

Measuring multipartite quantum correlations by thermodynamic work extraction

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(Received 31 July 2024; accepted 14 October 2025; published 17 December 2025)

While bipartite quantum correlations have been extensively studied across various fields, the role of multipartite quantum correlations in many-body systems remains elusive due to their complex structure. A primary challenge lies in the fact that the calculation of multipartite quantum correlation measure often requires an exponential cost with respect to the system size. In this work, we address this problem by adopting a thermodynamic approach: We introduce a measure of multipartite quantum correlations based on the difference in extractable thermodynamic work between global operations and LOCC (local operations and classical communication). This can be regarded as a multipartite generalization of the bipartite work deficit, which has attracted attention as a thermodynamic measure of bipartite quantum correlation. Importantly, we develop an efficient method for computing the multipartite work deficit in a special class of quantum many-body systems described by matrix product states (MPS). The numerical cost of this method scales linearly with system size, significantly reducing the exponential overhead required for direct calculations. We apply this method to an MPS family and show that a quantum phase transition is well captured by the multipartite work deficit, which exhibits singular behavior at the transition point. Our work shows that the multipartite work deficit not only highlights the fundamental connection between multipartite quantum correlations and quantum thermodynamics, but also serves as an efficiently computable probe of the structures of quantum many-body systems.

DOI: [10.1103/s8h3-5ptz](https://doi.org/10.1103/s8h3-5ptz)

I. INTRODUCTION

In light of recent developments in quantum technologies [1–6], quantum correlations are becoming increasingly important not only in quantum computation and quantum communication [7–9] but also in various fields of physics, including condensed matter physics [10,11] and high-energy physics [12–14]. For example, quantum correlations have been utilized as useful probes for understanding critical phenomena [15–17], topological order [18,19], and information scrambling [20]. While the understanding on bipartite quantum correlations has been well established through various measures with clear operational meanings [21–24], multipartite quantum correlations remain a very active research avenue [25–56], mainly because of their rich and complicated structure [57,58]. For example, even in tripartite quantum states, there are different types of quantum correlations represented by the W state and the Greenberger-Horne-Zeilinger (GHZ) state.

Another fundamental aspect of quantum correlations is its connection to thermodynamics [59]. A crucial issue is

how quantum correlations affect energetic quantities such as extractable work and free energy. This connection between quantum correlations and thermodynamics is twofold: It not only reveals the extractable work from quantum correlations [60–71], but also enables the quantification of quantum correlations themselves based on thermodynamics. Specifically, a measure of quantum correlation, called the work deficit, is introduced as the difference in extractable works through global operations and LOCC (local operations and classical communication) [72–78]. While the work deficit is widely investigated in bipartite systems, the multipartite work deficit is almost unexplored except for simple demonstrations in the seminal works such as Refs. [72,74]. Now, the critical questions are the following: (1) how to formulate multipartite work extraction, (2) how the thermodynamic approach is useful for multipartite quantum correlations, and (3) how one can efficiently compute the multipartite work deficit.

In this work, we introduce the multipartite work deficit defined with work extractions as shown in Fig. 1, for which the above points are clarified. By formulating the multipartite work extraction through nonadaptive LOCC, we obtain its expressions exactly calculable for general few-body states. For example, we show that the tripartite work deficit is given by $\ln 2$ in the GHZ state and $\ln 3$ in the W state. This quantitatively demonstrates that the W state has larger tripartite quantum correlation than the GHZ state, in terms of thermodynamically extractable work.

Furthermore, we develop an efficient calculation method of the multipartite quantum correlations for a special class

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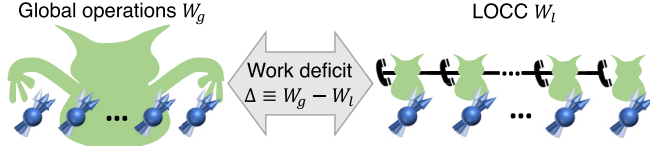


FIG. 1. Schematic of the definition of the multipartite work deficit. The multipartite work deficit, denoted by Δ , is defined as the difference between the extractable work through global operations, W_g , and that through LOCC, W_l , expressed as $\Delta \equiv W_g - W_l$. It is defined for arbitrary multipartite systems with finite local dimensions, and the explicit expressions for W_g , W_l , and Δ are given in Eqs. (2), (4), and (5), respectively. Note that in this framework, work is extracted in contact with a heat bath with inverse temperature β .

of quantum many-body systems described by matrix product states (MPS) [79–83]. While the cost of naive direct calculation of the multipartite work deficit grows exponentially with the system size as is the case for many other measures of multipartite quantum correlations [25–43], the cost of our efficient method is proportional to the system size enabling the significant cost reduction (Table I). It is noteworthy that this efficient method is not restricted to the work deficit but also is applicable to another measure of multipartite quantum correlation (i.e., global quantum discord [38]), thereby enabling the same reduction in numerical cost. This suggests the potential applicability of our method to various measures of multipartite quantum correlation.

By utilizing our efficient method, we demonstrate the multipartite work deficit in an MPS family introduced in Ref. [84]. In this example, we observe that the multipartite work deficit shows a sharp kink at the quantum phase transition point. This showcases that the multipartite work deficit serves as an efficiently computable probe of quantum phase transitions. We further show that the kink at the transition point becomes sharper under coarse graining, which confirms that our probe indeed captures the singularity that is physically relevant (i.e., not from the artifact of optimization).

TABLE I. Numerical costs for calculating the multipartite work deficit in N -site MPS and MPS in the thermodynamic limit, up to constant multiples. Direct calculation scales exponentially with the system size N , making it infeasible in the thermodynamic limit. Such exponential computational cost is a common issue for other measures of multipartite quantum correlations [25–43]. On the other hand, by employing the efficient calculation method introduced in this work, the costs are reduced to scale linearly with respect to N . Furthermore, this method is applicable even in the thermodynamic limit, for translationally invariant normal MPS [81,82], achieving a constant cost dependent only on the desired error bound ε , which scales as $e^{\mathcal{O}(\frac{1}{\varepsilon})}$.

	Direct calculation	Efficient calculation with error bound ε
N -site MPS	$e^{\mathcal{O}(N)}$	$Ne^{\mathcal{O}(\frac{1}{\varepsilon})}$
Normal MPS in thermodynamic limit	Not applicable	$e^{\mathcal{O}(\frac{1}{\varepsilon})}$

The present work establishes a fundamental relationship between multipartite quantum correlations and thermodynamics, introducing measures of quantum correlations with clear operational meaning based on thermodynamic work extraction. Since the introduced measure is efficiently computable for quantum many-body systems described by MPS, it is useful for probing the structure of quantum many-body systems including quantum phase transitions. It is also noteworthy that because of the operational definition of the multipartite work deficit, our framework can also be applied to real experimental setups such as ultracold atoms [1,2] and superconducting qubits [3,4].

This paper is organized as follows. In Sec. II, we introduce the multipartite work deficit in terms of thermodynamic work extraction and discuss its basic properties. In Sec. III, we propose an efficient calculation method of this measure in many-body systems and demonstrate it in an MPS family. In Sec. IV, we introduce the framework of coarse graining and apply it to the MPS family. In Sec. V, we summarize our work and discuss the future perspectives.

II. MULTIPARTITE WORK DEFICIT

A. Definition of multipartite work deficit

We here introduce a measure of multipartite quantum correlations, defined for a given state ρ of an N -partite system composed of d -dimensional subsystems $\{a_i\}_{i=1}^N$. This measure is based on thermodynamic work extraction and is therefore referred to as the multipartite work deficit. It is defined as the gap between extractable thermodynamic work through global operations W_g and LOCC W_l , as

$$\Delta \equiv W_g - W_l. \quad (1)$$

We consider the situation where the work is extracted under the interaction with a heat bath at inverse temperature β (with $\beta = 1$ set for notational simplicity), and the system Hamiltonian is trivial. In this case, the energy levels are completely degenerate and the change in the system's internal energy is negligible. While this framework for quantifying quantum correlations has already been studied in bipartite systems [72–78], we introduce it here in a self-contained manner for N -partite systems, for any $N \geq 2$. We note that our framework of considering work extraction from the heat bath is distinct from the previous works [64–69,85–88], where the work extraction from system's internal energy without utilizing a heat bath is discussed.

We first quantify the extractable work through the global operations W_g . It is given by

$$W_g = N \ln d - S(\rho), \quad (2)$$

where $S(\rho) \equiv -\text{Tr}[\rho \ln \rho]$ denotes the von Neumann entropy. This equation shows that the extractable work W_g is characterized with the gap between the maximum entropy of the system $N \ln d$ and the entropy $S(\rho)$ of the total system. This can be understood as the consequence of the second law of thermodynamics, which states that a larger amount of work can be extracted from a state with high purity. Concrete protocols to achieve the work extraction in Eq. (2) have been discussed, for example, in Refs. [89–92], and are also described in detail in Sec. S1 of the Supplemental Material [93].

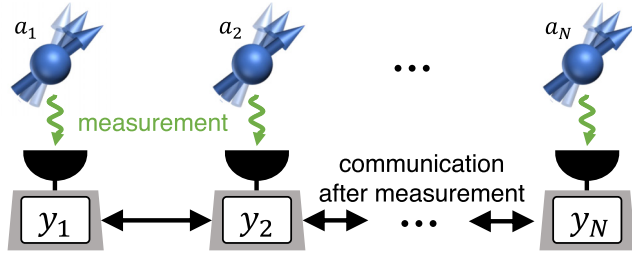


FIG. 2. Schematic of nonadaptive local measurements and classical communication. Projective measurements are performed at each local party, and the outcomes are shared among the parties after the measurements. Note that in this setup local feedback operations conditioned on the outcomes of other parties are not allowed.

