcal{I}_\rho(A:B)$ between two subsystems A and B 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, i.e., $S_\rho(A) := \mathrm{tr}\left[-\rho_A \log(\rho_A)\right]$ with ρ_A being the reduced density matrix on A [see Eq. (14)]

Previous studies [80, 81] provided the following clustering theorem, which holds at arbitrary temperatures as $\beta \lesssim \log(n)$ (see also [82]):

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) [80]:*

$$\mathrm{C}_{\rho_\beta}(O_A, O_B) \le \mathrm{poly}(|A|, |B|) \exp\left(-\frac{R}{e^{\Omega(\beta)}}\right), \quad (27)$$

where $d_{A,B} = R$, and the notation $\Omega(\beta)$ denotes $\Omega(\beta) \propto \beta^{1+z}$ $(z \ge 0)$. In addition, the mutual information $\mathcal{I}_\rho(A:B)$ decays exponentially with distance [81]:

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

A similar result holds in arbitrary dimensional systems:

Lemma 3 (2D– clustering theorem)**.** *Under the same setup as in the statement 2, the following inequality holds at arbitrary temperatures, such that $\beta < \beta_c$ (n: system size) in arbitrary dimensional systems [83–87]:*

$$\mathrm{C}_{\rho_\beta}(O_A, O_B) \le \mathrm{poly}(|A|, |B|) \exp\left(-\frac{R}{\mathcal{O}(1)}\right), \quad (29)$$

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

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

Lemmas 2 and 3 immediately imply the exponential decay of the bi-partite quantum entanglement. Using Pinsker's inequality (23) and the equation

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

, we immediately obtain the following corollary:

Corollary 4. *In the temperature regimes $\beta \lesssim \log(n)$ (1D) and $\beta < \beta_c$ (2D–), the trace distance of $\|\rho_{AB} - \rho_A \otimes \rho_B\|_1$ exponentially decays with the distance between regions A and B:*

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

Because of $\rho_A \otimes \rho_B \in \mathrm{SEP}(A:B)$, the above corollary implies $\delta_{\rho_{AB}} \lesssim e^{-\mathcal{O}(R)}$. For the relative entanglement (22), we have $E_R(\rho_{AB}) \le \mathrm{poly}(|A|, |B|) e^{-\mathcal{O}(R)}$ from the continuity bound [78]. Therefore, in high-temperature regimes, we know that the problem of bi-partite entanglement clustering can be easily proved using the established results [88]. Based on this fact, we focus on the low-temperature regimes, where thermal phase transitions can occur and the clustering of bi-partite correlations may be no longer satisfied.

III. QUANTUM CORRELATION

Before moving on the entanglement clustering theorem, we consider the quantum correlation function which is defined as a convex roof of the standard correlation function $\mathrm{C}_\rho(O_A, O_B)$ in Eq. (25). Quantum correlation is a natural quantum analogue of the standard correlation function and has a significant relationships with quantum entanglement (see Sec. III B). There are two main reasons for introducing quantum correlation:

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

A. Definition

For an arbitrary many-body quantum state ρ, we define the quantum correlation for observables O_A and O_B by the convex roof of the standard correlation function (25), i.e., $\mathrm{C}_\rho(O_A, O_B)$ $[= \mathrm{tr}(\rho O_A O_B) - \mathrm{tr}(\rho O_A) \cdot \mathrm{tr}(\rho O_B)]$:

$$\mathrm{QC}_\rho(O_A, O_B) := \inf_{\{p_s, \rho_s\}} \sum_s p_s |\mathrm{C}_{\rho_s}(O_A, O_B)|, \tag{33}$$

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. Note that we adopt the mixed convex roof instead of the pure convex roof, where decomposed states $\{\rho_s\}$ are restricted to the pure state, i.e., $\rho_s = |\phi_s\rangle\langle\phi_s|$ for $\forall s$. The main reason for using it is to ensure the inequality (37) in Lemma 5. The mixed convex roof has been considered in Refs. [89–92] for example.

We notice that the definition immediately implies

$$\mathrm{QC}_\rho(O_A, O_B) = \big|\mathrm{C}_\rho(O_A, O_B)\big| \tag{34}$$

when ρ is given by pure state.

The quantum correlations for a density matrix ρ may be different from those for a reduced density matrix ρ_L ($L \subset \Lambda$), i.e., $\mathrm{QC}_{\rho_L}(O_A, O_B) \neq \mathrm{QC}_\rho(O_A, O_B)$ [see also Ineq. (37)]. For example, let us consider the case in which ρ is given by the Greenberger-Horne-Zeilinger (GHZ) state as follows:

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

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 non-zero 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 has no correlations. Hence, no quantum correlations exist in the reduced density matrix of the GHZ state.

As basic properties of $\mathrm{QC}_\rho(O_A, O_B)$, we prove the following lemma:

Lemma 5. *Let O_A and O_B be arbitrary operators supported on A and B, respectively. We then obtain the following inequalities:*

$$\mathrm{QC}_\rho(O_A, O_B) \le |\mathrm{C}_\rho(O_A, O_B)|, \tag{36}$$

and

$$\mathrm{QC}_{\rho_L}(O_A, O_B) \le \mathrm{QC}_\rho(O_A, O_B), \tag{37}$$

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 arbitrary two quantum states ρ and σ, the difference between $\mathrm{QC}_\rho(O_A, O_B)$ and $\mathrm{QC}_\sigma(O_A, O_B)$ is upper-bounded as

$$|\mathrm{QC}_\sigma(O_A, O_B) - \mathrm{QC}_\rho(O_A, O_B)| \le 7\sqrt{2}\epsilon^{1/2}, \tag{38}$$

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

Proof. The proof of the inequality (36) is proved by choosing decomposition as $\rho = p_1\rho_1$ with $p_1 = 1$ and $\rho_1 = \rho$ in the definition (33). On the second inequality, we consider the decomposition $\{p_s, \rho_s\}$ such that

$$\sum_s p_s |\mathrm{C}_{\rho_s}(O_A, O_B)| = \mathrm{QC}_\rho(O_A, O_B). \tag{39}$$

For the reduced density matrix ρ_L, we choose the decomposition using $\{p_s, \rho_s\}$ as

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

Then, we have $|\mathrm{C}_{\rho_s}(O_A, O_B)| = |\mathrm{C}_{\rho_{s,L}}(O_A, O_B)|$, and hence, the inequality (37) is derived as

$$\begin{aligned} \mathrm{QC}_{\rho_L}(O_A, O_B) &\le \sum_s p_s |\mathrm{C}_{\rho_{s,L}}(O_A, O_B)| \\ &= \mathrm{QC}_\rho(O_A, O_B). \end{aligned} \tag{41}$$

Finally, we prove the inequality (38) by applying the method in Ref. [89, Proposition 5]. For standard correlation $\mathrm{C}_\rho(O_A, O_B)$, straightforward calculations yield

$$|\mathrm{C}_\rho(O_A, O_B)| \le 1, \tag{42}$$

and

$$|\mathrm{C}_\rho(O_A, O_B) - \mathrm{C}_\sigma(O_A, O_B)| \le 3\|\rho - \sigma\|_1, \tag{43}$$

where we use $\|O_A\| = \|O_B\| = 1$. Hence, we can take $K = 3/\log(d_X)$ and $M = 1/\log(d_X)$ in Ref. [89, Ineqs. (29) and (30)], where d_X is the total Hilbert space dimension for ρ, i.e., $d_X = \mathcal{D}_\Lambda$ in our notations. Then, we can obtain the inequality (38) from Ref. [89, Ineq. (31) and Proposition 5]. 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 $\mathrm{QC}_{\rho_{AB}}(O_A, O_B)$ 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., $\rho_{AB} \in \mathrm{SEP}(A:B)$):*

$$\rho_{AB} \in \mathrm{SEP}(A:B) \longrightarrow \mathrm{QC}_{\rho_{AB}}(O_A, O_B) = 0 \tag{44}$$

for arbitrary pairs of O_A, O_B. By taking the contraposition of the lemma, we know that

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

Proof. From the definition (19) of $\mathrm{SEP}(A:B)$, there exists the decomposition

$$\rho_{AB} = \sum_s p_s \rho_{s,A} \otimes \rho_{s,B} \tag{46}$$

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

$$\begin{aligned}\mathrm{QC}_{\rho_{AB}}(O_A, O_B) &\le \sum_s p_s |\mathrm{C}_{\rho_{s,A}\otimes\rho_{s,B}}(O_A, O_B)| \\ &= 0.\end{aligned} \tag{47}$$

This completes the proof. □

Thus, we have shown that zero entanglement is a sufficient condition for the zero quantum correlation as in Eq. (44). Then, we immediately wonder whether the converse is true, i.e.,

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

On this question, we have the following conjecture:

Conjecture 7. *The statement (48) is true. That is, the zero quantum correlation for arbitrary pairs of O_A, O_B is necessary and sufficient for zero entanglement.*

The reason why we believe the conjecture is true is that we have the following relationship for the standard correlation function:

$$\begin{aligned}&\mathrm{C}_{\rho_{AB}}(O_A, O_B) = 0 \text{ for arbitrary pairs of } O_A, O_B \\ &\longleftrightarrow \rho_{AB} \text{ is a product state.}\end{aligned} \tag{49}$$

Hence, it is natural to expect that the quantum version of the above relationship also holds. Regarding the above conjecture, we can at least prove the following statement:

Lemma 8. *If $\mathrm{QC}_{\rho_{AB}}(O_A, O_B) = 0$ for arbitrary pairs of O_A, O_B, the Peres-Horodecki separability criterion [93, 94], i.e., PPT (positive partial transpose) condition, is satisfied. That is, 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 $\mathrm{QC}_{\rho_{AB}}(O_A, O_B) = 0$ for arbitrary pairs of O_A, O_B implies $\epsilon = 0$ in (51). Hence, we have $\mathrm{tr}|\rho_{AB}^{T_A}| = \mathrm{tr}(\rho_{AB}^{T_A}) = 1$ from the inequality (52). This completes the proof. □

The above lemma shows that the conjecture 7 rigorously holds for some class of quantum systems such as 2×2, 2×3 quantum systems, and so on [94, 95]. If we try to prove/disprove the conjecture in general cases, we must consider existence of the bound entanglement [96, 97]. A possible route to prove the conjecture 7 is to rely on the entanglement witness [98–101]. The challenging task is to appropriately reduce the calculations of the witnesses to those of the quantum correlations. As shown in the proofs of Proposition 9 and Lemma 25 below, we can relate the calculation of the partial transpose to the quantum correlations.

C. PPT (Positive partial transpose) relative entanglement

Finally, we relate the quantum correlation to the PPT relative entanglement. As shown in Lemma 8, quantum correlation is proved to be deeply related to the PPT condition. By using this property, we relate the quantum correlations to the following PPT relative entanglement [102–105]:

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

where we choose $\mathcal{X} = \mathrm{PPT}$ in Eq. (20) with PPT as a set of the quantum states σ_{AB} that satisfy the PPT condition, i.e., $\sigma_{AB}^{T_A} \succeq 0$ for $\sigma_{AB} \in \mathrm{PPT}$. Because the PPT set includes the separable set SEP (PPT ⊇ SEP), $E_R^{\mathrm{PPT}}(\rho_{AB})$ is smaller than or equal to $E_R(\rho_{AB})$ except for special cases. As shown in Ref. [73], the PPT relative entanglement satisfies all basic conditions for the entanglement measure (i.e., the four conditions in Ref. [71]). It also gives an upper bound for the Rains' bound [106, 107], which is deeply related to the distillable entanglement [102, 106].

As shown in the following proposition, the quantum correlation (33) gives an upper bound for the PPT relative entanglement:

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

$$\mathrm{QC}_{\rho_{AB}}(O_A, O_B) \le \epsilon \|O_A\| \cdot \|O_B\| \tag{51}$$

for two arbitrary operators O_A and O_B. We then obtain

$$\begin{aligned}&E_R^{\mathrm{PPT}}(\rho_{AB}) \le 4\mathcal{D}_{AB}\bar{\delta}\log(1/\bar{\delta}) \le 4\mathcal{D}_{AB}\bar{\delta}^{1/2}, \\ &\bar{\delta} := 4\epsilon \min(\mathcal{D}_A, \mathcal{D}_B),\end{aligned} \tag{52}$$

where the second inequality is trivially derived from $x\log(1/x) \le x^{1-1/e} \le x^{1/2}$ for $0 \le x \le 1$. Recall that $\mathcal{D}_{AB}$ is the Hilbert space dimension in the region AB.

From the proposition, if there are no quantum correlations, i.e., $\epsilon = 0$ in (51), we can ensure $E_R^{\mathrm{PPT}}(\rho_{AB}) = 0$, which also yields Lemma 8. We can thus connect the clustering theorem for the quantum correlation to that for quantum entanglement. In the following section, we show that the generic quantum Gibbs states satisfy the exponential clustering for the quantum correlations at arbitrary temperatures, and hence, the entanglement clustering theorem also holds.

IV. EXPONENTIAL CLUSTERING FOR QUANTUM CORRELATIONS

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

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. 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 $\mathrm{QC}_{\rho_\beta}(O_A, O_B)$ is upper-bounded as follows:*

$$\begin{aligned}&\mathrm{QC}_{\rho_\beta}(O_A, O_B)\\ &\le C_\beta(|\partial A| + |\partial B|)\,(1 + \log|AB|)\,e^{-R/\xi_\beta},\end{aligned} \tag{53}$$

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

$$\begin{aligned}\xi_\beta &:= \frac{4}{\mu}\left(1 + \frac{v\beta}{\pi}\right), \quad c_{\beta,1} := e^{2/\xi_\beta}\left(\frac{12}{\pi} + \frac{6C}{v\beta}\right),\\ c_{\beta,2} &:= e^{2/\xi_\beta}\left(\frac{12+3C}{\pi} + \frac{3C}{v\beta}\right)[3 + \log(1 + 2g\beta)],\end{aligned} \tag{54}$$

and the basic parameters are summarized in Table I.

