Bounding entanglement entropy using zeros of local correlation matrices

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Correlation functions and entanglement are two different aspects to characterize quantum many-body states. While many correlation functions are experimentally accessible, entanglement entropy (EE), the simplest characterization of quantum entanglement, is usually difficult to measure. In this Letter, we propose a protocol to bound EE by local measurements. This protocol utilizes local correlation matrices and focuses on their (approximate) zero eigenvalues. Given a quantum state, each (approximate) zero eigenvalue can be used to define a set of local projection operators. An auxiliary Hamiltonian can then be constructed by summing these projectors. When the construction only involves projectors of zero eigenvalues, we prove the EE of a subsystem is bounded by the ground-state degeneracy of the auxiliary Hamiltonian on this subsystem. When projectors from nonzero eigenvalues are included, we show the EE can be bounded by a thermal entropy of the subsystem. Our protocol can be applied experimentally to investigate exotic quantum many-body states prepared in quantum simulators.

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Introduction. Entanglement not only plays an essential role in quantum information science but also becomes more and more important in modern studies of quantum matters [1–3]. Entanglement entropy (EE) can characterize quantum thermalization [4], describe quantum critical [5–9] and topologically ordered states [10,11], and bridge quantum correlation and the geometric metric in holographic quantum matter [12–14]. On the other hand, conventional characterizations of quantum matters are based on correlation functions and physical observables [15]. It is therefore natural to seek connections between EE and correlation functions or physical observables.

There are several well-established connections. It is known that the mutual information can be used to bound correlation functions [16,17]. The scrambling of entanglement is also directly related to the out-of-time-ordered correlator [18–23]. Experimentally, the Rényi entropy can be determined by measuring the shift operator between multiple copies of the target quantum state [24–28] or averaging over randomized measurements on single copies of a given quantum state [29–34]. Nevertheless, these protocols usually suffer from large statistical fluctuations as the subsystem size increases. Hence, experimental measurements of EEs so far are limited to small subsystem sizes.

In this Letter, we bring out a connection between the bound of the EE and the (approximate) zeros in the correlation matrix. The correlation matrix is first introduced [35] in the Hamiltonian reconstruction problem of “recovering” the Hamiltonian from one of its excited states [36]. Here, we introduce a slightly generalized local version of the correlation matrix and use it to bound the EE of a state. The local correlation matrix is Hermitian and positive semidefinite with non-negative eigenvalues. We focus on (approximate) zeros among all eigenvalues of the correlation matrix. Each (approximate) zero gives rise to a set of projection operators $\hat{P}_i$ which (approximately) satisfies $\hat{P}_i |\psi\rangle = 0$ and constrains $|\psi\rangle$. To quantify the extent of these constraints and give an upper bound of the EE, we introduce a positive semidefinite auxiliary Hamiltonian as the sum of these projectors multiplied by positive prefactors. When only projectors of zero eigenvalues are included, we prove that the von Neumann EE is upper bounded by the logarithm of the ground-state degeneracy of the auxiliary Hamiltonian constructed on the subsystem. When projectors of approximate zeros are included, the EE of a subsystem can be bounded by the thermal entropy at a temperature determined by the subsystem energy of the state.

Protocol. We first present our protocol, schematically shown in Fig. 1, of including only projectors from zero eigenvalues in the auxiliary Hamiltonian. It follows stepwisely from the following three statements and connects correlation functions and EE. It is schematically shown in Fig. 1 and is discussed in detail below.

Statement 1: From correlation matrix to eigenoperators. We consider a continuous region of $k$ sites and a set of linearly independent $k$-local operators $\{ \hat{L}_i \}$ acting only in this region. For a given quantum many-body state $|\psi\rangle$, we introduce its
Intuitively, the existence of a set of such projectors $\hat{P}_i$ means the wave function $|\psi\rangle$ tends to have a simple form and be low entangled. This is in contrast to a generic volume-law eigenstate where such local projectors $\hat{P}_i$ do not exist as implied by the uniqueness of the Hamiltonian reconstruction process [35]. This also means we should find as many such projectors as we can if we want to give a good upper bound on the EE of $|\psi\rangle$ of a subsystem $A$. To this end, we first exhaust all continuous regions of $k$ sites in $A$ and collect all $k$-local projection operators $\hat{P}_i$ constructed above (refer to Sec. I of the Supplemental Material [37] for a visual demonstration). We then construct a positive semidefinite auxiliary Hamiltonian on $A$ by summing these projectors multiplied by positive numbers,

$$\hat{H}_{aux}^A = \sum_\alpha c_\alpha \hat{\lambda}_\alpha = \sum_i c_i \hat{P}_i, \quad c_\alpha > 0, \quad c_i > 0,$$

where $\alpha$ enumerates $\hat{\lambda}_\alpha$ operators of zero eigenvalues of local correlation matrices on all $k$-site regions and $c_i = \sum_\alpha \bar{c}_\alpha a_i$ according to Eq. (5). The introduction of $\hat{H}_{aux}^A$ will prove to be convenient for us to discuss the bound of EE.