We next consider the extractable work through LOCC W_l . When we denote the work extraction with a certain protocol Λ as W_Λ , W_l can be defined as the optimization of W_Λ over the set of allowed LOCC protocols. In this section, we consider the LOCC class called zero-way closed LOCC, where the nonadaptive local projective measurement and classical communication are allowed, as shown in Fig. 2. Correspondingly, we can refer to the work deficit (1) mainly focused in this paper as the zero-way work deficit, while we often call it just the work deficit for simplicity. The extractable work with such a protocol Λ can be quantified as

$$W_\Lambda \equiv \sum_{n=1}^N \left\{ \ln d - \sum_{y_n} p_\Lambda(y_n) S(\tilde{\rho}_n^{\Lambda, y_n}) \right\} - H_\Lambda(Y_N), \quad (3)$$

where $Y_N \equiv (y_1, y_2, \dots, y_N)$ represents the measurement outcomes for all parties, with y_n denoting the outcome of the n th party. Here, $H_\Lambda(Y_N) \equiv -\sum_{Y_N} P_\Lambda[Y_N] \ln P_\Lambda[Y_N]$ is the Shannon entropy for Y_N , where $P_\Lambda[Y_N]$ denotes the probability for the measurement outcomes Y_N with measurement protocol Λ . The conditional density operator $\tilde{\rho}_n^{\Lambda, y_n}$ represents the conditional state of n th party when the measurement outcome y_n is obtained, and $p_\Lambda(y_n)$ denotes the corresponding probability.

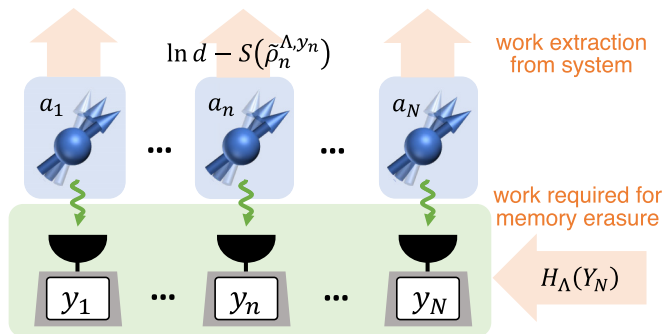


FIG. 3. Schematic for extractable work through a measurement protocol Λ . Extractable work from n th party a_n is $\ln d - S(\tilde{\rho}_n^{\Lambda, y_n})$ when the measurement outcome y_n is obtained, and the averaged work extraction becomes $\ln d - \sum_{y_n} p_\Lambda(y_n) S(\tilde{\rho}_n^{\Lambda, y_n})$. On the other hand, the work required to erase the measurement outcomes Y_N is $H_\Lambda(Y_N)$. Therefore, the net work extraction can be quantified as the gap between these two contributions as shown in Eq. (3).

As shown in Fig. 3, the net work extraction W_Λ is decomposed into two contributions: work extraction from the system after the measurement and the work needed to erase the memory. The first contribution corresponds to the terms in the curly brackets in Eq. (3). Since we cannot feed back the measurement outcomes of the different party in the current setup, the extractable work from each party is the gap between the maximum entropy $\ln d$ and the entropy of conditional state $S(\tilde{\rho}_n^{\Lambda, y_n})$. By taking the average over the measurement outcome y_n , we can derive the expression in Eq. (3). The second contribution of the memory erasure corresponds to the Shannon entropy term $H_\Lambda(Y_N)$. Since the measurement outcomes can be communicated among parties, we can collectively erase all the outcomes $Y_N \equiv (y_1, y_2, \dots, y_N)$. This enables the memory erasure with work cost $H_\Lambda(Y_N)$, which is less than that in the case without classical communication $\sum_{n=1}^N H_\Lambda(y_n)$.

The extractable work W_l can be calculated by further optimizing the measurement protocol Λ . Since we can show that the optimal local measurement becomes always rank 1 as detailed in Appendix A, W_l can be represented as

$$W_l = N \ln d - \min_{\Lambda \in \mathcal{M}_N} H_\Lambda(Y_N). \quad (4)$$

Here, $\mathcal{M}_N$ is the set of measurement protocols whose measurement operators are denoted as $\{\Pi_{y_1} \otimes \Pi_{y_2} \otimes \dots \otimes \Pi_{y_N}\}$, where $\{\Pi_{y_n}\}$ is a set of rank-1 projectors on n th party. By combining the expressions of Eqs. (2) and (4), we can derive a formula for the multipartite work deficit as

$$\Delta = \min_{\Lambda \in \mathcal{M}_N} H_\Lambda(Y_N) - S(\rho). \quad (5)$$

This equation shows that Δ involves the minimization over N sets of local measurement basis, which can be carried out by brute-force optimization when the system size N is small.

For example, consider the GHZ state in a three-qubit system, defined as

$$|\text{GHZ}\rangle \equiv \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle).$$

By brute-force optimization, the optimal measurement protocol for this state is given by the projective measurement in the computational basis $|0\rangle, |1\rangle$ on all parties, and therefore the work deficit is $\Delta = \ln 2$. Similarly, for the W state,

$$|W\rangle \equiv \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle),$$

the work deficit is $\Delta = \ln 3$, with the same optimal measurement protocol as in the GHZ state. These results indicate that the W state possesses a larger amount of multipartite quantum correlation than the GHZ state in terms of work deficit.

B. Expression with quantum relative entropy

By simple transformation, Eq. (5) can be reformulated as the following expression:

$$\Delta = \min_{\sigma \in \mathcal{C}_N} S(\rho \| \sigma), \quad (6)$$

where $S(\rho \| \sigma) \equiv \text{Tr}[\rho(\ln \rho - \ln \sigma)]$ denotes the quantum relative entropy. Here, $\mathcal{C}_N$ represents the set of classically

correlated states, which can be represented as

$$\sigma \equiv \sum_{Y_N} q(Y_N) \Pi_{y_1} \otimes \Pi_{y_2} \otimes \cdots \otimes \Pi_{y_N}, \quad (7)$$

with a set of orthogonal rank-1 projectors $\{\Pi_{y_n}\}$, and a certain probability distribution $q(Y_N)$. From Eq. (6), we can see that the multipartite work deficit Δ is the optimization over the local bases of the relative entropy of coherence.

We remark that multipartite work deficit, reduced to Eq. (6), is equivalent to other measures of multipartite quantum correlations introduced in the previous works [94–98], in the contexts totally different from thermodynamics. Here, we have formulated the multipartite work deficit based on thermodynamics. More importantly, we emphasize that the efficient calculation method discussed in Sec. III has not been proposed in any of the previous works.

We also remark the relationship between the multipartite work deficit and entanglement. For the bipartite pure state, it has been shown in the previous work [72] that the work deficit is reduced to the entanglement entropy $\Delta = S(\rho_1)$, where ρ_1 is the reduced density operator for a single party. On the other hand, for the mixed states in bipartite and multipartite systems, the work deficit can take positive values even for separable states, as is the case for the quantum discord [99,100]. This indicates that the notion of multipartite quantum correlation for the work deficit is broader than that of entanglement theory. This can be understood from the fact that the set of classically correlated states [Eq. (7)] is included by the set of separable states, represented as

$$\sigma \equiv \sum_x q(x) \sigma_1^x \otimes \sigma_2^x \otimes \cdots \otimes \sigma_N^x.$$

III. EFFICIENT CALCULATION IN MANY-BODY SYSTEMS

While the multipartite work deficit can be calculated exactly with a reasonable numerical cost in few-body systems, the calculations in many-body systems are challenging due to the exponential growth of the numerical cost. The reason for such a cost explosion is the necessity of optimizing all the local bases: We need to optimize N sets of measurement bases in order to calculate the work deficit (5), which requires an exponential cost in the brute-force optimization. Such a difficulty in optimizing local bases is not unique to the multipartite work deficit but is a common issue across various measures of multipartite quantum correlations; for example, the relative entropy of entanglement [25,26], geometric entanglement [27–29], and global quantum discord [38] involve optimization parameters proportional to the system size, similarly to the multipartite work deficit. While there have been some attempts to overcome this problem [101], systematic methods to calculate these measures with polynomial costs are yet to be established.

In this section, we propose an efficient calculation method for the multipartite work deficit, which is applicable for MPS with fixed bond dimension. MPS can efficiently represent the ground state of gapped one-dimensional local Hamiltonians [102,103] and has played a significant role in condensed matter physics and quantum information science. An N -site MPS

with bond dimension D_B is represented as [79–83]

$$|\psi\rangle \propto \sum_{\sigma_1, \dots, \sigma_N} \text{Tr}[A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_N} X] |\sigma_1, \sigma_2, \dots, \sigma_N\rangle, \quad (8)$$

where A^{σ_n} is D_B -dimensional square matrix corresponding to the orthogonal basis $|\sigma_n\rangle$ for n th site, and X is the matrix of the same size that represents the boundary condition (e.g., $X = \mathbb{1}_{D_B}$ for periodic boundary condition and $X = \mathbf{v}_R \mathbf{v}_L^T$ for open boundary condition, with certain D_B -dimensional vectors $\mathbf{v}_R$ and $\mathbf{v}_L$). In what follows, we introduce the efficient calculation method for this class of states, which enables significant cost reduction as shown in Table I. We also note that this method can be extended to another measure of multipartite quantum correlation called global quantum discord [38], as detailed in Sec. S4 of the Supplemental Material [93].