Remark. The constant C_β depends on the inverse temperatures; however, it increases most logarithmically with β, i.e., $C_\beta = \mathcal{O}(\log(\beta))$. In contrast, in the limit of $\beta \to +0$, the upper bound for $\mathrm{QC}_{\rho_\beta}(O_A, O_B)$ apparently breaks down. However, the temperatures of $\beta \ll 1$ corresponds to the high-temperature regime, and hence, a much stronger statement (e.g., exponential decay of the mutual information, see Sec. II D) can be proved by using the cluster expansion technique [27]. Therefore, the important temperature regime is $\beta \gg 1$, which cannot be captured by the cluster expansion. The inequality (53) yields non-trivial upper bounds even for $\beta = \mathcal{O}(n^z)$ $(z > 0)$.

A. Exponential entanglement clustering

By combining Proposition 9 with Theorem 10, we immediately obtain 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*

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

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

In the above upper bound, the correlation length exponentially increases with sizes of A and B. Hence, the inequality is meaningless when A and B depend on the system size (i.e., $\mathcal{D}_{AB} = e^{\mathcal{O}(n)}$). Unfortunately, we cannot improve it if we only utilize the decay of the quantum correlations. To highlight this point, let us consider a random state $|\mathrm{rand}\rangle$, which has the same property as the infinite temperature states as long as we look at the local regions. As shown in Ref. [108, 109], the state $|\mathrm{rand}\rangle$ satisfies exponential clustering for the standard correlation functions (25), which clearly implies exponential decay of quantum correlations. However, the state $|\mathrm{rand}\rangle$ has a large quantum entanglement between A and B. This point means that we need to take advantage of the characteristics of the quantum Gibbs state.

Using the quantum belief propagation technique [55, 56], we can significantly improve the inequality (55) in one-dimensional cases:

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

$$E_R^{\mathrm{PPT}}(\rho_{\beta,AB}) \le \bar{C}_\beta \log(\mathcal{D}_{AB}) e^{-R/[16\log(d_0)\xi_\beta^2] + 7gk\beta}, \tag{56}$$

where d_0 is defined as the one-site Hilbert space dimension and $\bar{C}_\beta := 20\left(\tilde{C}_\beta + 16 d_0^4 C_\beta\right)^{1/2}$ with C_β defined in Eq. (54) and $\tilde{C}_\beta$ defined in Eq. (F6) as

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

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

Here, the PPT relative entanglement has been considered. The definition of $E_R^{\mathrm{PPT}}(\rho_{\beta,AB})$ is also significantly associated with that of the entanglement negativity [49], which is another popular entanglement measure, especially in the context of numerical calculations. A part of the above results on the PPT relative entanglement can be applied to the entanglement negativity (See Appendix G)

V. QUANTUM CORRELATIONS BASED ON THE SKEW INFORMATION

We here consider another type of quantum correlation based on the WYD skew information [110–112]:

$$\mathcal{I}_\rho^{(\alpha)}(K) := \mathrm{tr}(\rho K^2) - \mathrm{tr}\left(\rho^{1-\alpha} K \rho^\alpha K\right) \tag{58}$$

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. As a representative application, it is utilized in formulating the Heisenberg uncertainty relation for mixed states [113–116]. More recently, the WYD skew information has attracted significant attention in the context of the quantum coherence theory [59, 117–120].

In Refs. [57, 58, 121, 122], the following quantity has been defined to characterize quantum correlations:

$$\bar{Q}_\rho(O_A, O_B) := \int_0^1 Q_\rho^{(\alpha)}(O_A, O_B) d\alpha$$
$$= \mathrm{tr}(\rho O_A O_B) - \int_0^1 \mathrm{tr}\left(\rho^{1-\alpha} O_A \rho^\alpha O_B\right) d\alpha \qquad (59)$$

with

$$Q_\rho^{(\alpha)}(O_A, O_B) := \mathrm{tr}(\rho O_A O_B) - \mathrm{tr}\left(\rho^{1-\alpha} O_A \rho^\alpha O_B\right). \qquad (60)$$

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

The authors in Ref. [57, 58] 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 the observations hold universally at arbitrary temperatures remains unclear. We resolve the problem by the following theorem:

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

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

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

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

We notice that the same upper bound trivially holds for $\bar{Q}_\rho(O_A, O_B)$ *in Eq.* (59).

By using Theorem 13, we immediately obtain a general upper bound on the WYD skew information:

Corollary 14. *Let* K *be an operator given by*

$$K = \sum_{i \in \Lambda} O_i \quad (\|O_i\| \le 1), \qquad (63)$$

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

$$\mathcal{I}_{\rho_\beta}^{(\alpha)}(K) := \mathrm{tr}(\rho_\beta K^2) - \mathrm{tr}\left(\rho_\beta^{1-\alpha} K \rho_\beta^\alpha K\right)$$
$$\le \tilde{C}'_\beta \xi_\beta'^D n = \mathcal{O}(\beta^D) n, \qquad (64)$$

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

A. Quantum Fisher information

As a relevant quantity, we here consider the quantum Fisher information $\mathcal{F}_\rho(K)$, which is defined as follows [123]:

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

where $K = \sum_{i\in\Lambda} O_i$ and $\rho = \sum_s \lambda_s |\lambda_s\rangle\langle\lambda_s|$. Here, we define λ_s and $|\lambda_s\rangle$ by the spectral decomposition $\rho_\beta = \sum_s \lambda_s |\lambda_s\rangle\langle\lambda_s|$. The quantum Fisher information was introduced in the field of quantum metrology [124–126]. In the context of the entanglement theory, it is also regarded as one of the representative measures for macroscopic quantum entanglement [6, 123, 127–130]. In recent studies, the quantum Fisher information has attracted significant attention in the development of quantum technologies (see Refs. [6, 131, 132] for recent reviews).

Quantum Fisher information is associated with the WYD skew information by the inequality of $(\mathcal{F}_{\rho_\beta}(K)/4) \le 2\mathcal{I}_{\rho_\beta}^{(\alpha=1/2)}(K)$, which has been proven in Ref. [133, Theorem 2] (see also [134]). Hence, from the inequality (64), we immediately obtain the upper bound of

$$\mathcal{F}_{\rho_\beta}(K) \le 8\tilde{C}'_\beta \xi_\beta'^D n, \qquad (66)$$

where $\tilde{C}'_\beta$ and ξ'_β are defined in Corollary 14. In the opposite direction, a general lower bound for quantum Fisher information is given in Ref. [135].

To discuss macroscopic entanglement by the quantum Fisher information, the scaling exponent is considered, i.e., $\mathcal{F}_{\rho_\beta}(K) \propto n^p$ $(p \le 2)$. When $p = 2$, the state is composed of a superposition of macroscopically different quantum states; for example, the GHZ state has $p = 2$ [123, 127]. In contrast, when $p = 1$, scaling is the same as the product states, and no macroscopic superposition exists. From the inequality (66), the scaling of the Fisher information is always given by $\mathcal{O}(n)$ (i.e., $p = 1$) as long as $\beta = \mathrm{poly\text{-}log}(n)$. Thus, our result gives the rigorous proof for the absence of macroscopic superposition at finite temperatures.

At the quantum critical point (i.e., $\beta = \infty$), a scaling of the quantum Fisher information usually behaves as $p > 1$ [135, Eq. (22)]; for example, $p = 7/4$ for the critical transverse Ising model [136, 137]. Our upper bound (66) characterizes the necessary temperature required while applying the many-body macroscopic entanglement to quantum metrology [60–64], which has attracted considerable attention in recent studies.

VI. FURTHER DISCUSSION

A. Macroscopic quantum effect v.s. quantum entanglement

We have discussed entanglement properties in the finite-temperature Gibbs state. Here, we state that our observation on the entanglement properties for the finite-temperature mixed state is considerably different from that for pure states in general. 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 show off-diagonal-long-range orders (ODLRO [1]). In Refs. [138, 139], Vedral discussed η-pairing states, which are eigenstates in the Hubbard, and similar models to explain high-temperature superconductivity. He argued that such states have a vanishing entanglement between two sites as the distance diverges, whereas classical correlations remain finite even in the thermodynamic limit. Maximally mixed states with η-paring states also exhibit this property. This observation suggests that ODLRO is not directly associated with the quantum entanglement discussed in this study. We remark that the quantum entanglement properties in the finite-temperature Gibbs state have not been analytically scrutinized so far in a general framework. We note that recent large-scale numerical computation in the two-dimensional transverse field Ising models reveal that entanglement measured via the Renyi negativity is short-ranged even at finite critical temperatures [53, 54]. This observation is consistent with our general statement.

B. Relation to the quantum Markov property

In this subsection, we briefly show a relation between the clustering of quantum entanglement and the approximate quantum Markov property.

For the purpose, we consider the squashed entanglement [79, 140, 141]. It is defined using the conditional mutual information $\mathcal{I}_{\rho_{ABE}}(A:B|E)$ for tripartite quantum systems:

$$\mathcal{I}_{\rho_{ABE}}(A:B|E) := S_{\rho_{ABE}}(AE) + S_{\rho_{ABE}}(BE) - S_{\rho_{ABE}}(ABE) - S_{\rho_{ABE}}(E). \quad (67)$$

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

$$E_{\rm sq}(\rho_{AB}) := \inf_E \left\{ \frac{1}{2}\mathcal{I}_{\rho_{ABE}}(A:B|E) \middle| {\rm tr}_E(\rho_{ABE}) = \rho_{AB} \right\}, \quad (68)$$

where $\inf_E$ is taken over all extensions of ρ_{AB} such that ${\rm tr}_E(\rho_{ABE}) = \rho_{AB}$. Different from the PPT relative entanglement (50), squashed entanglement is equal to zero if and only if the quantum state is not entangled [140].

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

$$\mathcal{I}_\rho(A:B|C) = 0 \quad \text{for} \quad d_{A,B} \geq r_0, \quad (69)$$

where r_0 is a constant of $\mathcal{O}(1)$. When the Hamiltonian is short-range and commuting, the above Markov property strictly holds for quantum Gibbs states at arbitrary temperatures [142, 143]. The quantum Markov property has a useful operational meaning [144], and it plays a critical role in preparing the quantum Gibbs states on a quantum computer [27, 145–147]. For non-commuting Hamiltonians with short-range interactions, it is conjectured that the quantum Markov property generally 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:*

$$\mathcal{I}_{\rho_\beta}(A:B|E) \leq {\rm poly}(|A|,|B|) e^{-d_{A,B}/\xi_\beta} \quad (70)$$

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

If the inequality (70) holds, we immediately obtain the exponential clustering for the squashed entanglement:

$$E_{\rm sq}(\rho_{\beta,AB}) \leq \frac{1}{2}\mathcal{I}_{\rho_\beta}(A:B|E) \leq {\rm poly}(|A|,|B|) e^{-d_{A,B}/\xi_\beta}, \quad (71)$$

where $E = \Lambda \setminus (AB)$ and $\rho_{ABE} = \rho_\beta$ is taken in Eq. (68). Until now, the above conjecture has been proved only in high-temperature regimes where thermal transition cannot occur, i.e., $\beta \lesssim \log(n)$ in 1D cases [147], and $\beta < \beta_c$ ($\beta_c = \mathcal{O}(1)$) in high-dimensional cases [27]. In these temperature regimes, regarding entanglement, much stronger statements than (71) (i.e., Corollary 4) have been already derived.

Finally, we show that the inequality (71) cannot be used to prove the exponential clustering of other quantum entanglement measures [e.g., the relative entanglement (22), or the entanglement of formation (78)] in general.

To upper-bound other entanglement measures, we need to upper-bound the quantity $\delta_{\rho_{AB}}$, which has been defined in Eq. (24), i.e., $\delta_{\rho_{AB}} := \inf_{\sigma_{AB}\in {\rm SEP}(A:B)} \|\rho_{AB} - \sigma_{AB}\|_1$, which characterizes the distance between the quantum state ρ_{AB} and the non-entangled state. The squashed entanglement gives the following upper bound for $\delta_{\rho_{AB}}$ [140, 141]:

$$\delta_{\rho_{AB}} \leq 42\sqrt{\mathcal{D}_{AB} E_{\rm sq}(\rho_{AB})}, \quad (72)$$

where $\mathcal{D}_{AB}$ is the dimension of the Hilbert space of AB. If $E_{\rm sq}(\rho_{AB}) \ll 1/\mathcal{D}_{AB}$, we can ensure that $\delta_{\rho_{AB}}$ is sufficiently small. However, $\mathcal{D}_{AB}$ is exponentially large, with a size of $|AB|$. Hence, even if the quantum Markov conjecture 15 was proven, the distance $\delta_{\rho_{\beta,AB}}$ for the quantum Gibbs state might be still considerably large when subset A or B is as large as the system size n. Here, we encounter a similar problem to the one in the inequality (52) in Proposition 9. Thus, the clustering problem of the bi-partite entanglement cannot be generalized to other entanglement measures only by clarifying the quantum Markov property.

C. General upper bound on the quantum correlation

We here show that the entanglement formation [48, 148] is a simple upper bound for the quantum correlation ${\rm QC}_{\rho_{AB}}(O_A, O_B)$. The relation between the entanglement of formation and the quantum correlation ${\rm QC}_{\rho_{AB}}(O_A, O_B)$ is derived from that between mutual information $\mathcal{I}_{\rho_{AB}}(A:B)$ and standard correlation function ${\rm C}_{\rho_{AB}}(O_A, O_B)$. The entanglement of formation is defined as follows:

$$E_F(\rho_{AB}) := \inf_{\{p_s,|\psi_{s,AB}\rangle\}} \sum_s \frac{p_s}{2} \mathcal{I}_{|\psi_{s,AB}\rangle}(A:B) \\ = \inf_{\{p_s,|\psi_{s,AB}\rangle\}} \sum_s p_s S_{|\psi_{s,AB}\rangle}(A:B) \quad (73)$$

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 the subset A, respectively. Furthermore, $\inf_{\{p_s,|\psi_{s,AB}\rangle\}}$ is taken for arbitrary decomposition $\rho = \sum_s p_s |\psi_{s,AB}\rangle\langle\psi_{s,AB}|$ with $p_s > 0$. Note that $\mathcal{I}_{\rho_s}(A:B) = 2S_{\rho_{s,AB}}(A)$ when ρ_s is a pure state.