Statement 3: From auxiliary Hamiltonian to the EE bound—
the ground-state degeneracy and the entanglement entropy (GSD-EE) theorem. If $D^A$ denotes the ground-state degeneracy of $\hat{H}_{aux}^A$ under the open boundary condition (OBC), the von Neumann EE of $|\psi\rangle$ between this subsystem $A$ and the rest of the system $B$ is upper bounded by $\log D^A$.

Proof. Because $\hat{P}_i|\psi\rangle = 0$ and $\hat{P}_i$ only acts on the subsystem $A$, the reduced density matrix $\hat{\rho}_A = Tr_B|\psi\rangle\langle\psi|$ satisfies

$$Tr_A(\hat{P}_i \hat{\rho}_A) = Tr_A(Tr_B \hat{P}_i |\psi\rangle\langle\psi|) = 0.$$ (7)

Diagonalizing $\hat{\rho}_A$ with a set of orthonormal basis $\{|\psi_k\rangle\}$, $\hat{\rho}_A = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ where $p_k > 0$, we can cast the above relation into the following form,

$$Tr_A(\hat{P}_i \hat{\rho}_A) = \sum_k p_k |\langle\psi_k|\hat{P}_i|\psi_k\rangle|^2.$$ (8)

It becomes clear that $\hat{P}_i|\psi\rangle = 0$ for every $|\psi_k\rangle$ and $\hat{P}_i$. Therefore, $|\psi_k\rangle$ is the ground state of $\hat{H}_{aux}^A$ with zero energy since $\hat{H}_{aux}^A$ is positive semidefinite. Consequently, the number of nonzero $p_k$ is no bigger than the ground-state degeneracy $D^A$ of the $\hat{H}_{aux}^A$, and the von Neumann EE is upper bounded by $\log D^A$.

Bounding EE of a large subsystem $A$ requires the determination of $D^A$ on the same large subsystem $A$, and to this end we have specially designed an algorithm (refer to Sec. IV of the Supplemental Material [37] for details). For a one-dimensional (1D) system, as a corollary of our GSD-EE theorem, if $D^A$ is upper bounded by a power law of the subsystem size $\sim L_A^\eta$, the EE is then upper bounded by $\sim \log L_A$, indicating the state is subvolume entangled. A few remarks are in order before we move on to specific examples. First, the operator space that the set of eigenvectors $\{|\hat{O}_\alpha\rangle\}$ spans does not depend on the form of $\hat{O}_\alpha$ as long as they span the same operator space $\mathcal{V}$. Second, the EE upper bound does not depend on the form of $\hat{O}_\alpha$, i.e., the choice of $\{e_i\}$, in the case of the zero eigenvalue of $\mathcal{M}$ being degenerate (see Sec. II of the Supplemental Material [37] for a proof). Finally, larger $\mathcal{V}$

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FIG. 1. Correlation functions and entanglement entropy are two different tools to characterize a quantum many-body state. This work establishes a connection between correlation and entanglement, based on the three statements discussed in the text.

Hermitian correlation matrix $\mathcal{M}$ with element $\mathcal{M}_{ij}$ defined as

$$\mathcal{M}_{ij} = \langle \psi | \hat{L}_j \hat{L}_i | \psi \rangle - \langle \psi | \hat{L}_j | \psi \rangle \langle \psi | \hat{L}_i | \psi \rangle.$$ (1)

Denote the eigenvalues of $\mathcal{M}$ as $\lambda_i$ and the corresponding eigenvectors as $e_i$. For each zero eigenvalue $\lambda_0$, if exists, one can use $e_i$ to construct an eigenvector $\hat{O}$ of $|\psi\rangle$ where $\hat{O}|\psi\rangle = \xi|\psi\rangle$ for some constant $\xi$.