A. Overview of efficient calculation method

Since the work deficit Δ increases proportionally with the number of party N for typical N -partite states, we here focus on the work deficit density, which is defined as

$$\delta \equiv \frac{\Delta}{N}. \quad (9)$$

This quantifies the leading term of the work deficit in many-body systems, and does not diverge even in the thermodynamic limit. For the calculation of the work deficit density, we need to search for N sets of measurement bases $\{|y_1\rangle\}, \{|y_2\rangle\}, \dots, \{|y_N\rangle\}$, which minimize the Shannon entropy in Eq. (5). If we perform a brute-force optimization over these N sets of measurement bases, we must calculate the Shannon entropy for all possible combinations of meshed basis parameters, leading to an exponential computational cost with respect to N , regardless of the system's state.

To avoid such exponential computational overhead, we evaluate the work deficit density through its lower and upper bounds, instead of directly calculating it:

$$L_l \leq \delta \leq U_l. \quad (10)$$

Here, these bounds U_l and L_l are defined by dividing the entire system into l -site segments, and by optimizing the local measurement bases within each segment. The tightness of these bounds can be improved by increasing the locality parameter l , while the numerical costs also increase with l . Especially for the systems described with MPS, we can derive the following inequality, which is also depicted in Fig. 4(a):

$$U_l - L_l \leq \mathcal{O}\left(\frac{1}{l}\right). \quad (11)$$

This is one of the main results of this paper, along with Eq. (10). Since the computational costs for U_l and L_l in MPS scale as $N e^{\mathcal{O}(l)}$ (up to constant factor) as discussed later in Sec. III B, Eq. (11) implies that the evaluation of δ with an arbitrary accuracy ε can be achieved at the cost that scales as $N e^{\mathcal{O}(\frac{1}{\varepsilon})}$, as shown in Table I. Furthermore, these bounds are calculable even in the thermodynamic limit for translationally invariant normal MPS [81,82], where the direct calculation of δ is infeasible. Normal MPS is a class of MPS with finite correlation length and represents the unique ground state of gapped one-dimensional local Hamiltonians [79].

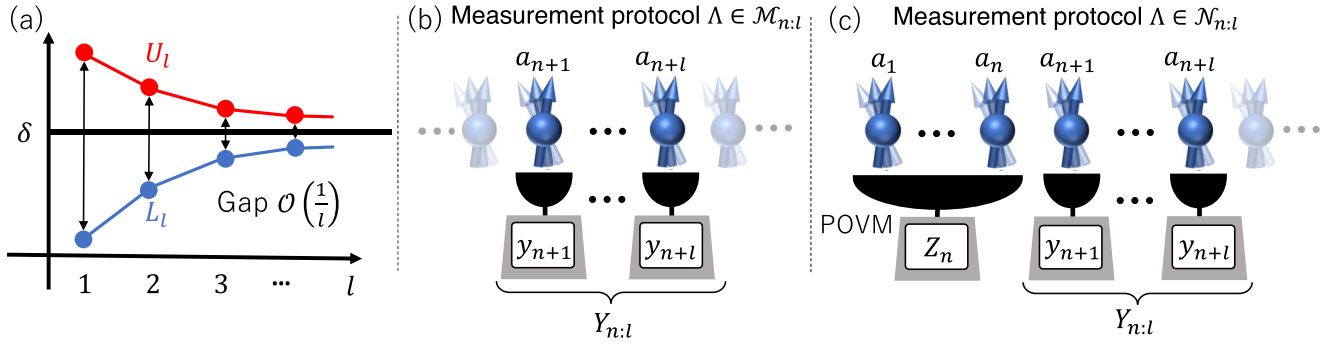


FIG. 4. Efficient calculation method for the work deficit density δ with systematically improvable upper and lower bounds. (a) Schematic of the systematic improvement of the lower and upper bounds, L_l and U_l , by increasing the locality parameter l . (b) The measurement protocol $\Lambda \in \mathcal{M}_{n:l}$, optimized to define the upper bound U_l . (c) The measurement protocol $\Lambda \in \mathcal{N}_{n:l}$, optimized to define the lower bound L_l .

B. Upper and lower bounds for work deficit density

We now explicitly express the lower and upper bounds for the multipartite work deficit density, which are utilized in its efficient calculation. The upper bound U_l is defined as

$$U_l \equiv \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\Lambda \in \mathcal{M}_{n:l}} H_{\Lambda}(Y_{n:l}) - S(\rho) \right\}, \quad (12)$$

where $I_l \equiv \{ml | m \in \mathbb{Z}, 0 \leq m < \frac{N}{l}\}$ is the set of the party labels. Here, $\mathcal{M}_{n:l}$ represents the set of measurement protocols composed of the local projective measurements on $\{a_i\}_{i=n+1}^{n+l}$, and $Y_{n:l} \equiv (y_{n+1}, \dots, y_{n+l})$ represents their outcomes, as shown in Fig. 4(b) [104]. By denoting the measurement outcomes from parties $\{a_i\}_{i=1}^n$ as $Y_n \equiv (y_1, \dots, y_n)$, this upper bound can be derived as follows:

$$\begin{aligned} \delta &= \frac{1}{N} \left\{ \min_{\Lambda \in \mathcal{M}_N} \sum_{n \in I_l} H_{\Lambda}(Y_{n:l} | Y_n) - S(\rho) \right\} \\ &\leq \frac{1}{N} \left\{ \min_{\Lambda \in \mathcal{M}_N} \sum_{n \in I_l} H_{\Lambda}(Y_{n:l}) - S(\rho) \right\} \\ &= \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\Lambda \in \mathcal{M}_{n:l}} H_{\Lambda}(Y_{n:l}) - S(\rho) \right\} \\ &= U_l. \end{aligned} \quad (13)$$

In the upper bound U_l defined as Eq. (12), the global optimization of δ is divided into the optimization of l -site segments. The cost for optimizing each term $\min_{\Lambda} H_{\Lambda}(Y_{n:l})$ is $e^{\mathcal{O}(l)}$, due to the necessity to optimize the local measurement bases on l sites. Since U_l is calculated as the sum of $\frac{N}{l}$ such terms, the total computational cost is represented as $Ne^{\mathcal{O}(l)}$, capturing the dominant factors of N and l . Furthermore, for translationally invariant normal MPS in the thermodynamic limit, U_l can be calculated with a cost of $e^{\mathcal{O}(l)}$. This is because almost all the terms in the summation $\{\min_{\Lambda} H_{\Lambda}(Y_{n:l})\}_{n \in I_l}$ are reduced to the same value due to the translation invariance and finite correlation length, eliminating the need for summation. More detailed discussion is provided as Theorem 3 in the Supplemental Material [93].

We remark that despite the universal applicability of this type of upper bound U_l , different types of upper bounds are more effective for some multipartite states. In fact, since δ is defined as the minimization over the measurement protocol, its upper bounds can be derived in various ways, e.g., by utilizing the ansatz protocol or restricting optimization region reasonably. For example, by employing arbitrary ansatz measurement protocol $\Lambda^* \in \mathcal{M}_N$, we can define the upper bound of δ as

$$U_{\Lambda^*} \equiv \frac{1}{N} \{H_{\Lambda^*}(Y_N) - S(\rho)\}, \quad (14)$$

where the inequality $\delta \leq U_{\Lambda^*}$ directly follows from the definition of δ . As another type of upper bound, we introduce $U_{l,k}$ with natural numbers l and k , which is derived by restricting the optimization region of the measurement protocols. This bound $U_{l,k}$ is the generalization of the upper bound U_l and is utilized in the numerical calculation in Sec. III C. The definition and derivation of this type of bound are provided in Appendix B.

The lower bound L_l is defined as

$$L_l \equiv \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\Lambda \in \mathcal{N}_{n:l}} H_{\Lambda}(Y_{n:l} | Z_n) - S(\rho) \right\}, \quad (15)$$

where $\mathcal{N}_{n:l}$ denotes the set of measurement protocols composed of an arbitrary POVM (positive operator valued measurement) on the parties $\{a_i\}_{i=1}^n$ and local projective measurements on l parties $\{a_i\}_{i=n+1}^{n+l}$ [105], and Z_n is the outcome of the POVM, as shown in Fig. 4(c). By denoting the set of the local projective measurements on $\{a_i\}_{i=1}^{n+l}$ as $\mathcal{M}_{n+l}$, this bound is derived as follows:

$$\begin{aligned} \delta &= \frac{1}{N} \left\{ \min_{\Lambda \in \mathcal{M}_N} \sum_{n \in I_l} H_{\Lambda}(Y_{n:l} | Y_n) - S(\rho) \right\} \\ &\geq \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\Lambda \in \mathcal{M}_{n+l}} H_{\Lambda}(Y_{n:l} | Y_n) - S(\rho) \right\} \\ &\geq \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\Lambda \in \mathcal{N}_{n:l}} H_{\Lambda}(Y_{n:l} | Z_n) - S(\rho) \right\} \\ &= L_l, \end{aligned} \quad (16)$$

where the inequality in the third line follows from the inclusion relationship of the set of measurement protocols $\mathcal{M}_{n+l} \subset \mathcal{N}_{n:l}$.

From Eq. (15), we can see that this lower bound L_l is defined as the sum of the local terms $\min_{\Lambda} H_{\Lambda}(Y_{n:l}|Z_n)$, which is similar to the upper bound U_l . The difference is that in the lower bound L_l , we need to optimize the POVM on the d^n -dimensional subsystem $\{a_i\}_{i=1}^n$, whose numerical cost seems to grow exponentially with the subsystem size n . However, in MPS with fixed bond dimension D_B , we can perform this optimization at a constant numerical cost, since the subsystem $\{a_i\}_{i=1}^n$ can be effectively regarded as a fixed-dimensional system (D_B -dimensional for open boundary conditions and D_B^2 -dimensional for periodic boundary conditions). Because of this reduction of subsystem dimension, the numerical cost for L_l becomes $Ne^{\mathcal{O}(l)}$ up to constant multiple in N -site MPS, and $e^{\mathcal{O}(l)}$ for the translationally invariant normal MPS in the thermodynamic limit.