The mutual information $\mathcal{I}_{|\psi_{s,AB}\rangle}(A:B)$ captures the full correlations between two subsystems [44]. Hence, it is quite plausible that entanglement of formation gives an upper bound of quantum correlations. Indeed, the following lemma connects the quantum correlation $\mathrm{QC}_{\rho_{AB}}(O_A, O_B)$ and the entanglement of formation:

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

$$\mathrm{QC}_\rho(O_A, O_B) \le 2\|O_A\| \cdot \|O_B\| \sqrt{E_F(\rho_{AB})}. \quad (74)$$

Proof. For the first, we note that

$$\sum_s p_s |\mathrm{C}_{\rho_{s,AB}}(O_A, O_B)|^2 \\ \ge \left(\sum_s p_s |\mathrm{C}_{\rho_{s,AB}}(O_A, O_B)| \right)^2, \quad (75)$$

which yields

$$\inf_{\{p_s,\rho_{s,AB}\}} \sum_s p_s |\mathrm{C}_{\rho_{s,AB}}(O_A, O_B)|^2 \ge [\mathrm{QC}_{\rho_{AB}}(O_A, O_B)]^2. \quad (76)$$

Hence, we aim to upper-bound the LHS in the above inequality.

Second, we consider the classical squashed (c-squashed) entanglement [92], which is given by the mixed convex roof of mutual information [149]:

$$E^c_{\mathrm{sq}}(\rho_{AB}) := \inf_{\{p_s,\rho_{s,AB}\}} \sum_s \frac{p_s}{2} \mathcal{I}_{\rho_{s,AB}}(A:B), \quad (77)$$

where $\inf_{\{p_s,\rho_{s,AB}\}}$ is taken 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 [150]. Trivially, the entanglement of formation $E_F(\rho_{AB})$ is lower-bounded as

$$E_F(\rho_{AB}) \ge E^c_{\mathrm{sq}}(\rho_{AB}). \quad (78)$$

We finally compare $E^c_{\mathrm{sq}}(\rho_{AB})$ with the LHS in (76). For this purpose, we utilize the following inequality in Ref. [44, Inequality (5)]:

$$\mathcal{I}_{\rho_{AB}}(A:B) \ge \frac{|C_{\rho_{AB}}(O_A, O_B)|^2}{2\|O_A\|^2 \cdot \|O_B\|^2}. \quad (79)$$

By applying the above inequality to the definition (77), we have

$$E^c_{\mathrm{sq}}(\rho_{AB}) \ge \inf_{\{p_s,\rho_{s,AB}\}} \sum_s \frac{p_s}{2} \cdot \frac{|C_{\rho_{AB}}(O_A, O_B)|^2}{2\|O_A\|^2 \cdot \|O_B\|^2} \\ \ge \frac{[\mathrm{QC}_{\rho_{AB}}(O_A, O_B)]^2}{4\|O_A\|^2 \cdot \|O_B\|^2}, \quad (80)$$

where we use (76) in the last inequality. By combining the above inequality with (78), we prove the main inequality (74). This completes the proof. □

D. Optimality of the obtained bounds

We here discuss the optimality of the correlation length ξ_β or ξ'_β in Theorems 10 and 13. We show that the β-dependence of the correlation length ξ_β (i.e., $\xi_\beta \propto \beta$) is qualitatively optimal and cannot be improved in general. This point is ensured by corresponding the inverse temperatures and the spectral gap, as follows:

$$\beta \longleftrightarrow 1/\Delta \quad (81)$$

with Δ being the spectral gap between the ground state and the first excited state. From the correspondence, the correlation length of $\mathcal{O}(\Delta^{-1})$ in the gapped ground states [66, 68, 151] implies the correlation length of $\mathcal{O}(\beta)$ in the thermal states.

To highlight this point in more detail, we first assume the following inequality for the number of energy eigenstates in an arbitrary energy shell $(E-1, E]$ [152–154]:

$$\mathcal{N}_{E,1} \le n^{cE}, \quad (82)$$

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, we set the energy origin such that the ground state's energy is equal to zero. Note that the above condition is satisfied in various types of quantum many-body systems [152].

Under the condition (82), the quantum Gibbs states ρ_β is close to the ground state ρ_∞ in the sense that

$$\|\rho_\beta - \rho_\infty\|_1 \le \text{const.} \times \frac{e^{-(\beta - c\log(n))\Delta}}{\beta - c\log(n)}. \quad (83)$$

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

$$\|\rho_\beta - \rho_\infty\|_1 = 1/\mathrm{poly}(n). \quad (84)$$

When the ground state is non-degenerate and gapped, the correlation function $\mathrm{C}_{\rho_\infty}(O_A, O_B)$ is given by

$$\mathrm{C}_{\rho_\infty}(O_A, O_B) = \mathrm{QC}_{\rho_\infty}(O_A, O_B) = \text{const.} \times e^{-\mathcal{O}(\Delta)R}, \quad (85)$$

where we use Eq. (34) for the pure state in the first equation. Using the continuity bound (38), we obtain

$$\mathrm{QC}_{\rho_\beta}(O_A, O_B) = \mathrm{C}_{\rho_\infty}(O_A, O_B) - 1/\mathrm{poly}(n) \\ = \text{const.} \times e^{-\mathcal{O}(\Delta)R} - 1/\mathrm{poly}(n) \\ = \text{const.} \times e^{-\mathcal{O}(R)/(\beta/\log(n))} - 1/\mathrm{poly}(n), \quad (86)$$

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 $R \gtrsim \beta/\log(n)$, and hence, the correlation length is proportional to β at sufficiently small temperatures.

In contrast, regarding the WYD skew information and the quantum Fisher information, room still exists for improvement of the β-dependences, which have been given the inequalities (64) and (66). In the ground states, the WYD skew information and the quantum Fisher information reduce to the variance of the operator. For arbitrary operator K given in Eq. (63), the variance $(\Delta K)^2 = \mathrm{tr}\left(\rho_\infty K^2\right) - [\mathrm{tr}\left(\rho_\infty K\right)]^2$ is upper-bounded by [155, 156]:

$$\mathcal{I}^{(\alpha)}_{\rho_\infty}(K) = (\Delta K)^2 \le \text{const.} \times \Delta^{-1} n. \tag{87}$$

Remarkably, the above inequality holds in infinite dimensional systems and long-range interacting systems. Hence, the (β, Δ) correspondence (81) indicates the improvement of the current upper bounds to

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

, which gives better bounds in dimensions greater than 1 ($D \ge 2$).

E. Beyond quantum Gibbs states

Throughout the discussion, we consider the equilibrium situation at a finite temperature. When we consider a non-equilibrium density matrix, the entanglement properties show different properties in general [157]. A natural question arises on whether the current results hold for more general quantum states. From the definition (33) of the quantum correlation, the concavity is satisfied, i.e.,

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

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

$$\rho = \int_0^\infty a(t) e^{-tH} dt \tag{88}$$

with $a(t)$ being a non-negative function, we can apply Theorem 10 to the state ρ. Then, the state ρ has a finite quantum correlation length, and the entanglement clustering is also satisfied. The same discussion can be also applied to the WYD skew information $\mathcal{I}^{(\alpha)}_\rho(K)$ and the quantum Fisher information $\mathcal{F}_\rho(K)$ due to their concavities [158]. Note that if the state ρ includes extremely low-temperature states, e.g., $\int_{t_0}^\infty a(t)\mathrm{tr}(e^{-tH}) \approx 1$ with $t_0 \approx \mathcal{O}(n)$, the state ρ is similar to low-temperature Gibbs states and the quantum correlation length may become large.

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

$$\rho = \frac{F(H)}{\mathrm{tr}\left[F(H)\right]}, \tag{89}$$

where $F(x) \ge 0$. This class of the quantum state is called the passive state [159, 160] and plays a crucial role in quantum thermodynamics [161–164]. The quantum Gibbs state trivially corresponds to the case, i.e., $F(x) = e^{-\beta x}$. From the Bernstein-Widder theorem [165–167], the passive state (89) can be represented in the form of Eq. (88) if and only if the function $F(x)$ is completely monotonic, as follows:

$$(-1)^m \frac{d^m}{dx^m} F(x) \ge 0 \tag{90}$$

for arbitrary $m \ge 0$. Therefore, for every passive state with the condition (90), the same structural restrictions must be imposed as the quantum Gibbs state.

VII. SUMMARY AND FUTURE WORKS

In this work, we mainly tackled the conjecture of the exponential clustering of the bipartite entanglement (91), which reveals the fundamental aspect of the long-range entanglement. To access the entanglement, we introduced a novel concept called the quantum correlation $\mathrm{QC}_\rho(O_A, O_B)$, which is defined by the convex roof of the standard bipartite correlation function as in Eq. (33). As a fundamental theorem, we derived the exponential clustering of the quantum correlation, which holds at arbitrary temperatures, including even the critical point of thermal phase transition. Based on its definition and the fact that it uses the convex roof, quantum correlation has properties similar to those of entanglement. On this point, we derived several basic statements in Sec. III including the relationship between the quantum correlation and the PPT relative entanglement (Proposition 9). From the clustering theorem for the quantum correlation, we have given the entanglement clustering theorems (Corollary 11 and Theorem 12) for PPT relative entanglement (2). Using similar analytical techniques, we also derived the exponential clustering of another type of quantum correlation based on the WYD skew information (Theorem 13). It yielded the fundamental limitations of the WYD skew information and the quantum Fisher information (Corollary 14), which serve as representative measures for quantum coherence and macroscopic entanglement.

Based on the present results, the strongest form of the bi-partite entanglement clustering may be given in the following form:

[The strongest conjecture]

$$E_R(\rho_{\beta,AB}) \le \mathrm{poly}(|A|, |B|) e^{-R/\tilde{\xi}_\beta}, \tag{91}$$

for arbitrary choice of A and B such that $d_{A,B} = R$, where $\tilde{\xi}_\beta = \mathrm{poly}(\beta)$ and $\mathrm{poly}(x)$ denote a finite degree polynomial. As shown in Sec. II C, from the continuity bounds, the inequality (91) yields the same upper bound for other entanglement measures. Our main theorems have not arrived at this form of entanglement clustering, and we still need a lot of work to refine the current results.

In conclusion, we unveiled a fundamental limit on the characteristic length scale such that some types of quantum effects can exist. The present results do not depend on system details and hold at arbitrary temperatures. Little has been known regarding the universal structural constraints in low-temperature physics that must be satisfied by every quantum many-body system. Identifying these constraints is a critical task in understanding the complicated quantum many-body phases as well as developing efficient algorithms for quantum many-body simulations. We hope that our work has paved a new way to access this profound problem.

Finally, we leave the following topics as specific open questions.

- The first point is to derive a clustering theorem for the relative entanglement instead of the PPT relative entanglement. One possible way for the purpose is to resolve the conjecture 7. Then, we would be able to improve Proposition 9; that is, under the condition of (almost) zero quantum correlations [i.e., Ineq. (51)], similar inequality to (52) may hold for the relative entanglement $E_R(\rho_{AB})$ instead of $E_R^{\rm PPT}(\rho_{AB})$. The improvement immediately yields the entanglement clustering for other popular measures such as the entanglement of formations [see also the discussion after Ineq. (24)].

- As a related problem, the $(|A|,|B|)$ dependence in Corollary 11 may be improved in dimensions greater than one. In the present form, the independence is in the exponential form, and hence, we cannot obtain a meaningful bound when $|A|$ and $|B|$ are as large as the system size. For improvement, as has been discussed after Corollary 11, it is not enough to consider only the operator correlations ${\rm QC}_\rho(A,B)$. We instead need to consider the full information between the two subsystems. At the current stage, the problem may be challenging since it should include an analogous difficulty to the data hiding problem in the context of the area law conjecture at zero temperature [108, 109, 152].

- Third, it is an intriguing problem to identify the class of quantum coherence measures [168] which is always short range at non-zero temperatures. In this study, we showed that bi-partite entanglement cannot exist at long distances, but as has been demonstrated in Sec. VI A, macroscopic quantum effects do not necessarily imply long-distance entanglement. For example, quantum discord, one of the well-known measures for quantum correlation [169, 170], only decays algebraically at thermal critical points [57]. It is still open to extending our current results to other coherence measures.

- Finally, can we apply entanglement clustering to more practical problems such as the efficient simulation of the quantum Gibbs states? The clustering of entanglement imposes a strong constraint to the structure of the quantum Gibbs states. Hence, it is likely that we may be able to utilize the property to reduce the computational complexity.

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CONTENTS

Appendix A: Spectral decomposition of operators

As a convenient notation, we define O_ω for arbitrary operator O as follows [55]:

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

where $\{|E_i\rangle\}$ and $\{E_i\}$ are eigenstates and the corresponding eigenvalues of H, respectively. The operator O_ω picks up terms like $\langle E+\omega|O|E\rangle|E+\omega\rangle\langle E|$. From the above definition, we can immediately obtain

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

and

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

where we define $\mathrm{ad}_H(\cdot) := [H, \cdot]$.

Appendix B: Beyond short-range interacting spin systems

1. Long-range interacting cases

We also discuss how to generalize our current analyses to systems with long-range interactions, where decay of the function $J(x)$ in Eq. (10) is given by a polynomial form, i.e.,

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

When $\alpha > 2D$, the Lieb-Robinson bound (15) can be generalized to long-range interacting systems [171–177]. We obtain the Lieb-Robinson bound in the following form:

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

where η_α and $\tilde{\alpha}$ depend on the spatial dimension D and the decay exponent α. For example, a loose estimation gives $\eta_\alpha = \alpha - D - 1$ and $\tilde{\alpha} = \alpha - 2D$ [175]. The quantitatively optimal estimation of the parameters η_α and $\tilde{\alpha}$ is still an open question.