**Proof.** Let us denote $\{e_i = (w_1, w_2, \ldots, w_n)\}$ and construct an operator $\hat{O} = \sum_i w_i \hat{L}_i$. Then, if $\lambda_0 = 0$, we have

$$\langle \psi | \hat{O}^\dagger \hat{O} | \psi \rangle - \langle \psi | \hat{O}^\dagger | \psi \rangle \langle \psi | \hat{O} | \psi \rangle = \sum_{ij} w_i^* \mathcal{M}_{ij} w_j = 0.$$ (2)

On the other hand, let $\hat{O}|\psi\rangle = \xi|\psi\rangle + |\psi\rangle$ with $|\psi\rangle = 0$, and the above relation translates to

$$0 = \langle \psi | \hat{O}^\dagger \hat{O} | \psi \rangle - \langle \psi | \hat{O}^\dagger | \psi \rangle \langle \psi | \hat{O} | \psi \rangle = \langle \psi | \psi \rangle,$$

meaning $\hat{O}|\psi\rangle = \xi|\psi\rangle$. Clearly, the number of independent eigenvectors $\hat{O}$ one can construct in this way equals the geometric/algebraic multiplicity of eigenvalue zero. □

**Statement 2:** From eigenoperators to auxiliary Hamiltonian. From each eigenvector $\hat{O}$, one can construct a set of projection operators $\{\hat{P}_i\}$, each of which annihilates the state, $\hat{P}_i|\psi\rangle = 0$.

**Proof.** Let us denote $\hat{\lambda}$ the positive semidefinite operator defined as ($\hat{I}$ being the identity operator)

$$\hat{\lambda} = (\hat{O}^\dagger - \xi^2 \hat{I})(\hat{O} - \xi \hat{I}).$$ (4)

and $|i\rangle$ the basis that diagonalizes $\hat{\lambda}$,

$$\hat{\lambda} = \sum_i a_i |i\rangle \langle i| \equiv \sum_i a_i \hat{P}_i,$$ (5)

where $a_i > 0$. Since $\hat{\lambda}$ annihilates the state and $0 = \langle \psi | \hat{\lambda} | \psi \rangle = \sum_i a_i \langle \psi | \hat{P}_i | \psi \rangle = \sum_i a_i \langle \psi | \hat{P}_i^2 | \psi \rangle = \sum_i a_i \|\hat{P}_i | \psi \rangle \|^2$, it follows that each $\hat{P}_i$ annihilates the state, $\hat{P}_i|\psi\rangle = 0$. Moreover, the projectors $\hat{P}_i$ are k-local operators since $\hat{O}$ is k-local. □
in general leads to a better upper bound with, however, more numerical/experimental effort to obtain $M$. Consequently, we should make a balance and choose a moderate number of operators. Nevertheless, using the 1-local operator basis, our protocol already gives the perfect EE upper bound of zero for product states (this is proved in Sec. III of the Supplemental Material [37]).

**Examples.** Below we shall apply the GSD-EE theorem to the scar states in the generalized Affleck-Kennedy-Lieb-Tasaki (AKLT) model and the ground state of the toric code model.

**Example 1: Scar states in the AKLT model.** The 1D AKLT model and its generalizations are known to host a series of quantum many-body scar states described the spectrum generating algebra [38,39]. These scar states admit the following analytical expression,

$$|\psi_n\rangle = (\hat{Q}^i)^n |G\rangle ,$$

where $\hat{Q} = \sum_i (-1)^i \hat{S}_i^z \hat{S}_i^x$ with $i$ being the site index and $\hat{S}_i^z$ being the spin raising operator at site $i$, and $|G\rangle$ is the ground state of the AKLT model under the periodic boundary condition (PBC). Here, the system size $L$ is assumed to be even, $n = 0, 1, \ldots, L/2 - 1$ for odd $L/2$, and $n = 0, 1, \ldots, L/2$ for even $L/2$.

To construct the correlation matrices, we choose 3-local operators ($\hat{L}_i$) that are constructed as tensor products of the Gell-Mann matrices,

$$\hat{L}_i = \lambda_a^{(1)} \otimes \lambda_b^{(2)} \otimes \lambda_c^{(3)},$$

where $a, b, c = 1, \ldots, 8$ are the indices of the eight standard Gell-Mann matrices and the superscripts 1, 2, 3 denote three successive sites. As an illustrative example, we choose the state $|\psi_1\rangle = \hat{Q} |G\rangle$ and construct the auxiliary Hamiltonian, following the general protocol described above. Since our target state is translational invariant up to a sign, we just need to construct the local correlation matrix of arbitrary three neighboring sites: All the other projectors entering the auxiliary Hamiltonian are obtained by simply translating the local projectors of this correlation matrix. It turns out that projectors constructed from $|\psi_1\rangle$ also annihilate all the scar states $|\psi_n\rangle$ for all system sizes $L > 3$ (refer to Sec. V in the Supplemental Material [37] for details). Thus the EE scaling behavior obtained for our target state $|\psi_1\rangle$ will also bound all other scar states $|\psi_n\rangle$. Using our specially designed algorithm, we are able to determine the ground-state degeneracy $D^4$ of the auxiliary Hamiltonian up to system size $L_A$ of a few hundred. We numerically find that $D^4 = 2L_A + 2$, which means the EE at most scales with the logarithm of the subsystem size.