Finally, we discuss the tightness of these bounds L_l and U_l , which is directly related to the accuracy of our calculation method. In general states, we can show that the tightness of these bounds is improved with increasing the locality parameter l , as

$$L_l \leq L_{kl}, \quad U_{kl} \leq U_l, \quad (17)$$

where k is arbitrary natural number. Furthermore, for systems described with MPS, we can derive Eq. (11), which indicates that an arbitrary error bound is achieved with our method by increasing l . Since the numerical costs for calculating the bounds L_l and U_l scale as $e^{\mathcal{O}(l)}$ with the locality parameter l , Eq. (11) demonstrates that the cost scales with the inverse of the error bound, ε , as $e^{\mathcal{O}(\frac{1}{\varepsilon})}$ (Table I).

C. Demonstration in an MPS family

We next demonstrate our efficient calculation method of work deficit density, in an MPS family introduced in Ref. [84]. The MPS family is represented with the following set of matrices with one parameter g :

$$A^0 = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, \quad A^1 = \begin{pmatrix} 1 & g \\ 0 & 0 \end{pmatrix}. \quad (18)$$

We consider the region $-1 \leq g \leq 1$ and system under periodic boundary condition. These MPS are the ground states of the parametrized Hamiltonian

$$H_g \equiv \sum_n 2(g^2 - 1)\sigma_n^z \sigma_{n+1}^z - (g+1)^2 \sigma_n^x + (g-1)^2 \sigma_n^z \sigma_{n+1}^x \sigma_{n+2}^z, \quad (19)$$

where σ_n^x and σ_n^z are the pauli x and z matrices on n th site, respectively. As the special cases of this MPS family, the cluster state is realized at $g = -1$, the generalized GHZ state $\frac{1}{\sqrt{2}}(|00 \cdots 0\rangle + |11 \cdots 1\rangle)$ is realized at $g = 0$, and the product state $|+\rangle + \cdots + |+\rangle$ is realized at $g = 1$ with $|+\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$.

This MPS family is widely studied as a model that exhibits a quantum phase transition while maintaining a fixed bond dimension $D_B = 2$ [106–110]. The phase transition occurs at $g = 0$, transitioning from a symmetry-protected topological

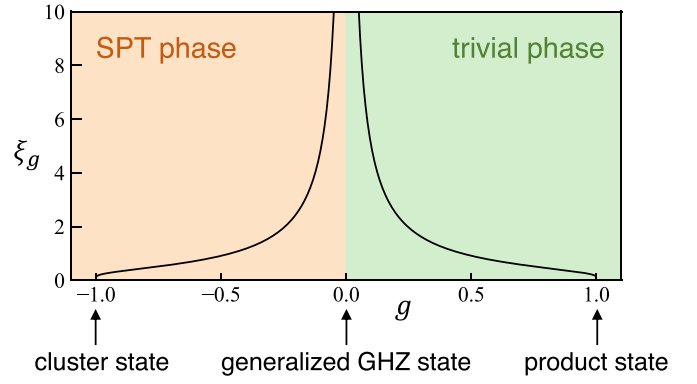


FIG. 5. Correlation length as a function of the system parameter g for the MPS family [Eq. (18)]. The correlation length diverges at the quantum phase transition point $g = 0$, indicating a transition from the SPT phase in $g < 0$ to the trivial phase in $g > 0$.

phase (SPT phase) when $g < 0$ to a trivial phase when $g > 0$. The correlation length ξ_g of this MPS family diverges at the transition point as follows, depicted in Fig. 5:

$$\xi_g = \begin{cases} \left(\ln \left| \frac{1-g}{1+g} \right| \right)^{-1} & (g < 0), \\ \left(\ln \left| \frac{1+g}{1-g} \right| \right)^{-1} & (g > 0). \end{cases} \quad (20)$$

We note that at $g = 0$, the system resides in a generalized GHZ state characterized by long-range, nondecaying correlation. This feature is distinct from conformal critical points, which are known for power-law decaying correlations. Previous studies have identified the point $g = 0$ in this MPS family as a multicritical point [106–108].

The result of our numerical calculation is shown in Fig. 6. In Fig. 6(a), the behavior of the work deficit density as a function of the system parameter g is depicted, while in Figs. 6(b) and 6(c) the lower and upper bounds for fixed g as a function of the locality parameter l are displayed. All of these figures illustrate that the lower and upper bounds are improved systematically with increasing locality parameter l , showcasing the validity of our calculation method.

From Fig. 6(a), we can observe the bimodal structure of δ , with its peaks in the regions $-1 \leq g \leq 0$ and $0 \leq g \leq 1$, respectively. The reasons for this bimodal structure can be attributed to two factors: long-range correlation around $g = 0$ and the short-range correlation around $g = \pm 1$. At $g = 1$, work deficit density δ becomes zero, since the system is in a product state and does not have intersite correlation at all. On the other hand, at $g = 0$, δ drop to zero due to the non-decaying correlation. The generalized GHZ state realized at $g = 0$ is the superposition of the completely aligned states $|00 \cdots 0\rangle$ and $|11 \cdots 1\rangle$, and therefore the multipartite work deficit remains the same value $\Delta = \ln 2$ independent of the system size N . In the thermodynamic limit $N \rightarrow \infty$, this leads to $\delta \equiv \frac{\Delta}{N} \rightarrow 0$. Consequently, the peak of δ occurs between these two extremes, where the system has the intermediate-scale correlation length. The peak in the region $-1 \leq g \leq 0$ occurs in a similar mechanism.

We further discuss the kinks observed in Fig. 6(a). In this figure, the unsmooth change in δ is observed at the phase transition point $g = 0$, reflecting the drastic change of the quantum

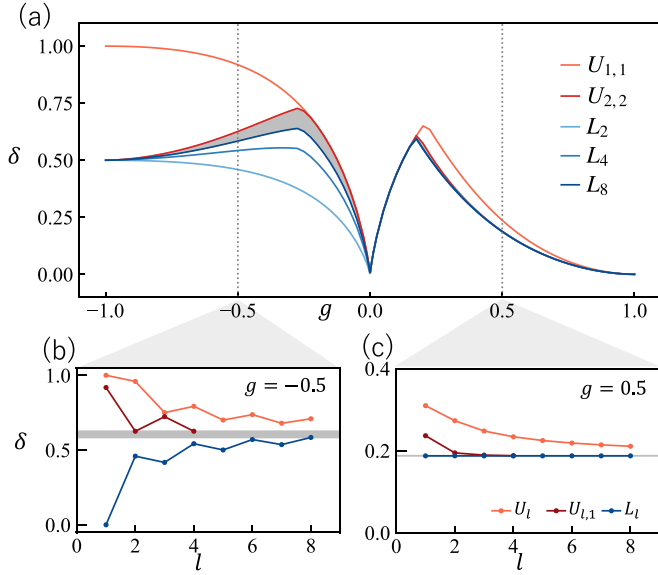


FIG. 6. Numerical calculation of the work deficit density in the MPS family [Eq. (18)]. (a) Work deficit density as a function of the system parameter g . The gray region, sandwiched by the lower and upper bounds, represents the range for the work deficit density δ . The step size for g is 0.025, except near $g = 0$, where the data points are more densely sampled at $g = \pm 0.025 \times 0.5^n$ for n ranging from 1 to 5. (b), (c) Lower and upper bounds of the work deficit density as a function of the locality parameter l at fixed system parameters $g = -0.5$ and 0.5 , respectively. Systematic improvement of the bounds with increasing l is observed. The data points for L_l , U_l , and $U_{l,k}$ are taken as the best value among results from numerical optimization for random initializations.

correlation structure. Around this point $g = 0$, the optimal measurement protocol Λ^* is kept unchanged; it is to perform the measurement on the basis $\{|0\rangle, |1\rangle\}$ for all sites. On the other hand, the kink observed around $g = 0.175$ in Fig. 6(a) is due to a discontinuous change in the optimal measurement protocol at this point; in the region $g < 0.175$, the optimal protocol is to perform projective measurements on the basis $\{|0\rangle, |1\rangle\}$ for all sites, while for $g \geq 0.175$, the optimal basis suddenly switches to $\{|+\rangle, |-\rangle\}$, where $|\pm\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$. Additionally, the kink may occur for the same reason in the region $1 \leq g \leq 0$, although it is not clearly observable in the current numerical calculation due to the gap in the lower and upper bounds. Such kinks, resulting from changes in the optimal measurement protocols, do not necessarily indicate a drastic change in the quantum correlation structure at those points. To distinguish between such kinks and the unsmoothness due to the phase transition at $g = 0$, we further introduce the framework of coarse graining in Sec. IV, demonstrating that the kink around $g = 0$ becomes sharper while the kinks at the other points shift or get dull under the coarse graining.

IV. COARSE GRAINING

In the foregoing sections, we have focused on the situation where each site is regarded as a single party. In this section, we calculate the work deficit density defined in a coarse-grained picture. Specifically, we consider the situation where m sites

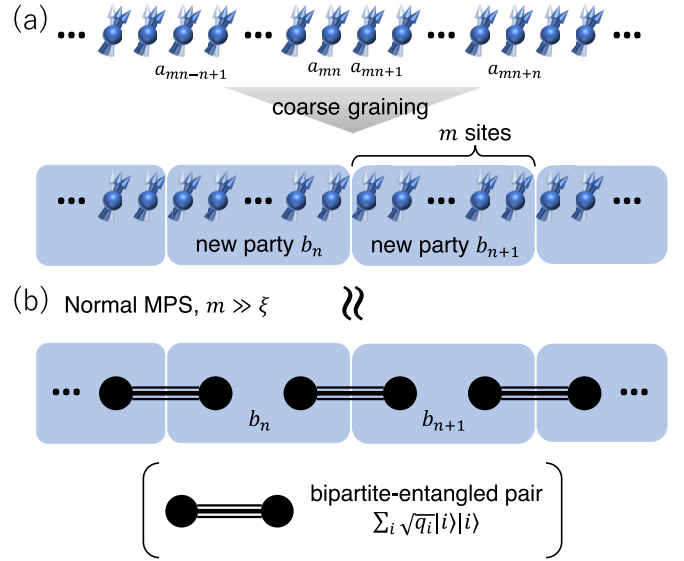


FIG. 7. (a) Schematic for the coarse graining. The neighboring m sites $\{a_{mn+1}, a_{mn+2}, \dots, a_{(m+1)n-1}\}$ are merged and regarded as a single party b_{n+1} . (b) Convergence of normal MPS to bipartite-entangled form under coarse graining. By taking the party size m much larger than the correlation length ξ , normal MPS converges to the form where bipartite-entangled pair $\sum_i \sqrt{q_i} |i\rangle |i\rangle$ is shared between the neighboring parties.

$\{a_{mn+1}, a_{mn+2}, \dots, a_{(m+1)n-1}\}$ are merged and regarded as a single party b_{n+1} , as shown in Fig. 7(a). To represent the work deficit density defined under such a partitioning, we introduce the notation δ_m , where the subscript m denotes the number of sites per a single party. In the case of $m = 1$, the subscript may be omitted, as has been done so far.

In the framework of coarse graining, we can get access to the structure of longer-range multipartite quantum correlation. For example, the work deficit density δ_m , defined under the partitioning of Fig. 7(a), does not account for the short-range quantum correlation among m sites $\{a_{mn+1}, \dots, a_{(m+1)n-1}\}$, while it captures the structure of longer-range quantum correlation well. This is contrary to δ_1 , which accounts for the effects of local quantum correlations across all sites. In this section, we analyze the long-range structure using the framework of coarse graining, demonstrating that the quantum phase transition in the MPS family (18) can be effectively probed with this framework.

A. Work deficit density for normal MPS under coarse graining

In this subsection, we show that the work deficit density δ_m converges to half of the entanglement entropy by increasing number of sites per party m . Especially, we focus on the translationally invariant normal MPS [81,82] under periodic boundary condition. We consider an N -site system divided into m -site parties, where the number of parties is denoted as $M \equiv \frac{N}{m}$. In this setup, we can derive the following equality, which is the main result of this section:

$$\delta_m = \frac{S_{EE}}{2} + \tilde{O}(e^{-\frac{m}{2\xi}}), \quad (21)$$

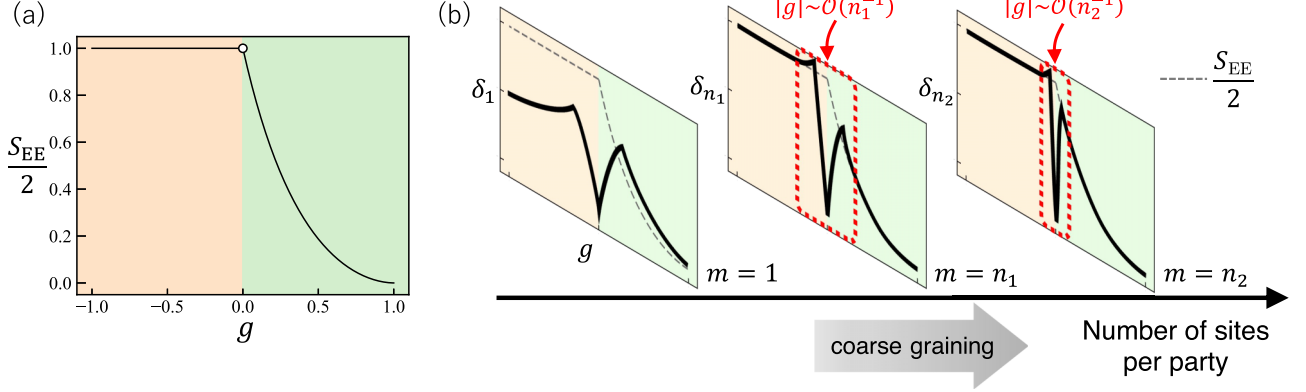


FIG. 8. (a) Entanglement entropy for the MPS family [Eq. (18)]. Here, S_{EE} is defined as the entanglement entropy of a subsystem whose size is much larger than the correlation length ξ_g , for each parameter g . Therefore, S_{EE} is ill-defined at $g = 0$ due to the divergence of the correlation length. (b) Rough sketch of the behavior of work deficit density δ_m in the MPS family under coarse graining. In the region $|g| \gg \frac{1}{m}$, δ_m converges to half of the entanglement entropy depicted in panel (a), while in the region $|g| \ll \frac{1}{m}$, δ_m is close to zero. Based on these analyses, we can conclude that δ_m undergoes drastic changes in the parameter region $|g| \sim \mathcal{O}(m^{-1})$. It is important to note that this figure is a rough sketch derived from analytical calculations in the regions $|g| \ll \frac{1}{m}$ and $|g| \gg \frac{1}{m}$ and is not based on the calculations in the entire parameter range $-1 \leq g \leq 1$.

where ξ is the correlation length of this MPS, S_{EE} is the entanglement entropy for subsystem much larger than ξ , and the notation $\tilde{\mathcal{O}}(x)$ represents $\mathcal{O}(x \ln x)$. In the following, we provide an intuitive discussion of why Eq. (21) is satisfied, while the rigorous proof is presented in the Supplemental Material [93] as Theorem 4.

The essence of the derivation of Eq. (21) is the fact that under coarse graining, a normal MPS converges to the state where the bipartite-entangled pairs are shared between the neighboring parties, as shown in Fig. 7(b). This convergence is the consequence of the renormalization group transformation, as discussed, e.g., in Refs. [81,82,111,112]. The state in Fig. 7(b) is represented as

$$|\psi\rangle \simeq \sum_{i_1, \dots, i_M} \sqrt{q_{i_1} q_{i_2} \dots q_{i_M}} \times |i_1\rangle_{1,1} |i_2\rangle_{1,2} |i_2\rangle_{2,1} |i_3\rangle_{2,2} \dots |i_M\rangle_{M,1} |i_1\rangle_{M,2}, \quad (22)$$

where $\{|j\rangle_{n,1} |k\rangle_{n,2}\}_{j,k=1}^{D_B}$ denotes the orthonormal basis of n th party b_n . In this representation, each m -site party is effectively regarded as a D_B^2 -dimensional system due to the fixed bond dimension of $|\psi\rangle$. Since Eq. (22) represents a state in which the bipartite-entangled pair $\sum_i \sqrt{q_i} |i\rangle_{n,2} |i\rangle_{n+1,1}$ is shared between neighboring parties, the work deficit density reduces to the bipartite contribution as follows:

$$\delta_m \simeq \frac{1}{M} \sum_{n=1}^M H(\{q_i\}) = H(\{q_i\}). \quad (23)$$

Here, the optimal measurement protocol for δ_m is to perform the projective measurement with basis $\{|j\rangle_{n,1} |k\rangle_{n,2}\}_{j,k}$ for all parties. Since $S_{EE} = 2H(\{q_i\})$ as shown in Fig. 7(b), we can derive Eq. (21). The error term $\tilde{\mathcal{O}}(e^{-\frac{m}{2\xi}})$ in Eq. (21) is the consequence of the error in the approximation in Eq. (22).

B. Detection of quantum phase transition with work deficit density

We apply the framework of coarse graining to the MPS family defined in Eq. (18), to reveal its long-range quantum correlation structure. We consider the system under periodic boundary condition in the thermodynamic limit, in the same way as Sec. III C. Instead of conducting numerical calculations across the entire parameter range $-1 \leq g \leq 1$ in a coarse-grained framework, we here perform the analysis solely within the regions $|g| \gg \frac{1}{m}$ and $|g| \ll \frac{1}{m}$ to grasp a rough sketch for the behavior of the work deficit density. Given that the correlation length [Eq. (20)] is approximately $\xi_g \simeq \frac{1}{2|g|}$ for $|g| \ll 1$, the regions $|g| \gg \frac{1}{m}$ and $|g| \ll \frac{1}{m}$ correspond to the situations of $\xi_g \ll m$ and $\xi_g \gg m$, respectively.

In the region $|g| \gg \frac{1}{m}$, we can utilize Eq. (21), since $\xi_g \ll m$ is satisfied. Therefore, the work deficit density converges to half of the entanglement entropy of subsystem much larger than the correlation length ξ_g , which can be calculated as follows:

$$\frac{S_{EE}}{2} = \begin{cases} \ln 2 & (g < 0), \\ h(\frac{1}{2} - \frac{\sqrt{g}}{1+g}) & (g > 0), \end{cases} \quad (24)$$

where $h(p) \equiv -p \ln p - (1-p) \ln(1-p)$ denotes the binary entropy function. It is depicted in Fig. 8(a).

On the other hand, in the region $|g| \ll \frac{1}{m}$, work deficit density deviates from the entanglement entropy since the party size m is smaller than the correlation length ξ_g . Therefore, in this region, we take a different strategy to evaluate δ_m . To be specific, we can derive the heuristic upper bound

$$\delta_m \leq \tilde{\mathcal{O}}(m|g|), \quad (25)$$

by utilizing a certain ansatz measurement protocol [93]. From this inequality, we can see that δ_m is close to zero in the region $|g| \ll \frac{1}{m}$. Such a behavior of work deficit density can be understood as the consequence of the long-range correlation around $g = 0$. For example, in the generalized GHZ state

at $g = 0$, the total work deficit remains the same value $\ln 2$ independent of the number of parties M , resulting in $\delta_m = 0$ in the thermodynamic limit $M \rightarrow \infty$.

Figure 8(b) shows the rough sketch of the behavior of work deficit density, reflecting these analytical calculations. This figure illustrates that δ_m converges to half of the entanglement entropy in the region $|g| \gg \frac{1}{m}$, while it rapidly approaches to zero in the region $|g| \ll \frac{1}{m}$. Therefore, by changing the size of the party m , the unsmoothness of the work deficit density around $g = 0$ becomes sharper, showcasing the drastic change in the long-range structure of multipartite quantum correlation. On the other hand, the other kinks observed in Fig. 6(c), such as the one at $g = 0.175$, shift or become dull under sufficient coarse graining, since δ_m converges to $\frac{S_{EE}}{2}$, which is smooth at these points as depicted in Fig. 8(a). This illuminates that these kinks are regarded as artifacts of optimization. We remark that Fig. 8(b) roughly predicts the behavior of the work deficit density based on the analysis in the regions $|g| \gg \frac{1}{m}$ and $|g| \ll \frac{1}{m}$. The behaviors in other parameter regions are merely interpolations from these extremes.

V. SUMMARY AND DISCUSSION

In this work, we introduced the multipartite work deficit, a measure that quantifies multipartite quantum correlation based on work extraction. It is defined as the difference in extractable works through global operations and nonadaptive LOCC. We obtained its expression [Eq. (5)] that is exactly calculable for general few-body states and computed its values in simple examples.

Importantly, we introduced an efficient calculation method for this measure in many-body systems described with MPS, in Secs. III A and III B. While the numerical cost for directly calculating the multipartite work deficit grows exponentially with system size N , the cost for our efficient method is linear with respect to N , enabling significant cost reduction (Table I). This method is applicable not only to the multipartite work deficit but also to another measure called global quantum discord [38], which highlights its potential applicability to various measures. In Sec. III C, we demonstrated this method in an MPS family [84]. We also introduced the framework of coarse graining of the multipartite work deficit in Sec. IV. By utilizing this framework in the MPS family, we observed the drastic change of multipartite quantum correlation structure at the quantum phase transition point.

A remaining issue of this work is to investigate whether our efficient calculation method for MPS can be applied to broader classes of many-body states. Such extension may be straightforward for the systems described with projected-entangled pair states, matrix product operators, and projected-entangled pair operators, which are the generalizations of MPS to higher-dimensional and/or mixed states [81,82]. In fact, these states can be represented with fixed bond dimensions independent of the system size, which is essential for our calculation method. On the other hand, extension to states that exhibit volume-law entanglement entropy is much more nontrivial, since the bond dimension for these states grows exponentially with the system size. It is an important open question to develop approaches for evaluating multipartite work deficit in such states.

Another future task is to study the multipartite work deficit defined with fully adaptive LOCC. In this work, we introduced the work deficit defined with zero-way LOCC, where only the nonadaptive local measurements are allowed. Furthermore, as discussed in detail in the Supplemental Material [93], we can formulate the work deficit based on the one-way LOCC, where the local measurement and one-way classical communication are allowed. These restrictions of the LOCC classes are crucial for deriving their closed formula that can be calculated exactly for general few-body states, while maintaining clear operational meanings based on work extraction. On the other hand, the investigation of the measure defined with fully adaptive LOCC, in which the adaptive local operations and arbitrary classical communication are allowed, poses a greater challenge due to the extensive range of allowable protocols. Since studies on such a case have so far been limited to demonstrations in a few examples [72,74], it remains a future task to establish calculation methods for general few-body and many-body systems.

It is also important to explore how the multipartite work deficit reveals the structures of quantum correlations in quantum many-body systems. While the quantum correlations of many-body systems at zero and finite temperature have been extensively studied in the previous works [113–123], they primarily focused on bipartite or tripartite measures, leaving the structure of multipartite quantum correlation largely unexplored. We expect that the multipartite work deficit introduced in this work would serve as a probe for elucidating such multipartite structures. Particularly, its convergence to entanglement entropy in normal MPS, as discussed in Sec. IV A, represents a significant step forward. Clarifying the conditions under which this convergence to bipartite entanglement occurs poses an open question.

Finally, we discuss the relevance of our work to experiments. Recently, single-site measurement and manipulation of quantum many-body systems [124,125], as well as thermodynamic work extraction from quantum systems [126–128], are becoming possible on real experimental platforms, such as ultracold atoms and superconducting qubits. The multipartite work deficit has fully operational meaning, as it is defined based on the work extraction through sitewise operations, which would be feasible with these current or near-future quantum technologies. Therefore, the multipartite work deficit is expected to serve as an experimental probe of multipartite structure of quantum correlations in many-body quantum systems. It would also be an interesting perspective to investigate the role of quantum correlations in thermodynamics in such experimental platforms.

ACKNOWLEDGMENTS

We thank Tsuyoshi Okubo and Yohei Fuji for fruitful discussions. T.Y. was supported by World-leading Innovative Graduate Study Program for Materials Research, Information, and Technology (MERIT-WINGS) of the University of Tokyo. T.Y. was also supported by JSPS KAKENHI Grant No. JP23KJ0672. N.Y. wishes to thank JST PRESTO No. JPMJPR2119, JST Grant No. JPMJPF2221, JST CREST Grant No. JPMJCR2314, IBM Quantum, and JST ERATO Grant No. JPMJER2302, Japan. T.S. was supported by JST ERATO-FS

Grant No. JPMJER2204, JST ERATO Grant No. JPMJER2302, Japan, JSPS KAKENHI Grant No. JP19H05796, and JST CREST Grant No. JPMJCR20C1. N.Y. and T.S. were also supported by Institute of AI and Beyond of the University of Tokyo.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: EXPRESSIONS OF MULTIPARTITE WORK DEFICIT

1. Expression of W_l

We here show that extractable work through zero-way closed LOCC is expressed as

$$W_l = N \ln d - \min_{\Lambda \in \mathcal{M}_N} H_\Lambda(Y_N). \quad (\text{A1})$$

To derive this expression from Eq. (3), we need to show that optimal measurement protocol is always rank 1. In the following, we prove that for any measurement protocol Λ that includes higher-rank projectors, there exists a certain protocol Λ' consisting solely of rank-1 projectors, such that $W_{\Lambda'} \geq W_\Lambda$ is satisfied.

In the zero-way closed LOCC, the allowed local measurement on each party is not arbitrary POVM but *projective* measurement. Therefore, the measurement protocol Λ is described by the sets of orthogonal projectors, represented as $\{\Pi_{y_1}\}, \{\Pi_{y_2}\}, \dots, \{\Pi_{y_N}\}$. In this case, the conditional density operator on the n th party is defined as

$$p_\Lambda(y_n) \tilde{\rho}_n^{\Lambda, y_n} \equiv \Pi_{y_n} \rho_n \Pi_{y_n},$$

where $p_\Lambda(y_n)$ represents the probability of the measurement outcome y_n . The rank-1 measurement protocol Λ' , which satisfies $W_{\Lambda'} \geq W_\Lambda$, can be constructed by replacing each higher-rank projector Π_{y_n} in Λ with its fine-grained rank-1 projectors $\{\Pi_{x_n}^{y_n} \Pi_{y_n}\}_{x_n}$, where $\{\Pi_{x_n}^{y_n}\}_{x_n}$ is the projectors on the diagonal basis of the conditional density operator defined as $\tilde{\rho}_n^{\Lambda, y_n} = \sum_{x_n} q^{y_n}(x_n) \Pi_{x_n}^{y_n}$. By representing the measurement outcomes for protocol Λ' as $(Y_n, X_n) \equiv (y_1, x_1, y_2, x_2, \dots, y_n, x_n)$, we can derive the inequality $W_{\Lambda'} \geq W_\Lambda$ as follows:

$$\begin{aligned} W_{\Lambda'} &= N \ln d - H_{\Lambda'}(Y_N, X_N) \\ &= N \ln d - \sum_{n=1}^N H_{\Lambda'}(y_n, x_n | Y_{n-1}, X_{n-1}) \\ &\geq N \ln d - \sum_{n=1}^N H_{\Lambda'}(y_n, x_n | Y_{n-1}) \\ &= N \ln d - \left\{ \sum_{n=1}^N H_{\Lambda'}(x_n | Y_n) + H_{\Lambda'}(y_n | Y_{n-1}) \right\} \\ &\geq N \ln d - \left\{ \sum_{n=1}^N H_{\Lambda'}(x_n | y_n) + H_{\Lambda'}(y_n | Y_{n-1}) \right\} \\ &= N \ln d - \sum_{n=1}^N \left\{ \sum_{y_n} p_\Lambda(y_n) S(\tilde{\rho}_n^{\Lambda, y_n}) \right\} - H_\Lambda(Y_N) = W_\Lambda. \end{aligned}$$