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

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

2. Disordered systems

Other interesting systems include disordered systems where randomness is added to the Hamiltonians. In such systems, one can prove that the Lieb-Robinson bound is improved as follows [178, 179]:

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

where C, η, μ are constants of $\mathcal{O}(1)$ which depend on 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 point leads to the quantum correlation length of $\mathcal{O}(\mathrm{polylog}(\beta))$ in the main theorem (i.e., Theorem 10, Theorem 13 and Theorem 12).

3. Quantum boson systems

Finally, in quantum boson systems, the Hamiltonian is locally unbounded (i.e., the parameter g is infinitely large, see Fig. I). In such systems, we do not usually obtain the Lieb-Robinson bound with a finite Lieb-Robinson velocity [180]. To extend our results, we may have to restrict ourselves to particular classes of quantum many-body boson systems, such as free boson systems [181, 182], spin-boson models [183, 184], and Bose-Hubbard type Hamiltonians [185–187]. The establishment of the Lieb-Robinson bound in the boson systems is still an active area of research.

Appendix C: Proofs of Theorem 13 and Corollary 14

In this section, we prove Theorem 13 before proving Theorem 10. The proof of Theorem 13 is much simpler than that of Theorem 10, but the essences of the both proofs are similar.

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

$$Q^{(\alpha)}_{\rho_\beta}(O_A,O_B) := \mathrm{tr}(\rho_\beta O_A O_B) - \mathrm{tr}\left(\rho_\beta^{1-\alpha} O_A \rho_\beta^\alpha O_B\right) \tag{C1}$$

and

$$\mathcal{I}^{(\alpha)}_{\rho_\beta}(K) := \mathrm{tr}(\rho_\beta K^2) - \mathrm{tr}\left(\rho_\beta^{1-\alpha} K \rho_\beta^\alpha K\right) \tag{C2}$$

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

For convenience of the readers, we give rough forms of the statements. In Theorem 13, we have given

$$Q^{(\alpha)}_{\rho_\beta}(O_A,O_B) \le C'_\beta \min(|\partial A|,|\partial B|) e^{-R/\xi'_\beta}, \tag{C3}$$

where the parameters are $\mathcal{O}(1)$ constants which have been given in Eq. (62). Furthermore, Corollary 14 given the following inequalities:

$$\mathcal{I}^{(\alpha)}_{\rho_\beta}(K) \le \tilde{C}'_\beta \xi'^D_\beta n = \mathcal{O}(\beta^D) n, \tag{C4}$$

for the WYD skew information.

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

We notice that it is not possible in general to obtain the same results for the parameter regime $\alpha \notin [0,1]$. Mathematically, the proof in Sec. C 3 breaks down for $\alpha\notin[0,1]$ because the function $g_{\alpha,\beta}(t)$ in (C20) no longer decays exponentially with t.

For example, when $\alpha=-1$, $\mathcal{I}^{(-1)}_\rho(K)$ is called the purity of coherence [188]:

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

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

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

For $\beta=\mathrm{poly}[\log(n)]$, under the same assumption as Eq. (82), the quantum Gibbs state ρ_β satisfies

$$\lambda_0\approx 1,\quad \lambda_j = e^{-\beta E_j}, \tag{C7}$$

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

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

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

Usually, we can only ensure $|\langle\lambda_j|K|\lambda_0\rangle|^2 \lesssim e^{-\mathrm{const.}\times E_j}$ from Ref. [189]. 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, we cannot obtain a meaningful upper bound $\mathcal{I}^{(\alpha)}_{\rho_\beta}(K)$ without the high-temperature condition.

2. Proof of Corollary 14

We first prove Corollary 14 based on Theorem 13. The proof can be immediately given as follows:

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

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

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

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

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

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

We thus obtain the inequality (C4) by using (C10) and $\xi'^{-1}_\beta \le \mu/2$:

$$\begin{aligned}\zeta_{0,\xi'_\beta} &= 1+\gamma e^{1/\xi'_\beta} \xi'^D_\beta D! = \xi'^D_\beta\left(\xi'^{-D}_\beta + \gamma e^{1/\xi'_\beta} D!\right) \\ &\le \xi'^D_\beta \left[(\mu/2)^D + \gamma e^{\mu/2} D!\right].\end{aligned} \tag{C12}$$

This completes the proof. □

3. Proof of Theorem 13

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

$$\begin{aligned}Q^{(\alpha)}_\rho(O_A,O_B) &\le \mathrm{tr}(\rho|O_AO_B|) + \frac{\mathrm{tr}(\rho|O_A|^2)+\mathrm{tr}(\rho|O_B|^2)}{2} \\ &\le \|O_A\|^2 + \|O_B\|^2 = 2,\end{aligned} \tag{C13}$$

where we use $\|O_A\| = \|O_B\| = 1$. For the proof of the inequality (C13), because $\mathrm{tr}(\rho O_A O_B) \le \mathrm{tr}(\rho|O_A O_B|)$ is trivial, we need to prove

$$|\mathrm{tr}\left(\rho^{1-\alpha} O_A \rho^\alpha O_B\right)| \le \frac{\mathrm{tr}(\rho|O_A|^2) + \mathrm{tr}(\rho|O_B|^2)}{2}. \tag{C14}$$

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

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

Using the Hölder inequality, we obtain

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

where we use $O_A O_A^\dagger = |O_A|^2$ in the last equation. By applying the inequality (C16) to (C15), we prove the inequality (C14). Therefore, we prove the inequality (C13).

We then consider the non-trivial upper bound given in Theorem 13, which utilizes the properties of the 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 [190]. To prove Theorem 13, we necessarily avoid directly treating the imaginary time evolution. The condition $\alpha \in [0,1]$ is utilized for this purpose. For $\alpha \notin [0,1]$, we cannot avoid the unboundedness of the norm of $e^{\beta\alpha H} O_A e^{-\beta\alpha H}$. This point is reflected that the function $g_{\alpha,\beta}(t)$ in (C20) converges only for $\alpha \in [0,1]$.

For this purpose, we transform the imaginary time evolution in a proper manner. Using the notation of Eq. (A1), we have

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

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

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

where we use Eq. (A3) in the last equation. Hence, using the identity $\mathrm{tr}\left([O_A, O_B] O_3\right) = \mathrm{tr}\left(O_A [O_B, O_3]\right)$, we obtain

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

From Eq. (A3), we consider

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

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

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

where the proof of the second equation is given in Sec. C 3 a. From the above form, we have

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

By combining Eqs. (C18) and (C19) with the inequality (C21), we obtain the following:

$$\begin{aligned}
&\left|Q_{\rho_\beta}^{(\alpha)}(O_A, O_B)\right| = \left|\int_{-\infty}^{\infty} g_{\alpha,\beta}(t) \mathrm{tr}\left(\rho_\beta [O_A(t), O_B]\right) dt\right| \\
&\le 2\beta^{-1} \int_{-\infty}^{\infty} \frac{e^{-2\pi|t|/\beta}}{1 - e^{-2\pi|t|/\beta}} \|[O_A(t), O_B]\| dt,
\end{aligned} \tag{C22}$$

where we use $\mathrm{tr}\left(\rho[O_A(t), O_B]\right) \le \|[O_A(t), O_B]\|$.

Using the Lieb-Robinson bound (15), we obtain

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

and we show the proof in Sec. C 3 b. For $R \le \xi'_\beta/2$, the RHS in (C23) is larger than the trivial upper bound (C13). Hence, we must consider $R \ge \xi'_\beta/2$, which yields

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

By applying the above inequality to (C22), we prove Theorem 13. □

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

We prove the equation (C20). For the proof, we rewrite the integral as follows:

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

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

We first consider the case of $t<0$. Then, using the residue theorem, we get

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

where $\mathrm{Res}_{\omega=(2\pi i m)/\beta}$ is the residue at $\omega=(2\pi i m)/\beta$. Because of

$$i\mathrm{Res}_{\omega=(2\pi i m)/\beta}\left(\frac{1-e^{\alpha\beta\omega}}{1-e^{\beta\omega}}e^{-i\omega t}\right) = i\beta^{-1}e^{2\pi m t/\beta}(-1+e^{2\pi i m\alpha}), \tag{C27}$$

we reduce Eq. (C26) to

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

In the same manner, we obtain

$$\frac{1}{2\pi}\int_{C_+}\frac{1-e^{\alpha\beta\omega}}{1-e^{\beta\omega}}e^{-i\omega t}d\omega = -i\sum_{m=1}^{\infty}\mathrm{Res}_{\omega=-(2\pi i m)/\beta}\left(\frac{1-e^{\alpha\beta\omega}}{1-e^{\beta\omega}}e^{-i\omega t}\right) = -i\beta^{-1}\sum_{m=1}^{\infty}e^{-2\pi m t/\beta}(-1+e^{-2\pi i m\alpha}). \tag{C29}$$

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

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

This completes the proof of Eq. (C20). □

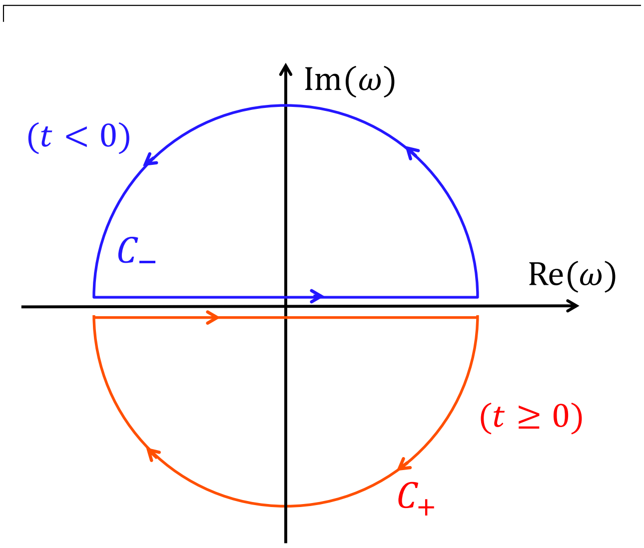

FIG. 3. Schematic picture of the integral paths in Eq. (C25).

b. Proof of the inequality (C23)

We first consider the decomposition

$$\int_{-\infty}^{\infty}\frac{e^{-2\pi|t|/\beta}}{1-e^{-2\pi|t|/\beta}}\|[O_A(t),O_B]\|dt \le \int_{|t|>t_0}\frac{e^{-2\pi|t|/\beta}}{1-e^{-2\pi|t|/\beta}}\|[O_A(t),O_B]\|dt + \int_{|t|\le t_0}\frac{e^{-2\pi|t|/\beta}}{1-e^{-2\pi|t|/\beta}}\|[O_A(t),O_B]\|dt, \tag{C30}$$

where we choose $t_0 := \mu R/(2v)$. For the first term in the RHS of (C30), from $1/(1-e^{-|x|}) \le 1+1/|x|$, we get

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

which yields

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

where we use $\|[O_A(t),O_B]\| \le 2\|O_A\|\cdot\|O_B\| = 2$ in the first inequality and use $\pi\mu/(v\beta) \ge \xi_\beta^{'-1} = \mu/[2+(v\beta)/\pi]$

in the last inequality. For the second term in the RHS of (C30), we use the Lieb-Robinson bound (15) as

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

which yields

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

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

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

where we use $e^{vt} - 1 = vt \int_0^1 e^{\lambda v t} d\lambda$ in the first inequality. The above inequality reduces the inequality (C33) to

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

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

By applying the inequalities (C32) and (C35) to Eq. (C30), we have the following:

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

which yields the inequality (C23). This competes the proof. □

Appendix D: Proof of Theorem 10

In this section, we prove one of our main theorems which gives the exponential decay of the quantum correlation defined by

$$\mathrm{QC}_\rho(O_A, O_B) := \inf_{\{p_s, \rho_s\}} \sum_s p_s |\mathrm{C}_{\rho_s}(O_A, O_B)|. \tag{D1}$$

In Theorem 10, we have proved the following inequality:

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

where ξ_β is a $\mathcal{O}(\beta)$ constant given in Eq. (54), and C_β has been given by $c_{\beta,1} + c_{\beta,2}$ with $c_{\beta,1}$ and $c_{\beta,2}$ defined in Eq. (54)

As a remark, 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 given in Claim 22.

1. Proof of Theorem 10

For an arbitrary quantum state ρ, we denote a spectral decomposition of ρ by

$$\rho = \sum_s \lambda_s |\lambda_s\rangle\langle\lambda_s|. \tag{D3}$$

In our proof, we aim to explicitly construct a set of ensemble $\{p_m, |\phi_m\rangle\}$ such that

$$\rho_\beta = \sum_m p_m |\phi_m\rangle\langle\phi_m|, \tag{D4}$$

which satisfies the inequality (33). To prove the statements, we take the following five steps. In the first and the second lemma (Lemmas 17 and 18), we consider the generic quantum states and give general statements on the quantum correlations. In the third section, the fourth and fifth lemmas (Lemmas 19, 20 and 21), we utilize the property of the quantum Gibbs states to upper-bound the quantum correlations.

In the first step, we prove the general upper bound for the quantum correlation as follows:

Lemma 17. *For an arbitrary operator O, let us define $\mathcal{L}_O$ as follows:*

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

Then, for the two operators O_A and O_B, if we have

$$[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0, \tag{D6}$$

the quantum correlation is bound from above as follows:

$$\begin{aligned}&\mathrm{QC}_\rho(O_A, O_B) \\ &\le \frac{1}{4} \left\| \left[\left(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}\right), \left(\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2}\right) \right] \right\|. \end{aligned} \tag{D7}$$

Usually, the condition (D6) is not satisfied. In the second lemma, we consider the case where Eq. (D6) holds only in an approximate sense. Then, we prove the following lemma:

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

$$[\tilde{\mathcal{L}}_{O_A}, \tilde{\mathcal{L}}_{O_B}] = 0 \tag{D8}$$

and

$$\|\mathcal{L}_{O_A} - \tilde{\mathcal{L}}_{O_A}\| \le \delta_1, \quad \|\mathcal{L}_{O_B} - \tilde{\mathcal{L}}_{O_B}\| \le \delta_2, \tag{D9}$$

we upper-bound the quantum correlation $\mathrm{QC}_\rho(O_A, O_B)$ as follows:

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

The remaining task is to upper-bound 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 show an integral form of $\mathcal{L}_O$ which comprises the time evolution of $t \approx \beta$. We prove the following lemma on the basic properties of the operator $\mathcal{L}_O$:

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:*

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

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

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

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

$$\|\mathcal{L}_O\| \le \|O\|. \tag{D13}$$

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 $t \approx \beta$. Using this fact, we can apply the Lieb-Robinson bound to prove the quasi-locality 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, we prove the following lemma which gives the upper bounds for δ_1 and δ_2:

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

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

This lemma gives the upper bound of the first term of the RHS in the inequality (D10) as follows:

$$\frac{3\delta_1 + 3\delta_2}{2} \le c_{\beta,1}(|\partial A| + |\partial B|) e^{-R/\xi_\beta}, \tag{D15}$$

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

Before detailing the estimation of the second term of the RHS of (D10), we show that for $R-2 \le \xi_\beta$, the upper bound (D15) results in a trivial upper bound for $\mathrm{QC}_\rho(O_A, O_B)$. Indeed, for $R - 2 \le \xi_\beta$, we have

$$\begin{aligned} &c_{\beta,1}(|\partial A| + |\partial B|) e^{-R/\xi_\beta} \ge c_{\beta,1} e^{-R/\xi_\beta} \\ &\ge e^{-(R-2)/\xi_\beta} \frac{12}{\pi} \ge \frac{12}{e\pi} \approx 1.4052, \end{aligned} \tag{D16}$$

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

The final task is to estimate the commutator

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

We need to characterize the quasi-locality of $\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}$. For $\rho = e^{-\beta H}$, it is given by the imaginary time-evolution of $\mathcal{L}_{O_A}$. For a large β, the unboundedness of imaginary time evolution usually occurs [190]. In fact, due to the specialty of $\mathcal{L}_{O_A}$, we can avoid such an unboundedness and prove the following lemma:

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

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

where we use $R - 2 > \xi_\beta$ in the second inequality.

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

$$\|\mathrm{ad}_H(O_X)\| \le \sum_{i \in X} \sum_{Z: Z \ni i} \|\mathrm{ad}_{h_Z}(O_X)\| \le 2 \sum_{i \in X} \sum_{Z: Z \ni i} \|h_Z\| \cdot \|O_X\| \le 2g|X|. \tag{D19}$$

Hence, using $\log(1+xy) \le \log(1+y) + \log(x)$ for $x \ge 1$ and $y \ge 0$, we have

$$
\begin{aligned}
&|\partial A|\Big(2+\log(1+\beta\|\mathrm{ad}_H(O_B)\|)\Big) + |\partial B|\Big(2+\log(1+\beta\|\mathrm{ad}_H(O_A)\|)\Big) \\
&\le (|\partial A|+|\partial B|)\Big(2+\log(1+2g\beta|AB|)\Big) \\
&\le (|\partial A|+|\partial B|)\left(\frac{2+\log(1+2g\beta)+\log|AB|}{\log|AB|+1}\right)(\log|AB|+1) \\
&\le (|\partial A|+|\partial B|)[3+\log(1+2g\beta)](\log|AB|+1).
\end{aligned} \tag{D20}
$$

By combining the above inequality with (D18), we upper-bound the second term of the RHS in the inequality (D10) by

$$
\frac{1}{4}\left\|\left[\left(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}\right),\left(\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2}\right)\right]\right\| \le c_{\beta,2}(|\partial A|+|\partial B|)(1+\log|AB|)e^{-R/\xi_\beta}, \tag{D21}
$$

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

By applying the inequalities (D15) and (D21) to Lemma 18, we obtain the desired inequality (D2). This completes the proof of Theorem 10. □

2. Proof of Lemma 17

In this proof, we utilize the techniques outlined in Ref. [191]. Let $\{|\psi_m\rangle\}$ be a set of orthonormal quantum states. We define the unitary matrix U which gives the quantum states $\{|\psi_m\rangle\}$ in the base of $\{|\lambda_s\rangle\}_s$:

$$
|\psi_m\rangle = \sum_s U_{m,s}|\lambda_s\rangle. \tag{D22}
$$

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

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

we rewrite the density operator ρ as

$$
\rho = \sum_m p_m|\phi_m\rangle\langle\phi_m|. \tag{D24}
$$

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

$$
\mathrm{QC}_\rho(O_A,O_B) \le \sum_m p_m|\mathrm{C}_{|\phi_m\rangle}(O_A,O_B)|, \tag{D25}
$$

where $\mathrm{C}_{|\phi_m\rangle}(O_A,O_B)$ has been defined as a standard correlation function, i.e., $\mathrm{C}_{|\phi_m\rangle}(O_A,O_B) = \langle\phi_m|O_AO_B|\phi_m\rangle - \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle$. Our task is to find a good set $\{|\psi_m\rangle\}$ such that $\{|\phi_m\rangle\}$ has a small correlation for O_A and O_B.

For an arbitrary operator O, we obtain

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

where we use the definition (D5) of $\mathcal{L}_O$ from the second equation to the third equation. We here show the definition again for the convenience of the readers:

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

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

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

and $\langle\phi_m|O_B|\phi_m\rangle = \alpha_{2,m}$, where we define $\alpha_{1,m}$ and $\alpha_{2,m}$ as the mth eigenstates of $\mathcal{L}_{O_A}$ and $\mathcal{L}_{O_B}$, respectively. We therefore obtain

$$
\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle = \alpha_{1,m}\alpha_{2,m} \tag{D29}
$$

for an arbitrary m.

We next consider $\langle\phi_m|O_AO_B|\phi_m\rangle$. From Eq. (D26), we immediately obtain

$$
\langle\phi_m|O_AO_B|\phi_m\rangle = \frac{1}{2p_m}\langle\psi_m|\{\rho,\mathcal{L}_{O_AO_B}\}|\psi_m\rangle. \tag{D30}
$$

From the equation, if we could obtain $\mathcal{L}_{O_AO_B} = \mathcal{L}_{O_A}\mathcal{L}_{O_B}$, we would be able to easily prove $\langle\phi_m|O_AO_B|\phi_m\rangle = \alpha_{1,m}\alpha_{2,m}$ in the same way as Eq. (D28). However, the challenging point is that we have $\mathcal{L}_{O_AO_B} \ne \mathcal{L}_{O_A}\mathcal{L}_{O_B}$ in general and need to take a different route.

For the purpose, we first consider

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

where we use $\mathcal{L}_{O\rho^{-1/2}} = \mathcal{L}_O\rho^{-1/2}$ from the definition (D5).

We then obtain

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

where we use $\sum_{m'}|\psi_{m'}\rangle\langle\psi_{m'}| = 1$. We further reduce Eq. (D32) to

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

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 reduces to

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

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

The remaining task is to estimate the error as

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

To obtain this, we consider

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

where we use $\mathcal{L}_{O_A}|\psi_m\rangle = \alpha_{1,m}|\psi_m\rangle$, $\mathcal{L}_{O_B}|\psi_m\rangle = \alpha_{2,m}|\psi_m\rangle$ from the second equation to the third equation. By applying Eq. (D36) to Eq. (D34), we finally obtain

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

By combining the above inequality and Eq. (D29) with (D25), we prove the inequality (D7). This completes the proof. □

3. Proof of Lemma 18

In this proof, we take the same approach as the proof of Lemma 17. We here choose $\{|\psi_m\rangle\}$ as the simultaneous eigenstates of $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$ instead of $\mathcal{L}_{O_A}$ and

$\mathcal{L}_{O_B}$:

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

We then have the same inequality as (D25):

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

We begin by estimating $\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle$. By using Eq. (D26), we have

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

where we define $\delta\mathcal{L}_{O_A} := \mathcal{L}_{O_A} - \tilde{\mathcal{L}}_{O_A}$. In the same way, we have $\langle\phi_m|O_B|\phi_m\rangle = \tilde{\alpha}_{2,m} + \frac{1}{2p_m}\langle\psi_m|\{\rho, \delta\mathcal{L}_{O_B}\}|\psi_m\rangle$. We thus obtain

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

which yields

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

For an arbitrary operator O, we have $|\langle\psi_m|O|\psi_m\rangle| \leq \langle\psi_m|\ |O|\ |\psi_m\rangle$, and hence,

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

where we use $\mathrm{tr}(|O|) = \|O\|_1$, $\|O+O'\|_1 \leq \|O\|_1 + \|O'\|_1$ and $\|OO'\|_1 \leq \|O\|_1 \cdot \|O'\|$ for arbitrary operators O and O'. By applying the inequality (D43) to (D41), we obtain

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

We next estimate the error which comes from $\langle\phi_m|O_AO_B|\phi_m\rangle$. We start from the same equation as Eq. (D34):

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

where in the second equation we use Eq. (D36) as follows:

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

In Eq. (D45), we have

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

In the same way, we obtain

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

Using the above equations, we reduce Eq. (D45) to

$$\langle\phi_m|O_AO_B|\phi_m\rangle = \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m} + \frac{1}{4p_m}\langle\psi_m|(\rho\delta\mathcal{L}_{O_A}\mathcal{L}_{O_B} + \delta\mathcal{L}_{O_A}\rho\mathcal{L}_{O_B} + \mathcal{L}_{O_A}\delta\mathcal{L}_{O_B}\rho + \delta\mathcal{L}_{O_B}\rho\mathcal{L}_{O_A})|\psi_m\rangle$$
$$+ \frac{1}{4}\langle\phi_m|\left[\left(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}\right), \left(\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2}\right)\right]|\phi_m\rangle, \tag{D49}$$

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

$$\sum_m p_m|\langle\phi_m|O_AO_B|\phi_m\rangle - \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m}|$$
$$\leq \frac{1}{2}\left(\|\delta\mathcal{L}_{O_A}\|\cdot\|\mathcal{L}_{O_B}\| + \|\mathcal{L}_{O_A}\|\cdot\|\delta\mathcal{L}_{O_B}\|\right) + \frac{1}{4}\left\|\left[\left(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}\right), \left(\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2}\right)\right]\right\|, \tag{D50}$$

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

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

By combining the inequalities (D44) and (D51), we finally obtain

$$\sum_m p_m|\langle\phi_m|O_AO_B|\phi_m\rangle - \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle|$$
$$= \sum_m p_m\left|\langle\phi_m|O_AO_B|\phi_m\rangle - \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m} - \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle + \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m}\right|$$
$$\leq \sum_m p_m\left(|\langle\phi_m|O_AO_B|\phi_m\rangle - \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m}| + p_m\left|\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle - \tilde{\alpha}_{1,m}\tilde{\alpha}_{2,m}\right|\right)$$
$$\leq \frac{3\delta_1+3\delta_2}{2} + \frac{1}{4}\left\|\left[\left(\rho^{-1/2}\mathcal{L}_{O_A}\rho^{1/2}\right), \left(\rho^{1/2}\mathcal{L}_{O_B}\rho^{-1/2}\right)\right]\right\|. \tag{D52}$$

By applying the above inequality to (D39), we prove the main inequality (D10). This completes the proof. □

4. Proof of Lemma 19

We first rewrite the eigenvalues $\{\lambda_s\}$ and the eigenstates $\{|\lambda_s\rangle\}$ as

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

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

$$\mathcal{L}_O = \sum_{s,s'}\frac{2\sqrt{e^{-\beta(E_s-E'_s)}}}{1+e^{-\beta(E_s-E'_s)}}\langle E_s|O|E_{s'}\rangle|E_s\rangle\langle E_{s'}|$$
$$= \int_{-\infty}^{\infty}\frac{2\sqrt{e^{-\beta\omega}}}{1+e^{-\beta\omega}}O_\omega d\omega, \tag{D54}$$

where we use the notation of Eq. (A1).

Using Eq. (A2), we reduce the above form to

$$\mathcal{L}_O = \int_{-\infty}^{\infty}\frac{2\sqrt{e^{-\beta\omega}}}{1+e^{-\beta\omega}}\frac{1}{2\pi}\int_{-\infty}^{\infty}O(t)e^{-i\omega t}dtd\omega$$
$$= \int_{-\infty}^{\infty}f_\beta(t)O(t)dt, \tag{D55}$$

with

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

By following the same analysis in Sec. C 3 a, we can prove that $f_\beta(t)$ is given by

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

This completes the proof of Eq. (D11).

The proof of the inequality (D13) is simply given as follows. Because of $f_\beta(t)\geq 0$, we have

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

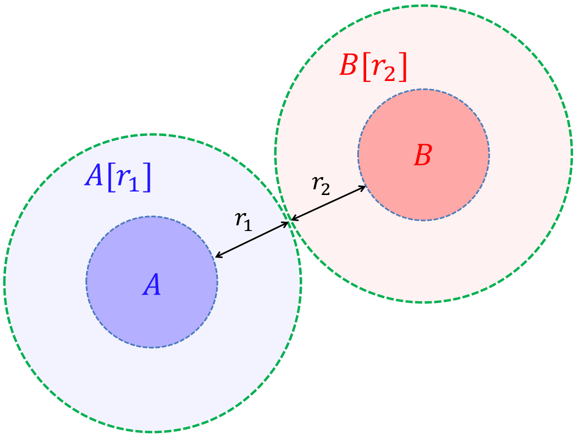

FIG. 4. Approximations of $\mathcal{L}_{O_A}$ and $\mathcal{L}_{O_B}$. In order to obtain the approximations $\tilde{\mathcal{L}}_{O_A}$ and $\tilde{\mathcal{L}}_{O_B}$ which commute with each other, we approximate $\mathcal{L}_{O_A}$ and $\mathcal{L}_{O_B}$ onto the extended regions $A[r_1]$ and $B[r_2]$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

Using the inverse Fourier transform

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

with $\omega=0$, we reduce the inequality (D57) to (D13). This completes the proof. $\square$

5. Proof of Lemma 20

We first show 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, we use Eq. (D11) in Lemma 19 and approximate the time-evolved operator $O_A(t)$ on $A[r_1]$, which yields

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

where the notation of $O_A(t,A[r_1])$ has been given in Eq. (16), and we choose r_1 appropriately. Note that $\tilde{\mathcal{L}}_{O_A}$ is now supported on the subset $A[r_1]$. In the same way, we define $\tilde{\mathcal{L}}_{O_A}$ as

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

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

Using Eq. (D59), we can estimate δ_1 as

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

For the estimation of the integral, we use a similar approach in Sec. C 3 b. We start from

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

where we choose $t_0 := \mu r_1/(2v)$. Because of

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

the first term is upper-bounded as

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

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

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

where we use $(e^{xy}-1)/x \le y(1+e^{xy})$ $(y\ge 0)$ in the third inequality. By applying the inequalities (D64) and (D65), we reduce Eq. (D62) to

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

where we use $r_1 \ge 1$. In the same way, we obtain

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

By applying $r_1=r_2=\lceil R/2-1\rceil$, we prove the inequality (D14). This completes the proof. $\square$

6. Proof of Lemma 21

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

$$e^{\pm\beta H/2} O_\omega e^{\mp\beta H/2} = e^{\pm\beta\omega/2} O_\omega, \tag{D68}$$

we have from Eq. (D54)

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

Using Eq. (A2), we reduce the above equation to

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

where we define $g_\beta(t)$ as

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

We have

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

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

As in Sec. C 3 a, we have

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

We thus obtain

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

For the proof of the lemma, we must prove the following two claims:

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*

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

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*

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

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

Using these claims, we can immediately upper-bound the norm of (D17). Let us approximate

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

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

$$\begin{aligned}
\|[\mathfrak{O}_1,\mathfrak{O}_2]\| &= \left\|[\mathfrak{O}_1 - \mathfrak{O}_{1,A[r_1]}, \mathfrak{O}_2] + [\mathfrak{O}_{1,A[r_1]}, \mathfrak{O}_2 - \mathfrak{O}_{2,B[r_2]}]\right\| \\
&\le 2\|\delta\mathfrak{O}_1\|\cdot\|\mathfrak{O}_2\| + 2\|\delta\mathfrak{O}_2\|\cdot\|\mathfrak{O}_1\| + 2\|\delta\mathfrak{O}_1\|\cdot\|\delta\mathfrak{O}_2\|,
\end{aligned} \tag{D78}$$

where we define $\delta\mathfrak{O}_1 := \mathfrak{O}_1 - \mathfrak{O}_{1,A[r_1]}$ and $\delta\mathfrak{O}_2 := \mathfrak{O}_2 - \mathfrak{O}_{2,B[r_2]}$, and use $\left\|\mathfrak{O}_{1,A[r_1]}\right\| \le \|\mathfrak{O}_1\| + \|\delta\mathfrak{O}_1\|$ in the inequality. For $\|\delta\mathfrak{O}_s\| > \|\mathfrak{O}_s\|$ ($s=1,2$), the above inequality is worse than the trivial inequality, i.e., $\|[\mathfrak{O}_1,\mathfrak{O}_2]\| \le 2\|\mathfrak{O}_1\|\cdot\|\mathfrak{O}_2\|$. Hence, we only must consider $\|\delta\mathfrak{O}_s\| \le \|\mathfrak{O}_s\|$, which yields

$$\|[\mathfrak{O}_1,\mathfrak{O}_2]\| \le 3\left(\|\delta\mathfrak{O}_1\|\cdot\|\mathfrak{O}_2\| + \|\delta\mathfrak{O}_2\|\cdot\|\mathfrak{O}_1\|\right). \tag{D79}$$

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

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

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

a. *Proof of Claim 22*

From the integral expression (D74), we first obtain

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

In a standard approach, we use

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

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

To obtain a refined bound, we parametrize $O(t)$ as $O(\lambda t)$ using a parameter λ. We then obtain

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

which yields

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

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

$$\left\|\int_{-\infty}^{\infty} g_\beta(t)O(t)dt\right\| \le \frac{2\|O\|}{\pi}\log\left(1+\frac{2\beta\|\mathrm{ad}_H(O)\|}{\pi\|O\|}\right) + \frac{2\|O\|}{\pi}, \tag{D85}$$

By combining the inequalities (D81) and (D85) with $2/\pi \le 1$, we prove the inequality (D75). $\square$

b. *Proof of Claim 23*

As in the proof of Lemma 20, we consider the approximation as Using the integral expression (D74), we have

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

which yields

$$\left\|\rho^{\pm 1/2}\mathcal{L}_O\rho^{\mp 1/2} - \left(\rho^{\pm 1/2}\mathcal{L}_O\rho^{\mp 1/2}\right)_{X[r]}\right\| \le \int_{-\infty}^{\infty}|g_\beta(t)|\cdot\|O(t, X[r]) - O(t)\|\,dt. \tag{D87}$$

Using $1/\sinh(x) \le 2e^{-x}(1+1/x)$ $(x \ge 0)$, we have

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

In addition, the Lieb-Robinson bound (18), we have

$$\|O(t) - O_X(t, X[r])\| \le \min\left(C|\partial X|\left(e^{v|t|} - 1\right)e^{-\mu r}, 2\right) \tag{D89}$$

Then, we can apply the same analyses as (C32), (C33) and (C35). For $t_0 = \mu r/(2v)$, we can obtain

$$\begin{aligned}
&\int_{-\infty}^{\infty} |g_\beta(t)| \cdot \|O(t, X[r]) - O(t)\|\, dt \\
&\le \int_{|t|>t_0} \frac{2e^{-\pi|t|/\beta}}{\beta}\left(1 + \frac{1}{\pi|t|/\beta}\right) \cdot 2dt + \int_{|t|\le t_0} \frac{2e^{-\pi|t|/\beta}}{\beta}\left(1 + \frac{1}{\pi|t|/\beta}\right) \cdot C|\partial X|\left(e^{v|t|} - 1\right)e^{-\mu r}dt \\
&\le \frac{8e^{-\pi t_0/\beta}}{\pi}\left(1 + \frac{1}{\pi t_0/\beta}\right) + \frac{4C}{\beta}|\partial X|\left(\frac{1}{v} + \frac{1}{\pi/\beta}\right)e^{-\mu R + vt_0} \\
&\le |\partial X|\left[\frac{8}{\pi}\left(1 + \frac{2v\beta}{\pi\mu r}\right)e^{-\pi\mu r/(2v\beta)} + 4C\left(\frac{1}{\pi} + \frac{1}{v\beta}\right)e^{-\mu r/2}\right] \le |\partial X|\left[\frac{8}{\pi}\left(1 + \frac{\xi_\beta}{2r}\right) + 4C\left(\frac{1}{\pi} + \frac{1}{v\beta}\right)\right]e^{-2r/\xi_\beta},
\end{aligned}$$

where we use the definition of $\xi_\beta := 4/\mu(1 + v\beta/\pi)$ in the last inequality. This completes the proof of Claim 23. □

Appendix E: Proof of Proposition 9

We here show the proof of Proposition 9 which connects the PPT relative entanglement and the quantum correlation. When the quantum correlation satisfies the following:

$$\mathrm{QC}_{\rho_{AB}}(O_A, O_B) \le \epsilon\|O_A\| \cdot \|O_B\| \tag{E1}$$

for arbitrary two operators O_A and O_B, Proposition 9 gives

$$E_R^{\mathrm{PPT}}(\rho_{AB}) \le 4\mathcal{D}_{AB}\bar{\delta}\log(1/\bar{\delta}) \le 4\mathcal{D}_{AB}\bar{\delta}^{1/2}, \tag{E2}$$

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

1. Proof

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

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

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

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

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

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

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

$$E_R^{\mathrm{PPT}}(\rho_{AB}) \le S(\rho_{AB}||\tilde{\sigma}_{AB}). \tag{E5}$$

Using the continuity bound on the relative entropy [192, Theorem 3] (or Ref. [78]), we have

$$\begin{aligned}
S(\rho_{AB}||\tilde{\sigma}_{AB}) \le &\delta_{AB}\log(\mathcal{D}_{AB}) - \delta_{AB}\log(\delta_{AB}) \\
&- \delta_{AB}\log[\lambda_{\min}(\tilde{\sigma}_{AB})],
\end{aligned} \tag{E6}$$

under the assumption of $\delta_{AB} \le 1/e$, where we define $\delta_{AB} := \|\rho_{AB} - \tilde{\sigma}_{AB}\|_1$ and $\lambda_{\min}(\tilde{\sigma}_{AB})$ is the minimum eigenvalue of $\tilde{\sigma}_{AB}$. From the definition (E4), we have $\lambda_{\min}(\tilde{\sigma}_{AB}) \ge \delta$ and

$$\delta_{AB} \le 2\mathcal{D}_{AB}\delta, \tag{E7}$$

and hence the inequality (E8) reduces to

$$\begin{aligned}
S(\rho_{AB}||\tilde{\sigma}_{AB}) &\le -2\mathcal{D}_{AB}\delta\log(2\delta^2) \\
&\le -4\mathcal{D}_{AB}\delta\log(\delta),
\end{aligned} \tag{E8}$$

which gives a trivial upper bound for $\delta > 1/e$. By combining the above inequality with (E5) and the upper bound (E3), we prove the main inequality (52). This completes the proof. □

2. Proof of Lemma 24

Our task now is to estimate

$$\min_i\langle\eta_i|\rho_{AB}^{T_A}|\eta_i\rangle = \inf_{|\eta\rangle}\mathrm{tr}\left(\rho_{AB}^{T_A}P_\eta\right). \tag{E9}$$

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

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

and prove the second term is 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 [93], we choose the basis which gives the Schmidt decomposition of $|\eta\rangle$ as follows:

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

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

To verify the point, we first consider the qubit case, i.e., $\mathcal{D}_A = \mathcal{D}_B = 2$. We can prove the following lemma:

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

$$\left|\mathrm{tr}\left[\rho_{AB}(P_\eta^{T_A} - P_\eta)\right]\right| \le 2\epsilon, \tag{E11}$$

where the parameter ϵ is given in (E1).

To generalize the results of two qubit to two qudit systems, we 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

$$\nu_s\nu_{s'}(-|s_A,s_B\rangle\langle s'_A,s'_B| + |s'_A,s_B\rangle\langle s_A,s'_B|) + \text{h.c.} = (\nu_s^2+\nu_{s'}^2)\left(|\eta_{s,s'}\rangle\langle\eta_{s,s'}|^{T_A} - |\eta_{s,s'}\rangle\langle\eta_{s,s'}|\right), \tag{E12}$$

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. We thus obtain from Lemma 25

$$\left|\mathrm{tr}\left[\rho_{AB}\left(|\eta_{s,s'}\rangle\langle\eta_{s,s'}|^{T_A} - |\eta_{s,s'}\rangle\langle\eta_{s,s'}|\right)\right]\right| \le 2\epsilon, \tag{E13}$$

which yields

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

We thus obtain

$$\mathrm{tr}\left(\rho_{AB}P_\eta^{T_A}\right) \ge \mathrm{tr}\left(\rho_{AB}P_\eta\right) - 4\epsilon\mathcal{D}_A \ge -4\epsilon\mathcal{D}_A, \tag{E15}$$

where we use $\mathrm{tr}\left(\rho_{AB}P_\eta\right) \ge 0$ in the second inequality. By using the above inequality, we have

$$\inf_{|\eta\rangle}\mathrm{tr}\left(\rho_{AB}^{T_A}P_\eta\right) \ge -4\epsilon\mathcal{D}_A. \tag{E16}$$

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

$$\delta \le 4\epsilon\min(\mathcal{D}_A,\mathcal{D}_B). \tag{E17}$$

By using it, we reduce the inequality (G4) 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

$$O_{AB} = \sum_{P=x,y,z}(J_P\hat\sigma_{1,P}\hat\sigma_{2,P} + h_{1,P}\hat\sigma_{1,P} + h_{2,P}\hat\sigma_{2,P}) \tag{E18}$$

by appropriately choosing the bases (see Ref. [193, Lemma 1] for 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 $\hat\sigma_{1,y} \to -\hat\sigma_{1,y}$, and hence,

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

In this way, we can always write

$$P_\eta^{T_A} - P_\eta = \Phi_A\otimes\Phi_B, \tag{E20}$$

where we can make $\|\Phi_A\| \le 2$ and $\|\Phi_B\| = 1$ because of $\|P_\eta^{T_A} - P_\eta\| \le 2$. Then, from the condition (E1) and the inequality (37) in Lemma 5, we get

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

which yields

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

where $\{\rho_{s,A}\}_s$ and $\{\rho_{s,B}\}_s$ are the reduced density matrices of $\{\rho_{s,AB}\}_s$ which are appropriately chosen.

We here aim to prove

$$\mathrm{tr}\left[\rho_A\otimes\rho_B(P_\eta^{T_A} - P_\eta)\right] = 0 \tag{E22}$$

for arbitrary ρ_A and ρ_B. Let u_A and u_B be unitary matrices which diagonalize ρ_A and ρ_B, respectively. We then obtain

$$\begin{aligned}&\mathrm{tr}\left[\rho_A\otimes\rho_B(P_\eta^{T_A} - P_\eta)\right] \\ &= \mathrm{tr}\left[\tilde\rho_A\otimes\tilde\rho_B(u_A\otimes u_B)(P_\eta^{T_A} - P_\eta)(u_A\otimes u_B)^\dagger\right] \\ &= \mathrm{tr}\left[\tilde\rho_A\otimes\tilde\rho_B(\tilde P_\eta^{\dagger_A} - \tilde P_\eta)\right],\end{aligned} \tag{E23}$$

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), we have $P_\eta^{T_A} = P_\eta^{\dagger_A}$ with $\dagger_A$ being the partial conjugate transpose, which gives

$$(u_A\otimes u_B)P_\eta^{\dagger_A}(u_A\otimes u_B)^\dagger = \tilde P_\eta^{\dagger_A}. \tag{E24}$$

In Eq. (E23), only the diagonal terms of $(\tilde P_\eta^{\dagger_A} - \tilde P_\eta)$ contribute to the value since $\tilde\rho_A\otimes\tilde\rho_B$ is a diagonal matrix. It is easy to see that all the diagonal terms in $(\tilde P_\eta^{\dagger_A} - \tilde P_\eta)$ is equal to zero, and hence, we conclude that Eq. (E23) reduces to Eq. (E22). By applying Eq. (E22) to the inequality (E21), we obtain the main inequality (E11). This completes the proof. □

Appendix F: Proof of Theorem 12

We here give the full proof of Theorem 12, where the following inequality has been obtained for one-dimensional quantum Gibbs states:

$$E_R^{\rm PPT}(\rho_{\beta,AB}) \le \bar{C}_\beta \log(\mathcal{D}_{AB}) e^{-R/[16\log(d_0)\xi_\beta^2]+7gk\beta}, \tag{F1}$$

where $\bar{C}_\beta := 20\left(\tilde{C}_\beta + 16 d_0^4 C_\beta\right)^{1/2}$ with C_β and $\tilde{C}_\beta$ defined in Eqs. (54) and (57), respectively. Here, the assumption of the finite interaction length has been imposed for Hamiltonian H.