To benchmark the effectiveness of our EE bounds, we numerically calculate the exact values of the bipartite EEs of all the scar states. Since our result bounds all the $|\psi_n\rangle$, we compare our bound with the maximum value of the numerically calculated values. As shown in Fig. 2, the numerical EE maximum is approaching $(\log L_A)/2$, and our bound is asymptotically $\log L_A$ (similar results are also obtained for scar states in the extended Fermi-Hubbard model—see Sec. VI of the Supplemental Material [37]). Further increasing the operator range to $k = 4$ and $k = 5$, we find that $D^4$ remains the same as that of $k = 3$ in both cases and that our upper bound no longer be improved. A natural guess is that our EE bound using $k = 3$ is already tight. The reason behind our conjecture is that our bound actually applies not only to pure states $(\hat{Q}^i)^n |G\rangle$, but also to linear superpositions of them and even to mixed states constructed from them.

**Example 2: Ground states of the toric code model.** Our formalism can be easily applied to stabilizer states [40–42]. Let us take the ground state of the toric code model [43] as a concrete example. Consider a 2D square lattice with qubits living on links and, say, with the PBC. The toric code model is defined by the following Hamiltonian,

$$H_{TC} = -\sum_{\text{vertices}} X + \sum_{\text{faces}} Z .$$

Each term in the first (second) sum is a product of four Pauli-\(X\) (Pauli-\(Z\)) operators around a vertex (face), and is dubbed a star (plaquette) term. All the terms in $H_{TC}$ commute with each other, and the ground state of the Hamiltonian is a simultaneous eigenstate of all the star and plaquette terms with eigenvalue +1. Now consider a rectangular subsystem as shown in Fig. 3(a) or 3(b), and let us try to evaluate the EE for such a ground state. Since each star or plaquette term is proportional to a projector up to a constant shift, we may skip the initial steps of our formalism and directly construct the auxiliary Hamiltonian $H_{aux}^T$, as the negative sum of all the star and plaquette terms that are completely inside $A$, and the EE

$$S^B \approx \log D^A ,$$

FIG. 2. Comparison between the upper bounds of the bipartite EE obtained by the ground-state degeneracy of the auxiliary Hamiltonian (green dots) and the computed maximum bipartite EEs of all the scar states (blue dots), Eq. (9), in the AKLT model.

FIG. 3. Two examples of a rectangular subsystem. The EE of the ground state of the toric code model takes the form $S = (\log P_v - 1) \log 2$ in both cases where $P_v$ is the perimeter of the shaded area.
is bounded from above by $\log D^A$. To compute $D^A$, notice that 

1. $\mu_{\beta^j}\Lambda^j$ form an independent set of stabilizers [40–42], which means (i) they are proportional to tensor products of the identity operator $I$ and Pauli operators $\hat{X}, \hat{Y}, \hat{Z}$, (ii) they square to the identity and mutually commute, and (iii) any product of a nonempty subset of those operators is not proportional to the identity (independence). 

These three properties imply that specifying the eigenvalue of each stabilizer will reduce the Hilbert space dimension by a half. Therefore, $D^A = 2^{n_A-n}$, where $n_A$ is the number of qubits in the subsystem, and $n$ is the number of stabilizers contained in $H^A_{\text{aux}}$. A simple counting shows $S_0 \leq \log D^A = (|\beta A| - 1) \log 2$, where $|\beta A|$ is the perimeter of the rectangular. This upper bound turns out to be exact. The first term proportional to $|\beta A|$ indicates the area law, and the subleading constant term is known as the topological entanglement entropy [10,11] signifying topological order.

Approximate zeros. In previous discussions, we have demonstrated we can obtain a useful upper bound on EE when the local correlation matrix contains exact zero eigenvalues. However, this protocol can easily fail. For one thing, the local correlation matrices of low entangled states, such as perturbed states of the ones considered in the previous section and many-body localized states, may contain only approximate zero eigenvalues. For another, errors are inevitable in experimentally measured correlation matrices. In this section, we extend previous results by providing an upper bound of EE when the correlation matrix contains approximate zero eigenvalues.