2. Expression with quantum relative entropy

We here show the equivalence of the two expressions of multipartite work deficit, namely, Eqs. (5) and (6). Equation (5) can be transformed into the representation with quantum relative entropy as

$$\begin{aligned} \min_{\Lambda \in \mathcal{M}_N} H_\Lambda(Y_N) - S(\rho) &= \min_{\Lambda \in \mathcal{M}_N} S(\mathcal{D}_\Lambda(\rho)) - S(\rho) \\ &= \min_{\Lambda \in \mathcal{M}_N} S(\rho \| \mathcal{D}_\Lambda(\rho)), \end{aligned} \quad (\text{A2})$$

where $\mathcal{D}_\Lambda$ denotes the dephasing map with respect to the measurement basis of Λ . Since $\mathcal{D}_\Lambda(\rho) \in \mathcal{C}_N$, the following inequality holds:

$$\min_{\Lambda \in \mathcal{M}_N} S(\rho \| \mathcal{D}_\Lambda(\rho)) \geq \min_{\sigma \in \mathcal{C}_N} S(\rho \| \sigma). \quad (\text{A3})$$

Furthermore, quantum relative entropy of ρ with respect to a classically correlated state $\sigma = \sum_{Y_N} q(Y_N) \Pi_{y_1} \otimes \Pi_{y_2} \otimes \dots \otimes \Pi_{y_N}$ can be decomposed as

$$S(\rho \| \sigma) = S(\rho \| \mathcal{D}_\sigma(\rho)) + S(\mathcal{D}_\sigma(\rho) \| \sigma),$$

where $\mathcal{D}_\sigma$ denotes the dephasing map with respect to the diagonal basis of σ . Therefore, we can derive the following inequality:

$$\begin{aligned} \min_{\sigma \in \mathcal{C}_N} S(\rho \| \sigma) &= \min_{\sigma \in \mathcal{C}_N} S(\rho \| \mathcal{D}_\sigma(\rho)) + S(\mathcal{D}_\sigma(\rho) \| \sigma) \\ &\geq \min_{\Lambda \in \mathcal{M}_N} S(\rho \| \mathcal{D}_\Lambda(\rho)). \end{aligned} \quad (\text{A4})$$

From Eqs. (A2), (A3), and (A4), we can derive the equivalence of Eqs. (5) and (6) as follows:

$$\min_{\Lambda \in \mathcal{M}_N} H_\Lambda(Y_N) - S(\rho) = \min_{\sigma \in \mathcal{C}_N} S(\rho \| \sigma). \quad (\text{A5})$$

APPENDIX B: EFFICIENT CALCULATION METHOD FOR WORK DEFICIT DENSITY δ

1. Upper bound $U_{l,k}$

We here introduce the definition of the upper bound $U_{l,k}$ of work deficit density δ , which is defined for the translationally invariant state with periodic boundary condition. This is regarded as a generalization of the upper bound U_l , which is defined as follows:

$$U_l \equiv \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\Lambda \in \mathcal{M}_{n:l}} H_\Lambda(Y_{n:l}) - S(\rho) \right\}, \quad (\text{B1})$$

where $\mathcal{M}_{n:l}$ describes the set of measurement protocols whose measurement operators are denoted as

$$\{\Pi_{y_{n+1}} \otimes \Pi_{y_{n+2}} \otimes \dots \otimes \Pi_{y_{n+l}}\}_{Y_{n:l}}.$$

Here, $\{\Pi_{y_{n+i}}\}$ represents the set of orthogonal rank-1 projectors on party a_{n+i} . For the translationally invariant system under periodic boundary condition, U_l is represented as

$$U_l = \frac{1}{l} \min_{\Lambda \in \mathcal{M}_{n:l}} H_\Lambda(Y_{n:l}) - \frac{S(\rho)}{N}, \quad (\text{B2})$$

since all the terms in the summation $\{\min_{\Lambda \in \mathcal{M}_{n:l}} H_\Lambda(Y_{n:l})\}_{n \in I_l}$ are identical.

For such states, the upper bound $U_{l,k}$ is defined as follows, which is reduced to Eq. (B2) when $k = 0$:

$$U_{l,k} \equiv \frac{kl}{N} \ln d + \frac{1}{l} \min_{\Lambda \in \mathcal{M}_l} H_{\Lambda^{\otimes(k+1)}}(Y_{n:l}|Y_{n-kl:kl}) - \frac{S(\rho)}{N}, \quad (\text{B3})$$

where $\mathcal{M}_l$ is the set of local projective measurements on the l -site segment, and the measurement protocol $\Lambda^{\otimes(k+1)}$ is to perform the identical measurement Λ on $(k+1)$ sequential l -site segments, specifically $\{a_i\}_{i=n-kl+1}^{n-kl+l}, \dots, \{a_i\}_{i=n+1}^{n+l}$. We note that in the thermodynamic limit $N \rightarrow \infty$, the first term in Eq. (B3) is negligible. We can derive the inequality $\delta \leq U_{l,k}$ as follows:

$$\begin{aligned} \delta &= \frac{1}{N} \min_{\Lambda \in \mathcal{M}_N} \left\{ \sum_{n \in I_l} H_{\Lambda}(Y_{n:l}|Y_n) \right\} - \frac{S(\rho)}{N} \\ &\leq \frac{1}{N} \min_{\Lambda \in \mathcal{M}_N} \left\{ \sum_{n \in I_l} H_{\Lambda}(Y_{n:l}|Y_{n-kl:kl}) \right\} - \frac{S(\rho)}{N} \\ &\leq \frac{1}{N} \min_{\Lambda \in \mathcal{M}_l} \left\{ \sum_{n \in I_l} H_{\Lambda^{\otimes(k+1)}}(Y_{n:l}|Y_{n-kl:kl}) \right\} - \frac{S(\rho)}{N} \\ &\leq \frac{1}{N} \min_{\Lambda \in \mathcal{M}_l} \left\{ \sum_{\substack{n \in I_l \\ n \geq kl}} H_{\Lambda^{\otimes(k+1)}}(Y_{n:l}|Y_{n-kl:kl}) \right\} + \frac{kl \ln d}{N} - \frac{S(\rho)}{N} \\ &= \left(\frac{1}{l} - \frac{k}{N} \right) \min_{\Lambda \in \mathcal{M}_l} H_{\Lambda^{\otimes(k+1)}}(Y_{n:l}|Y_{n-kl:kl}) + \frac{kl \ln d}{N} - \frac{S(\rho)}{N} \\ &\leq U_{l,k}. \end{aligned}$$

The equality in the fifth line follows from the fact that all the terms in the summation $\{H_{\Lambda^{\otimes(k+1)}}(Y_{n:l}|Y_{n-kl:kl})\}_{n \in I_l, n \geq kl}$ are identical due to the translation invariance of the system and measurement protocol.

2. Reduction of the optimization region for the lower bounds

We provide a detailed discussion on the optimization involved in the definition of the lower bound L_l . The lower bound is defined as

$$L_l \equiv \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\mu \in \mathcal{E}_n} \min_{\pi \in \mathcal{M}_{n:l}} H_{(\mu, \pi)}(Y_{n:l}|Z_n) - S(\rho) \right\}, \quad (\text{B4})$$

where $\mathcal{E}_n$ denotes the set of arbitrary POVMs on the parties $\{a_i\}_{i=1}^n$ and $\mathcal{M}_{n:l}$ represents the set of local projective measurements on the neighboring l parties $\{a_i\}_{i=n+1}^{n+l}$. Equation (B4) is equivalent to the representation in Eq. (15), since the measurement protocol $\Lambda \in \mathcal{N}_{n:l}$ is divided into $\mu \in \mathcal{E}_n$ and $\pi \in \mathcal{M}_{n:l}$ as $\Lambda = (\mu, \pi)$. The measurement operators for (μ, π) are given by

$$\{E_{Z_n} \otimes \Pi_{y_{n+1}} \otimes \Pi_{y_{n+2}} \otimes \dots \otimes \Pi_{y_{n+l}}\}_{Z_n, Y_{n:l}},$$

where $\{E_{Z_n}\}$ is the set of POVM operators for μ and $\{\Pi_{y_{n+i}}\}$ is the set of orthogonal projectors on party a_{n+i} . Since the Hilbert space dimension of the subsystem $\{a_i\}_{i=1}^n$ is d^n , the optimization cost for $\mu \in \mathcal{E}_n$ appears to grow exponentially with respect to n , at first glance.

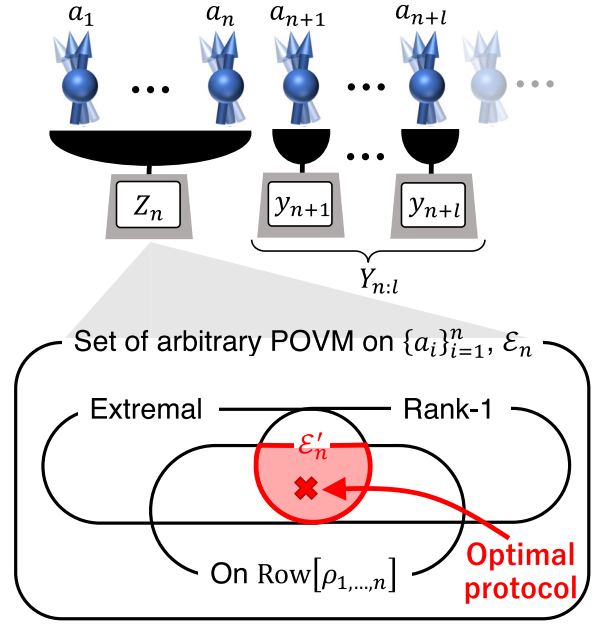


FIG. 9. Reduction of the optimization region in the calculation of lower bound L_l . Although the lower bound L_l includes the optimization over the set of arbitrary POVMs on the parties $\{a_i\}_{i=1}^n$, denoted as $\mathcal{E}_n$, this optimization region can be effectively reduced to the set of extremal rank-1 POVMs on $\text{Row}[\rho_{1,\dots,n}]$, denoted as $\mathcal{E}'_n$ (Theorem B1). Especially for the MPS with fixed bond dimension D_B , optimization over the reduced region $\mathcal{E}'_n$ can be performed at a constant cost independent of n .

However, we here show that this cost can be reduced to constant independent of n , for MPS with fixed bond dimension D_B . While we have only provided an intuitive explanation for this cost reduction in the main text, suggesting that the subsystem $\{a_i\}_{i=1}^n$ is regarded as a fixed-dimensional system, we present a more detailed discussion in this subsection. Specifically, we show that the optimization region $\mathcal{E}_n$ for the POVM μ can be reduced to the set of rank-1 extremal POVMs on $\text{Row}[\rho_{1,\dots,n}]$ denoted as $\mathcal{E}'_n$, as illustrated in Fig. 9. Here, $\text{Row}[\rho_{1,\dots,n}]$ is the row space of the reduced density operator $\rho_{1,\dots,n}$, namely, the subspace spanned by the row vectors of $\rho_{1,\dots,n}$. For an MPS with bond dimension D_B , the dimension for $\text{Row}[\rho_{1,\dots,n}]$ is fixed (D_B for open boundary condition and D_B^2 for periodic boundary condition). A rank-1 POVM is a class of POVM defined by rank-1 operators $\{E_{Z_n}\}$, and an extremal POVM is one that cannot be described as a convex combination of other POVMs [129,130]. This reduction of optimization region is stated as the following theorem:

Theorem B1. Let $\mathcal{E}_n$ be the set of arbitrary POVMs on parties $\{a_i\}_{i=1}^n$ and $\mathcal{E}'_n$ be the set of rank-1 extremal POVMs on $\text{Row}[\rho_{1,\dots,n}]$. Then, the following equality is satisfied:

$$\begin{aligned} L_l &\equiv \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\mu \in \mathcal{E}_n} \min_{\pi \in \mathcal{M}_{n:l}} H_{(\mu, \pi)}(Y_{n:l}|Z_n) - S(\rho) \right\} \\ &= \frac{1}{N} \left\{ \sum_{n \in I_l} \min_{\mu \in \mathcal{E}'_n} \min_{\pi \in \mathcal{M}_{n:l}} H_{(\mu, \pi)}(Y_{n:l}|Z_n) - S(\rho) \right\}. \quad (\text{B5}) \end{aligned}$$

The proof of this theorem is provided in the Supplemental Material [93]. Since the rank-1 extremal POVM on x -dimensional system is described with fewer than x^2 rank-1 measurement operators $\{E_{z_n}\}$ [129,130], the optimization of μ within $\mathcal{E}'_n$ can be performed at a constant cost independent of n . This is crucial for the lower bound L_l to be calculated with linear cost with respect to the system size N (Table I).

3. Lower and upper bounds for states approximated by MPS

While we have primarily focused on systems exactly represented by MPS, we here explain that our efficient calculation method is applicable also for states *approximated* by MPS. Specifically, we consider the state ρ that is approximated with an MPS ρ' with fixed bond dimension. To evaluate the lower bound $L_l(\rho)$, we utilize the fact that it is well approximated with $L_l(\rho')$, which is efficiently computable as the consequence of Theorem B1. To be more precise, we derive the following theorem:

Theorem B2. Let ρ and ρ' be the states satisfying $\|\rho - \rho'\|_{\text{tr}} \leq v$, where $\|X\|_{\text{tr}} \equiv \text{Tr}[|X|]$ denotes the trace norm. Then, the following inequalities are satisfied:

$$|U_l(\rho) - U_l(\rho')| \leq \tilde{\mathcal{O}}(v), \quad (\text{B6})$$

$$|L_l(\rho) - L_l(\rho')| \leq \tilde{\mathcal{O}}(v). \quad (\text{B7})$$

The proof of this theorem is provided in the Supplemental Material [93]. Since Eq. (B7) implies the inequality

$$\delta(\rho) \geq L_l(\rho) \geq L_l(\rho') - \tilde{\mathcal{O}}(v),$$

we can obtain the efficiently computable lower bound of $\delta(\rho)$ through the calculation in the MPS ρ' .

4. Tightness of the lower and upper bounds

We here derive the systematic improvement of our lower and upper bounds by increasing the locality parameter l . Especially for MPS with fixed bond dimension D_B , we can derive the inequality

$$U_l - L_l \leq \mathcal{O}\left(\frac{1}{l}\right). \quad (\text{B8})$$

This inequality shows that we can achieve arbitrary accuracy ε by increasing the locality l . In the derivation, we utilize the measurement protocol $\Lambda_{n:l}^* \in \mathcal{N}_{n:l}$, which achieves the minimum for $\min_{\Lambda \in \mathcal{N}_{n:l}} H_\Lambda(Y_{n:l}|Z_n)$. With this notation, we can derive the inequality (11) as follows:

$$\begin{aligned} U_l - L_l &\leq \frac{1}{N} \left\{ \sum_{n \in I_l} H_{\Lambda_{n:l}^*}(Y_{n:l}) - H_{\Lambda_{n:l}^*}(Y_{n:l}|Z_n) \right\} \\ &= \frac{1}{N} \sum_{n \in I_l} H_{\Lambda_{n:l}^*}(Y_{n:l} : Z_n) \\ &\leq \frac{1}{N} \sum_{n \in I_l} I_{\{a_i\}_{i=1}^n, \{a_i\}_{i=n+1}^{n+l}}(\rho) \end{aligned}$$

$$\begin{aligned} &\leq \frac{1}{N} \left\{ \sum_{n \in I_l} S(\rho_{1,\dots,n}) + S(\rho_{n+1,\dots,n+l}) \right\} \\ &\leq \frac{1}{l} 4 \ln D_B = \mathcal{O}\left(\frac{1}{l}\right). \end{aligned}$$

Here, $H_\Lambda(y : z) \equiv H_\Lambda(y) + H_\Lambda(z) - H_\Lambda(y, z)$ represents the classical mutual information between measurement outcomes y and z under the measurement protocol Λ , and $I_{a_1,a_2}(\rho) \equiv S(\rho_1) + S(\rho_2) - S(\rho_{1,2})$ represents the quantum mutual information between parties a_1 and a_2 . The inequality in the third line follows from the fact that quantum mutual information decreases monotonically under local CPTP (completely positive and trace-preserving map), which is the consequence of the monotonicity of quantum relative entropy [131]. In the derivation of the final line, we utilize that the system is described with an MPS with a fixed bond dimension D_B .

Additionally, we can derive the following inequalities, which are satisfied in general, not only in MPS:

$$L_l \leq L_{kl}, \quad U_{kl} \leq U_l. \quad (\text{B9})$$

The inequality $L_l \leq L_{kl}$ can be derived as

$$\begin{aligned} L_{kl} &= \frac{1}{N} \left\{ \sum_{n \in I_{kl}} \min_{\Lambda \in \mathcal{N}_{n:kl}} H_\Lambda(Y_{n:kl}|Z_n) - S(\rho) \right\} \\ &= \frac{1}{N} \left\{ \sum_{n \in I_{kl}} \min_{\Lambda \in \mathcal{N}_{n:kl}} \sum_{j=0}^{k-1} H_\Lambda(Y_{n+jl:l}|Y_{n:jl}, Z_n) - S(\rho) \right\} \\ &\geq \frac{1}{N} \left\{ \sum_{n \in I_{kl}} \sum_{j=0}^{k-1} \min_{\Lambda \in \mathcal{N}_{n:(j+1)l}} H_\Lambda(Y_{n+jl:l}|Y_{n:jl}, Z_n) - S(\rho) \right\} \\ &\geq \frac{1}{N} \left\{ \sum_{m \in I_l} \min_{\Lambda \in \mathcal{N}_{m:l}} H_\Lambda(Y_{m:l}|Z_m) - S(\rho) \right\} \\ &= L_l, \end{aligned} \quad (\text{B10})$$

where subscript m in the fourth line corresponds to $n + jl$ in the third line, and therefore the inequality in the fourth line follows from the inclusion relation $\mathcal{N}_{n:(j+1)l} \subset \mathcal{N}_{n+jl:l}$. The inequality $U_{kl} \leq U_l$ can be derived as follows:

$$\begin{aligned} U_{kl} &= \frac{1}{N} \left\{ \sum_{n \in I_{kl}} \min_{\Lambda \in \mathcal{M}_{n:kl}} H_\Lambda(Y_{n:kl}) - S(\rho) \right\} \\ &= \frac{1}{N} \left\{ \sum_{n \in I_{kl}} \min_{\Lambda \in \mathcal{M}_{n:kl}} \sum_{j=0}^{k-1} H_\Lambda(Y_{n+jl:l}|Y_{n:jl}) - S(\rho) \right\} \\ &\leq \frac{1}{N} \left\{ \sum_{n \in I_{kl}} \min_{\Lambda \in \mathcal{M}_{n:kl}} \sum_{j=0}^{k-1} H_\Lambda(Y_{n+jl:l}) - S(\rho) \right\} \\ &\leq \frac{1}{N} \left\{ \sum_{m \in I_l} \min_{\Lambda \in \mathcal{M}_{m:l}} H_\Lambda(Y_{m:l}) - S(\rho) \right\} \\ &= U_l, \end{aligned} \quad (\text{B11})$$

where the subscript m in the fourth line corresponds to $n + jl$ in the third line.

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