1. Proof

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

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

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

$$h_{\partial A_1} = \sum_{Z: Z\cap A_1 \neq \emptyset, Z\cap A_2 \neq \emptyset} h_Z,$$
$$h_{\partial B_1} = \sum_{Z: Z\cap B_1 \neq \emptyset, Z\cap B_2 \neq \emptyset} h_Z. \tag{F3}$$

Then, we formally describe the quantum Gibbs state ρ_β as

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

where Φ is an appropriate operator. We can prove that Φ is given by a quasi-local operator and is 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:*

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

where we define $\delta_{1,\ell} := \tilde{C}_\beta e^{-2\ell/\xi_\beta + 14gk\beta}$, and ξ_β is defined in Eq. (54) and

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

We also have

$$\|\tilde{\Phi}\| \le e^{2gk\beta}. \tag{F7}$$

In the following, we prove the main inequality (F1) based on the above two lemmas. For the purpose, we first define $\tilde{\rho}_\beta$ and $\tilde{Z}$ as follows:

$$\tilde{\rho}_\beta = \frac{e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}}{\tilde{Z}},$$
$$\tilde{Z} := \mathrm{tr}\left(e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}\right), \tag{F8}$$

Because we have

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

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

$$\tilde{\rho}_{\beta,AB} = \tilde{\rho}_{A_0A_1} \otimes \tilde{\rho}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1}. \tag{F10}$$

We here define $\tilde{\delta}$ for $\tilde{\rho}_{A_2B_2}$ in the same way as (E3), and define $\tilde{\sigma}_{A_2B_2}$ as

$$\tilde{\sigma}_{A_2B_2} = \tilde{\rho}_{A_2B_2} + \tilde{\delta} \cdot \hat{1}_{A_2B_2}. \tag{F11}$$

Using $\tilde{\sigma}_{A_2B_2}$ above, we define $\tilde{\sigma}_{AB}$ as

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

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

We can prove $\tilde{\sigma}_{AB}^{T_A} \succeq 0$ as follows. Because of $\tilde{\sigma}_{A_2B_2}^{T_A} \succeq 0$, we get

$$\left(\tilde{\rho}_{A_0A_1} \otimes \tilde{\sigma}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1}\right)^{T_A} \succeq 0. \tag{F13}$$

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

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

with $\tilde{\lambda}_i \ge 0$, we have

$$\begin{aligned} &\left(\tilde{\Phi} \tilde{\rho}_{A_0A_1} \otimes \tilde{\sigma}_{A_2B_2} \otimes \tilde{\rho}_{B_0B_1} \tilde{\Phi}^\dagger\right)^{T_A} \\ &= \sum_i \tilde{\lambda}_i \left(\Phi_{A_1,A_2}^* \otimes \Phi_{B_1,B_2}\right) |\tilde{\lambda}_i\rangle\langle\tilde{\lambda}_i| \left(\Phi_{A_1,A_2}^{T_A} \otimes \Phi_{B_1,B_2}^\dagger\right) \\ &\succeq 0. \end{aligned} \tag{F15}$$

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

$$\begin{aligned} &\|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1 \\ &\le \left\|\tilde{Z}\tilde{\Phi}\tilde{\rho}_{\beta,AB}\tilde{\Phi}^\dagger - \rho_{\beta,AB}\right\|_1 + \left\|\tilde{Z}\tilde{\Phi}\tilde{\rho}_{\beta,AB}\tilde{\Phi}^\dagger - \tilde{\sigma}_{AB}\right\|_1. \end{aligned} \tag{F16}$$

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

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

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

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

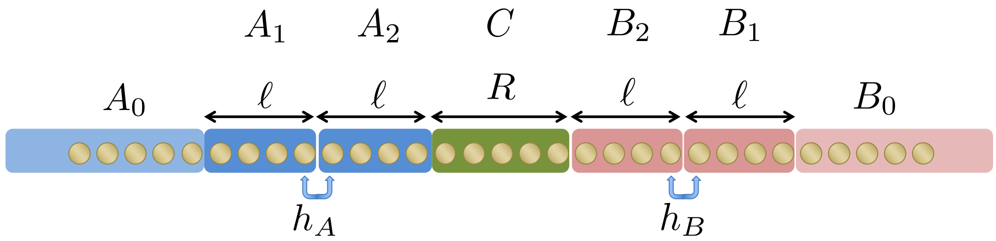

FIG. 5. For the proof, we decompose subsets A and B into three pieces. The decomposed subsets A_1, A_2, B_2, and B_1 are taken such that they have the same cardinality, i.e., $A_1 = A_2 = B_0 = B_1 = \ell$. We denote the interactions between the subsystems A_1 and A_2 (B_1 and B_2) by $h_{\partial A_1}$ ($h_{\partial B_1}$). 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. Using the quantum belief propagation, we prove that the effect of the regions A_0 and B_0 does not influence the entanglement value. Then, roughly speaking, the entanglement between A and B is characterized by the entanglement between A_1A_2 and B_1B_2. Because the size of these regions is 2ℓ, the dependence on the Hilbert space dimension in (55) is significantly improved.

where we use the inequality (F17) with $\|\rho_{\beta,AB}\|_1 = 1$ in deriving the first term of the RHS.

The remaining task is to estimate the parameters $\tilde{Z}$, $\tilde{\delta}$ and $Z_{\tilde{\sigma}}$. We can prove the following inequalities:

$$\tilde{Z} \le e^{4gk\beta}, \quad \tilde{\delta} \le \delta_{2,R},$$
$$\frac{1}{Z_{\tilde{\sigma}}} \le 1 + \delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}, \tag{F19}$$

where $\delta_{2,R} := 16 C_\beta e^{-R/\xi_\beta + 2\ell \log(d_0)}$.

Proof of inequalities in (F19). First, the first inequality in (F19) for the partition function $\tilde{Z}$ can be immediately derived using the Golden–Thompson inequality:

$$\begin{aligned}\tilde{Z} &= \mathrm{tr}\left(e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}\right) \\ &\le \mathrm{tr}\left(e^{-\beta H} e^{\beta(h_{\partial A_1} + h_{\partial B_1})}\right) \\ &\le \mathrm{tr}\left(e^{-\beta H}\right) e^{\beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|)} \le e^{4gk\beta},\end{aligned} \tag{F20}$$

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

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

$$\begin{aligned}\tilde{\delta} &\le 4 \min(\mathcal{D}_{A_2}, \mathcal{D}_{B_2}) \times C_\beta (|\partial A_2| + |\partial B_2|) \\ &\quad \times (1 + \log|A_2B_2|)\, e^{-R/\xi_\beta} \\ &\le 16 C_\beta e^{-R/\xi_\beta + 2\ell \log(d_0)} = \delta_{2,R},\end{aligned} \tag{F21}$$

where we use $|A_2| = |B_2| = \ell$, $|\partial A_2| = |\partial B_2| = 2$ and $1 + \log|A_2B_2| = 1 + \log(2\ell) \le d_0^\ell$ for $d_0 \ge 2$.

Finally, From Eq. (F12), we have

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

where in the last inequality, we use $\mathcal{D}_{A_2B_2} = d_0^{2\ell}$, $\tilde{Z} \le e^{4gk\beta}$ and $\left\|\tilde{\Phi}\right\| \le e^{2gk\beta}$ in (F7). Using $1/(1-x) \le 1 + x$ for $x \ge 0$, we can prove the third inequality in (F19) from the above inequality. This completes the proof of the inequalities (F19). □

By combining the inequalities (F18) and (F19), we obtain

$$\left\|\tilde{\Phi}\tilde{\rho}_{\beta,AB}\tilde{\Phi}^\dagger - \tilde{\sigma}_{AB}\right\|_1 \le \left(\delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}\right)(1 + \delta_{1,\ell}) + \delta_{2,R} e^{8gk\beta}\left(1 + \delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}\right). \tag{F23}$$

We then apply the inequalities (F17) and (F23) to (F16) and finally obtain

$$\begin{aligned}\|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1 &\le \min\left[2, \left(\delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}\right)\left(2 + \delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}\right)\right] \\ &\le 3\left(\delta_{1,\ell} + \delta_{2,R} d_0^{2\ell} e^{8gk\beta}\right),\end{aligned} \tag{F24}$$

where we use the trivial inequality of $\|\tilde{\sigma}_{AB} - \rho_{\beta,AB}\|_1 \le 2$. By choosing $\ell = \lceil R/(16\log(d_0)\xi_\beta) \rceil$, we obtain

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

Finally, we consider

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

which yields $\lambda_{\min}(\tilde{\sigma}'_{AB}) = \tilde{\delta}_{AB}\mathcal{D}_{AB}^{-1}$. Note that $\tilde{\sigma}'_{AB} \in$

PPT. We then obtain

$$\|\tilde{\sigma}'_{AB} - \rho_{\beta,AB}\|_1 \le 3\tilde{\delta}_{AB} + \|\tilde{\sigma}'_{AB} - \tilde{\sigma}_{AB}\|_1 \le 5\tilde{\delta}_{AB}. \tag{F27}$$

The inequality (E8) on the relative entropy gives

$$\begin{aligned} S(\rho_{\beta,AB}\|\tilde{\sigma}'_{AB}) &\le 5\tilde{\delta}_{AB}\log(\mathcal{D}_{AB}) - 5\tilde{\delta}_{AB}\log(5\tilde{\delta}_{AB}) \\ &\quad - 5\tilde{\delta}_{AB}\log[\lambda_{\min}(\tilde{\sigma}'_{AB})] \\ &\le 10\tilde{\delta}_{AB}\log\left(\mathcal{D}_{AB}\tilde{\delta}_{AB}^{-1}\right) \\ &\le 20\sqrt{\tilde{\delta}_{AB}}\log(\mathcal{D}_{AB}), \end{aligned} \tag{F28}$$

where we use $x\log(z/x) \le 2\sqrt{x}\log(z)$ for $0 \le x \le 2$ and $z \ge 2$. Because of $E_R^{\mathrm{PPT}}(\rho_{AB}) \le S(\rho_{\beta,AB}\|\tilde{\sigma}'_{AB})$, we prove the main inequality (F1) by applying the definition of $\tilde{\delta}_{AB}$ in (F25) to (F28). This completes the proof. □

a. *Proof of Lemma 26*

Using the quantum belief propagation [56], we can describe Φ as follows:

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

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

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

The explicit form of $f_\beta(t)$ can be calculated as follows [194, Eq. (103) in Supplementary Information]:

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

where we use $\log\left(\frac{e^x+1}{e^x-1}\right) \le 2/(e^x-1)$ and $1/(e^x-1) \le e^{-x}(1+x^{-1})$ for $x \ge 0$.

In the following sections, we adopt the following approximation:

$$\begin{aligned} &\tilde{\Phi} := \mathcal{T}e^{\int_0^1 \tilde{\phi}(\tau)d\tau}, \\ &\tilde{\phi}(\tau) := -\frac{\beta}{2}\int_{-\infty}^{\infty} F_\beta(t)\big[h_{\partial A_1}(H_\tau,t,A_1A_2) \\ &\qquad + h_{\partial B_1}(H_\tau,t,B_1B_2)\big]dt, \end{aligned} \tag{F31}$$

where we use the notation of Eq. (16). Here, $h_{\partial A_1}(H_\tau,t,A_1A_2)$ and $h_{\partial B_1}(H_{\tau'},t,B_1B_2)$ are supported on A_1A_2 and B_1B_2, respectively. Because of $[h_{\partial A_1}(H_\tau,t,A_1A_2), h_{\partial B_1}(H_{\tau'},t,B_1B_2)] = 0$, $\tilde{\Phi}$ is given by the form of

$$\tilde{\Phi} = \Phi_{A_1,A_2}\otimes\Phi_{B_1,B_2}. \tag{F32}$$

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

$$\left\|\Phi - \tilde{\Phi}\right\| \le e^{\int_0^1\left(\|\phi(\tau)\| + \|\tilde{\phi}(\tau)\|\right)d\tau}\int_0^1\left\|\phi(\tau) - \tilde{\phi}(\tau)\right\|d\tau, \tag{F33}$$

where we use the analysis in Ref. [45, Claim 25]. To estimate the RHS of (F33), we first consider

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

where we use $\|h_{\partial A_1}(H_\tau,t,A_1A_2)\| \le \|h_{\partial A_1}(H_\tau,t)\| = \|h_{\partial A_1}\|$ and $\int_{-\infty}^{\infty}F_\beta(t)dt = \tilde{F}(0) = 1$. Second, using the Lieb-Robinson bound (18), we have

$$\begin{aligned} &\|h_{\partial A_1}(H_\tau,t) - h_{\partial A_1}(H_\tau,t,A_1A_2)\| \\ &\le \|h_{\partial A_1}\|\min\left(2, 2C\left(e^{v|t|}-1\right)e^{-\mu(\ell-k)}\right), \end{aligned} \tag{F35}$$

where we use $|\partial\mathrm{Supp}(h_{\partial A_1})| = 2$ on a 1D chain, and we use the assumption that $h_{\partial A_1}$ has the interaction length k (i.e., $|\mathrm{Supp}(h_{\partial A_1})| \le 2k$). Note that $\|h_{\partial A_1}(H_\tau,t) - h_{\partial A_1}(H_\tau,t,A_1A_2)\|$ is trivially smaller than $2\|h_{\partial A_1}\|$.

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

$$\left\|\phi(\tau) - \tilde{\phi}(\tau)\right\| \le \frac{\beta(\|h_{\partial A_1}\| + \|h_{\partial B_1}\|)}{2}\int_{-\infty}^{\infty}F_\beta(t)\min\left(2, 2C\left(e^{v|t|}-1\right)e^{-\mu(\ell-k)}\right)dt. \tag{F36}$$

Because of the form of $F_\beta(t)$ in Eq. (F30), we can apply the same calculations as in Sec. C 3 b. For $t_0 = \mu\ell/(2v)$, we have

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

where we use the definition of $\xi_\beta := \frac{4}{\mu}\left(1+\frac{v\beta}{\pi}\right)$.

Because of inequality (F34), the LHS of (F37) is trivially smaller than 1. In contrast, for $\ell \le \xi_\beta/3$, the RHS of (F37) is larger than $20e^{-2/3}/\pi^2$, which is worse than the trivial upper bound. Hence, we need consider only the case of $\ell \ge \xi_\beta/3$, which reduces (F37) to

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

Using the upper bound of

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

we can reduce the inequalities (F34) and (F38) to

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

respectively. By applying the above inequalities to (F33), we obtain

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

Therefore, by letting $\tilde{\rho}_\beta := e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})}/\tilde{Z}$ with $\tilde{Z} = \mathrm{tr}(e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})})$, we obtain

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

where we use Eq. (F4), i.e., $e^{-\beta(H-h_{\partial A_1}-h_{\partial B_1})} = \Phi^{-1}\rho_\beta(\Phi^\dagger)^{-1}$. Using the above equation, we have

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

where we use the triangle inequality to obtain $\|\tilde{\Phi}\Phi^{-1}\| \le \|1-\tilde{\Phi}\Phi^{-1}\|+1$. From the inequality of $\|\Phi^{-1}\| \le e^{2gk\beta}$, which is derived in the same way as (F34), we have

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

from the inequality (F41), where we use $xe^{6x} \le e^{7x}$ for $x \ge 0$.

Therefore, by combining the inequalities (F42) and (F43), we obtain the inequality (F5) as follows:

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

Finally, on the norm $\|\tilde{\Phi}\|$, we can immediately obtain from (F34)

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

which gives the 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.

We here consider the entanglement negativity which is given by [49]

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

Using the Proposition 9, we can immediately obtain the following corollary:

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

$$\mathrm{QC}_\rho(O_A, O_B) \le \epsilon \|O_A\| \cdot \|O_B\| \tag{G2}$$

for two arbitrary operators O_A and O_B; we then obtain

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

where the first inequality is trivially derived from $\log(1+x) \le x$ for $x \ge 0$. Recall that $\mathcal{D}_{AB}$ is the Hilbert space dimension in the region AB. By applying Theorem 10 to the inequality (G3), we can derive a similar inequality to (55).

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

$$\|\rho_{AB}^{T_A}\|_1 = 1 + \sum_{i=1}^{M_0} 2|\langle \eta_i|\rho_{AB}^{T_A}|\eta_i\rangle| \le 1 + 2\delta M_0 \le 1 + 2\delta \mathcal{D}_{AB} \tag{G4}$$

with $\delta := -\min_i \langle \eta_i|\rho_{AB}^{T_A}|\eta_i\rangle$, where we use $M_0 \le \mathcal{D}_{AB}$. We note that the value M_0 can be as large as $(\mathcal{D}_A - 1)(\mathcal{D}_B - 1)$ in general (see Ref. [195]). Thus, using the upper bound on δ in Lemma 24, we prove the inequality (G3). This completes the proof. □

In contrast, we cannot derive a similar inequality to (F1) for 1D quantum Gibbs states if we consider the entanglement negativity. This point is explained as follows. As shown in Lemma 26, we have derived

$$\left\|\rho_\beta - \tilde{\Phi} e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}\tilde{\Phi}\right\|_1 \le e^{-\ell/\mathcal{O}(\beta) + \mathcal{O}(\beta)}, \tag{G5}$$

where $\tilde{\Phi}$ has been supported on $A_1A_2 \cup B_1B_2$. We thus conclude that for $\ell \gtrsim \beta^2$, we have

$$\rho_\beta \approx \tilde{\Phi} e^{-\beta(H - h_{\partial A_1} - h_{\partial B_1})}\tilde{\Phi}. \tag{G6}$$

The primary difficulty here is that the entanglement negativity cannot satisfy a convenient continuity inequality. In Ref. [196, Ineq. (16)], it has been proved that for arbitrary quantum states ρ_{AB} and ρ'_{AB}

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

Hence, even for $\|\rho - \rho'\|_1 = e^{-\mathcal{O}(n^z)}$ $(0 < z < 1)$, the difference of the entanglement negativity can be significantly large [197]. Therefore, we cannot utilize the error estimation (G5) for our purpose.

To take the same steps as in Sec. F, we need to calculate

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

instead of

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

to obtain a meaningful upper bound for the entanglement negativity. However, in general, the partial-transpose operation can significantly increase the operator norm, i.e., $\|O^{T_A}\|_1 \le \min(\mathcal{D}_A, \mathcal{D}_{A^c})\|O\|_1$ as shown in Ref. [198, 199]. Because of this difficulty, it is an open question whether we can derive a similar statement to Theorem 12 for the entanglement negativity (G1). We expect that we would be able to prove it for the entanglement negativity by employing a similar analysis to Ref. [200].

Appendix H: Quantum Fisher information matrix

We here compare our definition (33) for the quantum correlation $\mathrm{QC}_\rho(O_A, O_B)$ to the quantum Fisher information matrix. First, we note 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:

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

where $\rho = |\psi\rangle\langle\psi|$. For general state ρ, the quantum Fisher information is known to be equal to the convex roof of the variance [191, 201]:

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

where minimization is taken for all possible decompositions of ρ such that $\rho = \sum_s p_s |\psi_s\rangle\langle\psi_s|$ with $p_s > 0$. In this way, the quantum Fisher information has a kind of similarity to the quantum correlation $\mathrm{QC}_\rho(O_A, O_B)$.

To view the similarity in more detail, we consider the following quantum Fisher information matrix [131]:

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

We notice that

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

The quantum Fisher information matrix has been used in multiparameter quantum estimation theory [131, 202–204]. Then, can we associate the quantum Fisher information matrix with the convex roof of some observables in the analogy of Eq. (H2)?

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

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

which is the minimization of the absolute value of the average correlation. On the above quantity, we can prove the following statement, which is similar to Lemma 17:

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

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

we upper-bound the quantity $\mathrm{QC}^*_\rho(O_A, O_B)$ in Eq. (H5) as follows:

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

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

Remark. On the quantity $\mathrm{QC}^*_\rho(O_A, O_B)$ in (H5), at first glance, we find no meaningful constraints on the entanglement structure since $\mathrm{C}_{\rho_s}(O_A, O_B)$ can have a negative value. That is, even if $\mathrm{QC}^*_\rho(O_A, O_B)$ is equal to zero, $\mathrm{QC}_\rho(O_A, O_B)$ may be still large. Surprisingly though, we can prove the same statement as Lemma 8 for $\mathrm{QC}^*_\rho(O_A, O_B)$ on the Peres-Horodecki separability criterion (i.e., the PPT condition):

Lemma 29. *We prove the following satatement:*

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

From the statement (H8) and the inequality (H7), one can see that the quantum Fisher information matrix also plays some roles in quantum correlation measures.

1. Proof of Lemma 28

We here prove Lemma 28, which implies

$$\mathrm{QC}^*_\rho(O_A, O_B) \le \frac{1}{4} |\mathcal{F}_\rho(O_A, O_B)|. \quad \text{(H9)}$$

with

$$\mathrm{QC}^*_\rho(O_A, O_B) := \inf_{\{p_s,\rho_s\}} \left| \sum_s p_s \mathrm{C}_{\rho_s}(O_A, O_B) \right|, \quad \text{(H10)}$$

where $[\mathcal{L}_{O_A}, \mathcal{L}_{O_B}] = 0$ is assumed. Note that the operator $\mathcal{L}_O$ has been defined in Eq. (D5).

a. *Proof*

We follow the proof of Lemma 17. We consider the decomposition of ρ as follows:

$$\rho = \sum_m p_m |\phi_m\rangle\langle\phi_m|.$$
$$|\phi_m\rangle = \frac{1}{\sqrt{p_m}} \sqrt{\rho} |\psi_m\rangle, \quad p_m = \langle\psi_m|\rho|\psi_m\rangle, \quad \text{(H11)}$$

and choose $|\psi\rangle_m$ 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. We then reach the same equation as (D29):

$$\langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle = \alpha_{1,m}\alpha_{2,m}. \quad \text{(H12)}$$

We next prove that

$$\sum_m p_m \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle = \frac{1}{2} \mathrm{tr}(\{\rho, \mathcal{L}_{O_A}\mathcal{L}_{O_B}\}), \quad \text{(H13)}$$

where $\{\cdot, \cdot\}$ is the anticommutator. By expanding the RHS in Eq. (H13), we get

$$\frac{1}{2} \mathrm{tr}(\{\rho, \mathcal{L}_{O_A}\mathcal{L}_{O_B}\}) = \frac{1}{2} \sum_m \langle\psi_m|\{\rho, \mathcal{L}_{O_A}\mathcal{L}_{O_B}\}|\psi_m\rangle$$
$$= \sum_m \langle\psi_m|\rho|\psi_m\rangle \alpha_{1,m}\alpha_{2,m}, \quad \text{(H14)}$$

which reduces to the LHS in Eq. (H13) from $p_m = \langle\psi_m|\rho|\psi_m\rangle$ and Eq. (H12)

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

$$\frac{1}{2} \mathrm{tr}(\{\rho, \mathcal{L}_{O_A}\mathcal{L}_{O_B}\})$$
$$= \sum_{s,s'} \frac{2\lambda_s\lambda_{s'}}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O_A|\lambda_{s'}\rangle\langle\lambda_{s'}|O_B|\lambda_s\rangle, \quad \text{(H15)}$$

where we use the form of $\mathcal{L}_O$ in Eq. (D5). By combining Eqs (H13) and (H15), we have

$$\sum_m p_m \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle$$
$$= \sum_{s,s'} \frac{2\lambda_s\lambda_{s'}}{\lambda_s + \lambda_{s'}} \langle\lambda_s|O_A|\lambda_{s'}\rangle\langle\lambda_{s'}|O_B|\lambda_s\rangle. \quad \text{(H16)}$$

Finally, we have

$$\sum_m p_m \langle\phi_m|O_A O_B|\phi_m\rangle = \mathrm{tr}(\rho O_A O_B)$$
$$= \sum_{s,s'} \frac{\lambda_s + \lambda_{s'}}{2} \langle\lambda_s|O_A|\lambda_{s'}\rangle\langle\lambda_{s'}|O_B|\lambda_s\rangle, \quad \text{(H17)}$$

where we use $[O_A, O_B] = 0$. By subtracting Eq. (H16) from Eq. (H17), we obtain

$$\sum_m p_m \left(\langle\phi_m|O_A O_B|\phi_m\rangle - \langle\phi_m|O_A|\phi_m\rangle\langle\phi_m|O_B|\phi_m\rangle \right)$$
$$= \sum_{s,s'} \frac{(\lambda_s - \lambda_{s'})^2}{2(\lambda_s + \lambda_{s'})} \langle\lambda_s|O_A|\lambda_{s'}\rangle\langle\lambda_{s'}|O_B|\lambda_s\rangle$$
$$= \frac{1}{4} \mathcal{F}_\rho(O_i, O_j). \quad \text{(H18)}$$

By applying the above equation to (H5), we prove the inequality (H7). This completes the proof. □

2. Proof of Lemma 29

We here prove the statement of

$$\mathrm{QC}^*_{\rho_{AB}}(O_A, O_B) = 0 \text{ for arbitrary pairs of } O_A, O_B \longrightarrow \rho_{AB} \text{ satisfies the PPT condition.} \tag{H19}$$

This statement can be easily checked by the following discussion.

First, if we can prove the inequality (52) in Proposition 9 by assuming the inequality (51) for $\mathrm{QC}^*_\rho(O_A, O_B)$ instead of $\mathrm{QC}_\rho(O_A, O_B)$, we obtain the statement (H19). Second, in the proof of Proposition 9, the inequality (51) is used only in deriving the upper bound (E21) for the proof of Lemma 25. From the second line to the third line in (E21), we use $\mathrm{QC}_\rho(O_A, O_B)$ as an upper bound for

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

however, in fact, $\mathrm{QC}^*_\rho(O_A, O_B)$ also serves as the upper bound for the above quantity. This allows us to prove the inequality (52) only from the constraint on $\mathrm{QC}^*_\rho(O_A, O_B)$. This completes the proof. □

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[150] The deference between $E^c_{\rm sq}(\rho_{AB})$ and $E_F(\rho_{AB})$ can be significantly large. For example, the quantity $E^c_{\rm sq}(\rho_{AB})$ is trivially upper-bounded using the mutual information as $\mathcal{I}_{\rho_{AB}}(A:B)/2$. In contrast, as has been pointed out in Ref. [207], there exist quantum states [208] such that the entanglement of formation may be much larger than the mutual information, i.e., $E_F(\rho_{AB}) \gg \mathcal{I}_{\rho_{AB}}(A:B) \geq E^c_{\rm sq}(\rho_{AB})$. In Ref. [79, Example 9], an explicit example such that $E_F(\rho_{AB}) > \mathcal{I}_{\rho_{AB}}(A:B)/2$ has been given.

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