Statements 1 and 2 require minor revision: Instead of focusing only on zero eigenvalues, we also include eigenvalues $\lambda_\alpha < c$ with a finite cutoff $c$. Then following (4) and (5), we can define an additional set of projection operators $\hat{P}$. Except for including these extra projectors, the form of the auxiliary Hamiltonian (6) remains the same. Now, statement 3 needs to be modified.

Statement 3: From auxiliary Hamiltonian to the EE bound. Given the auxiliary Hamiltonian $H^A_{\text{aux}}$, we first compute its energy $E^A_{\text{aux}}$ of the state $|\psi\rangle$ as $E^A_{\text{aux}} = \text{Tr}_A(\hat{H}^A_{\text{aux}} \hat{\rho}_A) = \langle \psi | \hat{H}^A_{\text{aux}} | \psi \rangle$. We then consider the thermal reduced density matrix

$$\hat{\rho}^A_{\text{aux}}(\beta) = \exp \left( -\beta \hat{H}^A_{\text{aux}} \right)/Z^A_{\text{aux}}(\beta),$$

where $Z^A_{\text{aux}}$ is the partition function and determine the inverse temperature $\beta^*$ by matching the energy $\text{Tr}_A(\hat{H}^A_{\text{aux}} \hat{\rho}^A_{\text{aux}}(\beta^*)) = E^A_{\text{aux}}$. For all density matrices with the same energy, the thermal density matrix maximizes the entropy [44], the von Neumann EE of $|\psi\rangle$ is upper bounded by the thermal entropy $S_0(\beta^*) = -\text{Tr}_A[\hat{\rho}^A_{\text{aux}}(\beta^*) \log \hat{\rho}^A_{\text{aux}}(\beta^*)]$. When we only include projectors of exact zeros in the auxiliary Hamiltonian, the statement 3 can be reduced to the statement 3. In this case, we have $E^A_{\text{aux}} = 0$ and $\beta^* = \infty$, and consequently $S_0(\infty) = \log D^A$.

Example 3: Scar states in the PXP model. We apply our extended protocol to the scar states in the PXP model under the PBC [45–47]. We choose the range-$k$ operator basis $\hat{L}_i$ as

$$\hat{L}_i = \lambda^{(1)}_{aq_1} \otimes \lambda^{(2)}_{aq_2} \otimes \cdots \otimes \lambda^{(k)}_{aq_k},$$

with $[a_k] = \{0, 1, 2, 3\}$ being the indices of the identity matrix and Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$ (the identity operator where all $a_k$ are zero is excluded). In our numerical study, we choose the system size $L = 20$ and $k \in \{3, 4, 5\}$. Due to the Hilbert space restriction, the correlation matrices for both scar states and thermal eigenstates have the same number of trivial zero eigenvalues, but those for scar states have more approximate zeros. We only include the $\Delta_\alpha$ operators with a certain cutoff $\lambda_\alpha < c$ in the auxiliary Hamiltonian, and at the same time enforce the Hilbert space restriction, effectively setting $\tilde{c}_\alpha = \infty$ for the $\Delta_\alpha$ operators of trivial zeros. We then follow our protocol to compute the upper bounds (see Sec. VII of the Supplemental Material [37] for details). As shown in Fig. 4, for $k = 4, 5$, the upper bounds of EE from the thermal entropy $S(\beta^*)$ lead to a well separation between the thermal states and scar states.

Summary. In summary, we have developed a protocol that connects correlation and entanglement in a quantitative way, and tested it with exotic quantum states. Our method can be readily applied to experiments as an economic way of bounding the entanglement entropy of a quantum state. All one needs to measure are local physical observables that give rise to the matrix elements of the local correlation matrices (see Sec. VIII of the Supplemental Material [37] for an experimental protocol in cold atom systems). Different from methods that focus directly on the reduced density matrix [48–51], our method is divide-and-conquer in nature. This means our measurement cost to bound the EE of a subsystem $A$ only scales linearly with the subsystem size $L_A$. Moreover, for the exact zero case of eigenvalues of local correlation matrices, the numerical effort can be significantly reduced by our special algorithm. For the case of approximate zeros, however, using thermal entropy to bound entanglement entropy is costly and deserves further studies. Still, in this noisy intermediate-scale quantum era [52], we envision our protocol to be particular useful.

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[38] S. Mudgalay, N. Regnault, and B. A. Bernevig, Entanglement of exact excited states of Affleck-Kennedy-Lieb-Tasaki models:


