I. Illustration of Our Protocol of Exact Zeros Using 2-local Operator Basis

We shall further elucidate our protocol of bounding the entanglement entropy of a subsystem $A$ using $k = 2$-local operator basis $\{\hat{L}_i\}$ here. To facilitate understanding, we use a concrete example depicted in Fig. [S1]. The subsystem $A$ is shaded red, say with sites 2, 3, 4, 5, and of size $L_A = 4$. Our protocol is first to measure the correlation matrix on sites 2 and 3 (dotted black in the second row of Fig. [S1]), collect the $\hat{\Delta}$ operators (equivalently projection operators) following statements 1 and 2 in the main text. We then move to sites 3, 4 to repeat the above procedure, and then to sites 4, 5 for the same task. After exhausting all these continuous $k = 2$ subsystems inside $A$, we collect all those $\hat{\Delta}_\alpha$ to construct the auxiliary Hamiltonian $\hat{H}_A^{aux}$ following equation (6) in the main text. The final step is to utilize the GD-EE theorem to calculate the ground-state degeneracy $D_A$ that yields an upper bound of $\log D_A$ of the entanglement entropy of $A$.

![Diagram of steps of our protocol to bound entanglement entropy (EE) of subsystem A (shaded red) using 2-local operator basis \{\hat{L}_i\}. For every consecutive two sites (dotted black) in A, we use a set of 2-local operator basis \{\hat{L}_i\} acting on these two sites to construct the correlation matrix and determine the corresponding positive semidefinite operators \{\hat{\Delta}_{\alpha}^{(n)}\} where $n$ labels the choices of these two sites. The $\hat{\Delta}_\alpha$ operators that enters the auxiliary Hamiltonian comes from the union of these \{\hat{\Delta}_{\alpha}^{(n)}\}.]

II. Equivalence between Different Choices of Eigenvectors \{e_\alpha\} with Degeneracy

We shall show in the degenerate case where $\dim(\text{Ker}(M)) = n > 1$ the final result of $D_A$ does not depend on the choice of eigenvectors of zero eigenvalues (our Lemma 1 below). Let us denote the unitary matrix connecting two different sets of zero-eigenvalue basis $\{\tilde{e}_\alpha\}$ and $\{\check{e}_\alpha\}$ as $U$,

$$
\begin{pmatrix}
\tilde{e}_1 \\
\tilde{e}_2 \\
\vdots \\
\tilde{e}_n
\end{pmatrix} =
\begin{pmatrix}
U_{11} & U_{12} & \cdots & U_{1n} \\
U_{21} & U_{22} & \cdots & U_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
U_{n1} & U_{n2} & \cdots & U_{nn}
\end{pmatrix}
\begin{pmatrix}
e_1 \\
e_2 \\
\vdots \\
e_n
\end{pmatrix},
$$

(S1)
where we have used the shorthand notation \( \hat{\alpha} \). Summing the \( e \)

we can write the product state as

\[
|\psi\rangle = \sum_{\alpha} U_{\alpha\beta} |\psi\rangle = \sum_{\beta} U_{\alpha\beta} |\psi\rangle \equiv \tilde{\xi}_\alpha |\psi\rangle ,
\]

where we have identified \( \tilde{\xi}_\alpha = \sum_{\beta} U_{\alpha\beta} \xi_{\beta}. \) The corresponding positive semidefinite operator \( \hat{\Delta}_\alpha \) for the tilde version then reads

\[
\hat{\Delta}_\alpha = (\hat{O}_\alpha - \hat{\xi}_\alpha \hat{I})(\hat{O}_\alpha - \hat{\xi}_\alpha \hat{I}) = \sum_{\beta,\gamma} U_{\alpha\beta} U_{\alpha\gamma}^* (\hat{O}_\gamma^\dagger - \hat{\xi}_\gamma \hat{I})(\hat{O}_\beta - \hat{\xi}_\beta \hat{I}) .
\]

**Lemma 1.** The value of ground-state degeneracy of the auxiliary Hamiltonian, \( D^A \), is the same for different basis choices \( \{e_\alpha\} \) and \( \{\bar{e}_\alpha\} \).

**Proof.** It suffices to show if a ground state \( |G\rangle \) of the auxiliary Hamiltonian \( \hat{H}_{\text{aux}}^A \) satisfy \( \hat{\Delta}_\alpha |G\rangle = 0 \), \( \forall \alpha \), then \( \hat{\Delta}_\alpha |G\rangle = 0 \), \( \forall \alpha \) since we can reverse the role \( \{e_\alpha\} \) and \( \{\bar{e}_\alpha\} \) and repeat the whole process. From our condition \( \hat{\Delta}_\alpha |G\rangle = 0 \), \( \forall \alpha \) and Eq. (S4), we have

\[
\langle G | \sum_{\beta,\gamma} U_{\alpha\beta} U_{\alpha\gamma}^* (\hat{O}_\gamma^\dagger - \hat{\xi}_\gamma \hat{I})(\hat{O}_\beta - \hat{\xi}_\beta \hat{I}) |G\rangle = 0 .
\]

Summing the \( \alpha \) index and noting \( \sum_{\alpha} U_{\alpha\beta} U_{\alpha\gamma}^* = \delta_{\beta\gamma} \) (delta function), we have

\[
\langle G | \sum_{\beta} (\hat{O}_\gamma^\dagger - \hat{\xi}_\gamma \hat{I})(\hat{O}_\beta - \hat{\xi}_\beta \hat{I}) |G\rangle = \langle G | \sum_{\alpha} \hat{\Delta}_\alpha |G\rangle = 0 .
\]

where we have changed the dummy summation index from \( \beta \) to \( \alpha \). Since \( \hat{\Delta}_\alpha \) is positive semidefinite, the above equation implies

\[
\hat{\Delta}_\alpha |G\rangle = 0 , \quad \forall \alpha .
\]

Therefore, \( D^A \) does not depend on the choice of eigenvector basis in the degenerate space of zero eigenvalues.

**III. EE Bounds of Product States**

In this section, we take product states as an example for demonstrating the effectiveness of our GD-EE theorem. We shall prove the local correlation matrix of 1-local operator basis \( \{\tilde{L}_i\} \) is enough to give an EE upper bound of zero for produce state.

For definiteness, consider a spin-1/2 system and denote the local bases on a site as \( |0\rangle \) and \( |1\rangle \). Without loss of generality, we can write the product state as

\[
|\psi\rangle = \prod_i \otimes |0\rangle_i = |00\cdots0\rangle ,
\]

since one can always rotate local basis on every site freely. Now, choose the nontrivial 1-local operator basis as the standard Pauli operators \( \hat{X}, \hat{Y}, \) and \( \hat{Z} \). The correlation matrix, defined in Eq. (1) in our manuscript, is thus

\[
\mathcal{M}_{ij} = \langle \psi | \hat{\sigma}_i \hat{\sigma}_j | \psi \rangle - \langle \psi | \hat{\sigma}_i^+ | \psi \rangle \langle \psi | \hat{\sigma}_j | \psi \rangle
\]

where we have used the shorthand notation \( \hat{\sigma} \equiv (\hat{X}, \hat{Y}, \hat{Z}) \). The explicit form of \( \mathcal{M} \) can be easily written down

\[
\mathcal{M} = \begin{pmatrix}
1 & -i & 0 \\
-i & i & 0 \\
0 & 0 & 0
\end{pmatrix} .
\]
The eigenvalues of $\mathcal{M}$ are 0, 0, and 2, and two linear independent eigenvectors of $\mathcal{M}$ with zero eigenvalues can be taken as $\mathbf{e}_1 = (1/\sqrt{2}, -i/\sqrt{2}, 0)^T$ and $\mathbf{e}_2 = (0, 0, 1)^T$. The corresponding two eigenoperators are $\hat{O}_1 = (\hat{X} - i\hat{Y})/\sqrt{2}$ with $\xi_1 = 0$ and $\hat{O}_2 = \hat{Z}$ with $\xi_2 = -1$. The associated positive semidefinite operators, defined in Eq. (4) in the main text, $\hat{\Delta}_1$ and $\hat{\Delta}_2$ are
\begin{align}
\hat{\Delta}_1 &= (\hat{X} + i\hat{Y})(\hat{X} - i\hat{Y})/2 = \hat{I} + \hat{Z} = 2|1\rangle\langle 1|, \\
\hat{\Delta}_2 &= (\hat{Z} + \hat{I})(\hat{Z} + \hat{I}) = 2(\hat{Z} + \hat{I}) = 4|1\rangle\langle 1|.
\end{align}
This means the auxiliary Hamiltonian $\hat{H}_{\text{aux}}^A$, defined in Eq. (6) in the main text, takes the form
\begin{equation}
\hat{H}_{\text{aux}}^A = \sum_{i \in A} c_i |1\rangle_i\langle 1|_i, \quad c_i > 0,
\end{equation}
where $i$ labels the sites in subsystem $A$. Clearly, regardless of the value of $c_i$ as long as $c_i > 0$, the ground state of $\hat{H}_{\text{aux}}^A$ under the open boundary condition is unique: $|G\rangle = \prod_{i \in A} \otimes |0\rangle_i$. From our GD-EE theorem, the von Neumann entropy $S_v$ is upper bounded by $\log 1 = 0$. On the other hand, $S_v \geq 0$, and, therefore, our GD-EE theorem yields the exact result $S_v = 0$ for product states.

A remark is in order here. In practice we do not know the rotated basis, $|0\rangle$ and $|1\rangle$, and hence do not know $\hat{X}, \hat{Y}$, and $\hat{Z}$ defined above. However, the choice of bases $\{\hat{L}_i\}$ is immaterial. Indeed, if one repeats the above process for a general product state,
\begin{equation}
|\psi\rangle = \prod_i \otimes |\phi_i\rangle = \prod_i \otimes (\alpha_i |0\rangle + \beta_i |1\rangle),
\end{equation}
one will again find two zero eigenvalues of the correlation matrix. The two eigenvectors, up to some normalization constants, can be taken as
\begin{equation}
\mathbf{e}_1 = \left(\alpha\beta^* + \alpha^*\beta, i\alpha^*\beta - i\alpha\beta^*, 1\right)^T, \quad \mathbf{e}_2 = \left(\frac{\alpha^2 - \beta^2}{2\alpha\beta}, \frac{-\alpha^2 - \beta^2}{2\alpha\beta}, 1\right)^T.
\end{equation}
The eigenvalues $\xi_1$ and $\xi_2$ for $\hat{O}_1$ and $\hat{O}_2$ are $\xi_1 = 1/(|\beta|^2 - |\alpha|^2)$ and $\xi_2 = 0$, respectively. The two $\hat{\Delta}$ operators, up to some constant normalization factors, constructed for site $i$ are
\begin{equation}
\hat{\Delta}_1 = \hat{\Delta}_2 = \left(\frac{|\alpha_i|^2}{|\beta_i|^2}, \frac{-\alpha_i^*\beta_i}{|\beta_i|^2}, 1\right)^T = \langle \phi_i^+ | \phi_i^+ \rangle,
\end{equation}
where $|\phi_i^+\rangle = \beta_i^* |0\rangle - \alpha_i^* |1\rangle$ is orthogonal (zero inner product) to $|\phi_i\rangle$. The resulting auxiliary Hamiltonian then reads (up to some normalization constants)
\begin{equation}
\hat{H}_{\text{aux}}^A = \sum_i c_i |\phi_i^+\rangle\langle \phi_i^+|, \quad c_i > 0,
\end{equation}
and its ground state is unique with $D^A = 1$.

Having showed the special case of spin-1/2 systems where the local Hilbert space dimension $q$ equals two, we shall continue to give a formal constructive proof for the case of general $q$. Denote the local Hilbert basis as $|i\rangle, i = 0, 1, \cdots, q - 1$ and still, without loss of generality, the general form a product state $|\psi\rangle$ is taken to be
\begin{equation}
|\psi\rangle = \prod_i \otimes |0\rangle_i = |00 \cdots 0\rangle,
\end{equation}
as before. And we shall take the operator basis $\{\hat{L}_i\}$ to be the set of complete 1-local operators (still the trivial identity operator can be neglected as before). Then, a general 1-body eigenoperator $\hat{O}$ where $\hat{O}|\psi\rangle = \xi |\psi\rangle$ (they exist, for example we can construct $|0\rangle\langle 1|$ as one such operator) can be formally written as
\begin{equation}
\hat{O} = \xi |0\rangle\langle 0| + \sum_{i=1}^{q-1} |\phi_i\rangle\langle i|,
\end{equation}
where $|\phi_i\rangle = \hat{O}|i\rangle$. The positive semidefinite operator $\hat{\Delta}$ then reads

$$\hat{\Delta} = (\hat{O}^\dagger - \xi^* \hat{I})(\hat{O} - \xi \hat{I}) = \sum_{i,j=1}^{q-1} C_{ji}|j\rangle \langle i|$$

where

$$C_{ji} = \langle \langle \phi_j| - \xi^* \langle j|\rangle \langle \phi_i| - \xi \langle i| \rangle\rangle$$

is positive semidefinite (can be proven by showing $\sum_{i,j} x_j^* C_{ji} x_i \geq 0$ since it is the squared norm of $x_i(|\phi_i\rangle - \xi |i\rangle)$ as expected. Therefore, we can diagonalize $C_{ij}$ and bring $\Delta$ into diagonal form

$$\hat{\Delta} = \sum_{i,j=1}^{q-1} C_{ji}|j\rangle \langle i| = \sum_i a_i|\tilde{i}\rangle \langle \tilde{i}| \equiv \sum_{i} a_i \tilde{P}_i,$$

where $a_i \geq 0$ are the eigenvalues of matrix $C_{ij}$. The important thing to note is that $\tilde{P}_i |\tilde{i}\rangle = |\tilde{i}\rangle$ is a linear combination of $|i\rangle$ with $\tilde{i} = 1, 2, \ldots, q - 1$. Moreover, by taking a set of states $|\phi_j\rangle$ where the matrix $C_{ij}$ has rank $q - 1$ (for example, setting $|\phi_0\rangle = (\xi + 1)|i\rangle$ makes $C$ an identity matrix), $|0\rangle$ becomes the only state in the kernel of $\hat{\Delta}$. As a result, the ground state of $\hat{H}^A_{aux}$ under the open boundary condition is unique as in the spin-$1/2$ case: $|G\rangle = \prod_{i \in A} |0\rangle_i$, and our upper bound of the von Neumann entropy is exact, $S_v = \log 1 = 0$.

IV. Special Algorithm for the Ground-State Degeneracy of the Auxiliary Hamiltonian

Our GD-EE theorem states that the EE of a state $|\psi\rangle$ on a subsystem of size $L_A$ is upper bounded by the ground-state degeneracy $D^A$ of the auxiliary Hamiltonian $\hat{H}^A_{aux}$ under the open boundary condition. Because of the exponential increase of the Hilbert space dimension, the maximum size $L_A$ can be reached by directly attacking this problem using the exact diagonalization method is quite limited. We now explain a special algorithm that overcomes the difficulty.

For the simplicity of notations, consider the concrete example of AKLT scar states mentioned in the main text. Here, the exact diagonalization method is quite limited. We now explain a special algorithm that overcomes the difficulty.

Our GD-EE theorem states that the EE of a state $|\psi\rangle$ on a subsystem of size $L_A$ is upper bounded by the ground-state degeneracy $D^A$ of the auxiliary Hamiltonian $\hat{H}^A_{aux}$ under the open boundary condition. Because of the exponential increase of the Hilbert space dimension, the maximum size $L_A$ can be reached by directly attacking this problem using the exact diagonalization method is quite limited. We now explain a special algorithm that overcomes the difficulty.

For the simplicity of notations, consider the concrete example of AKLT scar states mentioned in the main text. Here, the exact diagonalization method is quite limited. We now explain a special algorithm that overcomes the difficulty.
degeneracy $D^A$ as well as $C_{kn,m}^{(L_A)}$. Since this recursive method is memory-cheap and we just need to diagonalize a matrix of dimension $D^{A'} \times q$ (where $q$ is the Hilbert space dimension of a single site) to get $D^A$, calculating the ground state degeneracy of system size $L_A$ of a few hundreds is very easy.

V. Projector Space of Scar States in the AKLT Model

To employ our GD-EE theorem to upper bound the bipartite entanglement entropies of all the scar states, \[ |\psi_n\rangle = (\hat{Q}^1)^n |G\rangle, \tag{S1} \]
we need to find a set of projection operators $\{\hat{P}_i\}$ such that each of them annihilates every $|\psi_n\rangle$, \[ \hat{P}_i |\psi_n\rangle = 0, \quad \forall \ i, n. \tag{S2} \]

Let $\hat{H}_{\text{aux},n}^A$ denotes an auxiliary Hamiltonian of $|\psi_n\rangle$, let $\hat{P}_i^{(n)} = |i^{(n)}\rangle \langle i^{(n)}|$ denotes the projectors entering $\hat{H}_{\text{aux},n}^A$. Since, as implied by Lemma 1, the kernel (ground-state manifold) of the auxiliary Hamiltonian is invariant for fixed operator space $V = \text{Span}\{\hat{L}_i\}$, the complement of the kernel, the state space $V^{(n)} = \text{Span}\{|i^{(n)}\rangle\}$, is also invariant. Therefore, the direct way to identify $\{\hat{P}_i\}$ annihilating all the scar states is to first calculate the common intersection $V_\cap \equiv \bigcap_n V^{(n)}$ and then form $\{|i\rangle \langle i|\}$ using a set of bases $\{|i\rangle\}$ in $V_\cap$. This is, however, computationally too expensive, for it requires calculating $V^{(n)}$ for every $|\psi_n\rangle$. Fortunately, making use of the special structure of the AKLT Hamiltonian and the ground state $|G\rangle$, we typically only need to deal with one $|\psi_n\rangle$, thus significantly reducing the computational cost. First note that the AKLT Hamiltonian under the periodic boundary condition (PBC) is a sum of projectors, \[ \hat{H}_{\text{AKLT}} = \sum_{i=1}^{L} \hat{P}_{i,i+1}^{(2)}, \tag{S3} \]
where $\hat{P}_{i,i+1}^{(2)}$ is the projection operator of two spin-1’s at site $i$ and $i+1$ onto total spin-2, and that the ground state $|G\rangle$ is annihilated by every $\hat{P}_{i,i+1}^{(2)}$, \[ \hat{P}_{i,i+1}^{(2)} |G\rangle = 0, \quad \forall \ i. \tag{S4} \]

If we partite the system into two parts, one consisting of $k$ consecutive sites and the other part containing the rest $L-k$ sites as shown in Fig. [S2], and denote the part of the Hamiltonian acting only in the $k$-site region as $\hat{H}_k$, i.e. \[ \hat{H}_k = \sum_{i=1}^{k-1} \hat{P}_{i,i+1}^{(2)}, \tag{S5} \]
it follows that the ground state is annihilated by $\hat{H}_k$, \[ \hat{H}_k |G\rangle = 0. \tag{S6} \]

Since $\hat{H}_k$ is nothing but the AKLT Hamiltonian of the $k$-site region under the open boundary condition (OBC),

\[ \begin{array}{cccccccc}
1 & 2 & \cdots & k & k+1 & \cdots & L-1 & L \\
\hline
\end{array} \]

FIG. S2. Partition of the system into $k$-site region and $(L-k)$-site region.

Eq. (S6) implies $|G\rangle$ can be decomposed in the following way,

\[ |G\rangle = \sum_{\eta=1}^{4} |G_{k,\eta}\rangle \otimes |\Psi_{\eta}\rangle \tag{S7} \]
where $|G_{k,n}\rangle$ is the ground state of the $k$-site AKLT Hamiltonian under the OBC with $\eta = 1, 2, 3, 4$ as labels of the four-fold degeneracy, and $|\Psi_\eta\rangle$ is a state vector in the Hilbert space of the rest $L-k$ sites. Similarly, we can write $\hat{Q}_k$ and $\hat{Q}_{L-k}^\dagger$, that act only in the $k$- and $(L-k)$-site regions respectively,

$$\hat{Q}_k = \sum_{i=1}^{k} (-1)^i \left( \hat{S}_i^x \right)^2 + \sum_{i=k+1}^{L} (-1)^i \left( \hat{S}_i^x \right)^2 \equiv \hat{Q}_k^\dagger + \hat{Q}_{L-k}^\dagger.$$  

(S8)

The key observation is that, using the decomposition of Eqs. (S7) and (S8), we can decompose a general scar state,

$$|\psi_n\rangle = \left( \hat{Q}_k^\dagger + \hat{Q}_{L-k}^\dagger \right)^n |G\rangle = \sum_{m=0}^{n} \sum_{\eta=1}^{4} (\hat{Q}_k^\dagger)^m |G_{k,\eta}\rangle \otimes |\tilde{\Psi}_{m,\eta}\rangle,$$

(S9)

where $|\tilde{\Psi}_{m,\eta}\rangle$ is a state vector in the Hilbert space the $L-k$ sites. Since $|G_{k,\eta}\rangle$ only contain $z$-component of the total spin, $S_z$, greater or equal than $-1$ and each $\hat{Q}_k^\dagger$ raises $S_z$ by two [7], the maximum value of $m$ we need to address is $\left[ \frac{k+1}{2} \right]$ where $[x]$ denotes the maximum integer no bigger than $x$. Let $\{|\Phi_i\rangle\}$ denotes a set of orthonormal bases where each basis has zero inner product with $(\hat{Q}_k^\dagger)^m |G_{k,\eta}\rangle$ for every possible values of $m$ and $\eta$,

$$\langle \Phi_i | (\hat{Q}_k^\dagger)^m |G_{k,\eta}\rangle = 0, \quad \forall \ i, m, \eta.$$  

(S10)

We can then easily construct a set of $k$-local projection operators $\{|\Phi_i\rangle\langle \Phi_i|\}$ and each $|\Phi_i\rangle\langle \Phi_i|$ annihilates all the scar states, Eq. (S1), for system size $L > k$. From construction, it is clear that the state space spanned by $\{|\Phi_i\rangle\}$, denoted as $V_\Phi$, is a subset of the common intersection $V_{\cap}$ we are looking for,

$$V_\Phi \equiv \text{Span} \{ |\Phi_1\rangle, |\Phi_2\rangle, \cdots \} \subseteq V_{\cap}.$$  

(S11)

On the other hand, for a scar state $|\psi_n\rangle$ with fixed $n \geq \left[ \frac{k+1}{2} \right]$ of a large enough system size $L$, the states $|\tilde{\Psi}_{m,\eta}\rangle$ in the decomposition of $|\psi_n\rangle$, Eq. (S9), are in general linearly independent. This implies that for such a scar state $|\psi_n\rangle$,

$$\tilde{P}_i^{(n)} |\psi_n\rangle = 0, \quad \iff \tilde{P}_i^{(n)} (\hat{Q}_k^\dagger)^m |G_{k,\eta}\rangle = 0, \quad \forall \ m, \eta.$$  

(S12)

In other words, $V^{(n)} = V_\Phi$ for such $|\psi_n\rangle$, which further implies $V_{\cap} \subseteq V_\Phi$. Together with Eq. (S11), we conclude

$$V_\Phi = V_{\cap},$$  

(S13)

and $V_{\cap}$ can be determined by such a scar state $|\psi_n\rangle$.

The above consideration holds generally for $k \geq 2$, and further simplification can happen for a given $k$. For example, for $k = 3$, a simple calculation shows that

$$\text{Span} \{ (\hat{Q}_3^\dagger)^2 |G_{3,\eta}\rangle \} \subset \text{Span} \{ |G_{3,\eta}\rangle, \hat{Q}_3^\dagger |G_{3,\eta}\rangle \}.$$  

(S14)

This means that a 3-local projector that annihilates $|\psi_1\rangle = \hat{Q}_3^\dagger |G\rangle$ will also annihilates all the other scar states $|\psi_n\rangle$ for all system sizes $L > 3$. Moreover, our 3-local operator basis

$$\hat{L}_i = \lambda_a^{(1)} \otimes \lambda_b^{(2)} \otimes \lambda_c^{(3)}, \quad a, b, c = 1, 2, \cdots, 8$$  

(S15)

is general enough for the constructed state space $V = \text{Span} \{ |i\rangle \}$ from $\{\hat{P}_i\}$ to contain $V_\Phi$. Similar result holds both for 4-local operator basis

$$\hat{L}_i = \lambda_a^{(1)} \otimes \lambda_b^{(2)} \otimes \lambda_c^{(3)} \otimes \lambda_d^{(4)}, \quad a, b, c, d = 1, 2, \cdots, 8$$  

(S16)

and 5-local operator basis

$$\hat{L}_i = \lambda_a^{(1)} \otimes \lambda_b^{(2)} \otimes \lambda_c^{(3)} \otimes \lambda_d^{(4)} \otimes \lambda_e^{(5)}, \quad a, b, c, d, e = 1, 2, \cdots, 8.$$  

(S17)
VI. EE Bounds of Scar States in the Fermi–Hubbard Model

The scar states in the 1D extended Fermi–Hubbard model for spin-1/2 fermions take a similar form to those of the AKLT model [1, 2]. They are known as the $\eta$-pairing states [3] and take the form of

$$|\psi_n\rangle = (\hat{\eta}^\dagger)^n |0\rangle,$$

where $|0\rangle$ is the vacuum state with no fermions and $\hat{\eta}^\dagger = \sum_i (-1)^i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger$ is the so-called $\eta$-pairing operator with $\hat{c}_{i\uparrow}^\dagger$ ($\hat{c}_{i\downarrow}^\dagger$) being the fermionic creation operator for spin up (down) at site $i$. The procedure to construct the local correlation function parallels that of the AKLT model. We choose our target scar state as the half-filled state $|\psi\rangle_{L/2}$ ($L$ is assumed to be even), and operators $\hat{L}_i$ as range-3 operators with a similar tensor product form, $\hat{L}_i = \lambda^{(1)}_a \otimes \lambda^{(2)}_b \otimes \lambda^{(3)}_c$ on three neighboring sites 1, 2 and 3. The Hilbert space is four-dimensional for each site, spanned by an unoccupied state, two singly occupied states with different spins, and one doubly occupied state. Thus, here we take $\lambda$ as the fifteen generators of SU(4) group and the identity ($a, b, c = 1, \cdots, 16$). The local correlation matrix is then calculated and the auxiliary Hamiltonian is constructed in a similar fashion. We find ground state degeneracy $D_A$ scales with the subsystem size $L_A$ as $D_A = L_A + 1$, meaning the EE of this state is bounded by the logarithm of the subsystem size. For reasons identical to the AKLT case, this bound is also valid for all other scar states of $n \neq L/2$. Finally, we compare the exact value of EE with our bound of the scar state $|\psi_{L/2}\rangle$. The exact value of EE is analytically known [4] to be asymptotically $S_v \propto (\log L_A)/2$. Therefore, apart from a ratio of two, our bound gives the correct log-volume scaling of the EE.

VII. Numerical Details for Bounding Entanglement Entropies in PXP Model

In this section, we shall elaborate on the numerical procedure we use to bound the EEs of the scar states in the PXP model. We start to construct the correlation matrix for given range-$k$ operator basis of the form (still the identity operator is excluded)

$$\hat{L}_i = \lambda^{(1)}_{a_1} \otimes \lambda^{(2)}_{a_2} \otimes \cdots \otimes \lambda^{(k)}_{a_k},$$

where $\{a_j\} = \{0, 1, 2, 3\}$ for $j = 1, 2, \cdots, k$ are the indices of the $2 \times 2$ identity matrix $I$ (where $a_j = 0$) and the three Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}$. We calculate the $(4^k - 1)$-dimensional local correlation matrix for every eigenstate and compare the correlation spectrum of a scar state with surrounding thermal states. As shown in Fig. S4, the correlation spectra of scar states are markedly different with more smaller eigenvalues. From such plot, we can determine a position $\alpha = N_1$ (labeled by pink arrow in Fig. S4) where the eigenvalue plot of the scar state is about to cross those of the surrounding thermal states. We shall use the $N_1 - N_0$ (we subtract $N_0$ to exclude the trivial zeros) eigenvalues to construct an auxiliary Hamiltonian $\hat{H}_\text{aux}^A$ to bound the EE. For such nonzero eigenvalue $\lambda_\alpha \neq 0$, we
FIG. S4. Plots of correlation spectra for a group of eigenstates (eigenstate indices \( n \) shown in the legends) around two quantum many-body scar states (marked as black) for the PXP model in the zero momentum and inversion even sector. The system size is \( L = 20 \) and the range of the operator basis \( \{ \hat{L}_i \} \) is \( k = 5 \). In both groups, the eigenvalues of the correlation matrix of the scar state noticeably fall below (excluding the first \( N_0 = 608 \) trivial zeros) those of the surrounding thermal eigenstates when \( \alpha \leq N_1 \) (corresponding points marked by pink arrows). The \( N_1 - N_0 \) positive semidefinite \( \hat{\Delta}_\alpha \) operators associated with these eigenvalues are then taken as the starting point to construct \( \hat{H}^A_{\text{aux}} \) to bound EE.

still proceed to define an operator \( \hat{O} \) using the corresponding eigenvector \( \mathbf{e}_\alpha = (w_1, w_2, \ldots, w_n) \) in a similar fashion, 
\[
\hat{O} = \sum_i w_i \hat{L}_i.
\]

In this case, \( \hat{O} \) is not an eigenoperator of \( |\psi\rangle \) anymore, 
\[
\hat{O} |\psi\rangle = \xi |\psi\rangle + |\psi_\perp\rangle, \quad \text{where} \quad \langle \psi_\perp |\psi_\perp\rangle > 0.
\]

(S2)

We can, however, still define a positive semidefinite operator \( \hat{\Delta}_\alpha \) as before,
\[
\hat{\Delta}_\alpha = \left( \hat{O}^\dagger - \xi^* \hat{I} \right) \left( \hat{O} - \xi \hat{I} \right).
\]

(S3)

The constructed auxiliary Hamiltonian still takes the same form
\[
\hat{H}^A_{\text{aux}} = \sum_\alpha \tilde{c}_\alpha \hat{\Delta}_\alpha, \quad \tilde{c}_\alpha > 0.
\]

(S4)

For given \( N_1 \), optimizing the value of \( \tilde{c}_\alpha \) to get the best upper bound is beyond the scope of our paper. Therefore, for demonstration purposes, we shall take the simplest case where \( \tilde{c}_\alpha = 1, \forall \alpha \). Since \( N_1 \) is handpicked, we choose to vary the value of \( N_1 \) to get a comparatively good upper bound of EE. We summarize the optimized result of the EE upper bounds of the scar states of the PXP model in Table I (see also [5]).

As can be seen from either Fig. 4 in the main text or Table. I here, the obtained optimal upper bound decrease with the increase of \( k \). For \( k = 4,5 \), our bounds of the scar states are well separated from the thermal continuum, signifying weak ergodicity breaking [7].

**VIII. Experimental Scheme to Measure the Correlation Matrix**

Here we will give a detailed description of the experimental measurement of correlation matrix \( \mathcal{M} \) in the context of cold atom systems. We also give an explicit example of expanding the product of two operators.
To be concrete, we consider a spin-1/2 chain in optical lattices, which can be realized by ultracold atoms with two hyperfine states and large on-site repulsion. The system is prepared in the state \(|\psi\rangle\), of which the entanglement property is to be bounded. As an example, we consider the measurement of the correlation matrix \(\mathcal{M}\) of the subsystem \(A\) that contains first two sites \(n = 1, 2\). Let us choose our operator basis \(\{\hat{L}_i\}\) as \({\hat{\sigma}}_a^n, \hat{\sigma}_a^n, \hat{\sigma}_b^n, \) where \(a, b = x, y, z\) labels the three Pauli operators, and add identity operator \(\hat{I}\) to form the complete set of hermitian operator basis \(\{\hat{L}_i\} = \{\hat{I}, \hat{\sigma}_a^n, \hat{\sigma}_b^n, \hat{\sigma}_a^1\hat{\sigma}_b^n\}\). To obtain the matrix element \(\mathcal{M}_{ij}\), we need to measure \(\langle \psi | \hat{L}_i^\dagger \hat{L}_j | \psi \rangle\) and \(\langle \psi | \hat{L}_i | \psi \rangle\). However, it is straightforward to see that \(\hat{L}_i^\dagger \hat{L}_j = \hat{L}_j \hat{L}_i\) is an element in \(\{\hat{L}_i\}\) using the fact that

\[
\hat{\sigma}_a^n \hat{\sigma}_b^n = \delta^{ab} \hat{I} + \sum_c i\epsilon_{abc} \hat{\sigma}_c^n, \tag{S1}
\]

where \(\epsilon_{abc}\) is the Levi-Civita symbol. In more general cases, when the set of operators \(\{\hat{L}_i\}\) is orthogonal under the matrix trace \(\text{Tr}(\hat{L}_i \hat{L}_j) \propto \delta_{ij}\), we can write

\[
\hat{L}_i \hat{L}_j = \sum_k C^k_{ij} \hat{L}_k, \quad C^k_{ij} = \frac{\text{Tr}(\hat{L}_i \hat{L}_j \hat{L}_k)}{\text{Tr}(\hat{L}_k^2)}. \tag{S2}
\]

As a result, knowing \(\{\langle \psi | \hat{L}_i | \psi \rangle\}\), or \(\{\langle \psi | \hat{L}_i^\dagger \hat{L}_j | \psi \rangle\}\), is enough to determine the correlation matrix \(\mathcal{M}\). We first consider the measurement of \(\hat{\sigma}_x^1, \hat{\sigma}_z^2\), and \(\hat{\sigma}_1^z \hat{\sigma}_2^z\), which directly corresponds to the (correlation of) atom occupation in different hyperfine states. The technique of quantum gas microscopy can be directly applied to measure these quantities by fluorescence imaging [8–13]. Repeated measurements produce the probability distribution of spin states in the \(z\) direction \(s_{n_1 n_2}\) where the subscript \(s_n = \uparrow, \downarrow\) labels the state of the \(n\)-th site. We have

\[
\langle \psi | \hat{\sigma}_x^1 | \psi \rangle = \sum_{s_2} (p_{\uparrow s_2} - p_{\downarrow s_2}), \quad \langle \psi | \hat{\sigma}_z^2 | \psi \rangle = \sum_{s_1} (p_{s_1 \uparrow} - p_{s_1 \downarrow}), \quad \langle \psi | \hat{\sigma}_1^z \hat{\sigma}_2^z | \psi \rangle = p_{\uparrow \uparrow} + p_{\downarrow \downarrow} - p_{\uparrow \downarrow} - p_{\downarrow \uparrow}, \tag{S3}
\]

which can be measured at the same time. Moreover, for systems with translation symmetry, one can use data on different sites to compute \(p_{s_1 s_2}\) efficiently in a single-shot measurement.

For other operators, the measurement can be done with an additional Raman pulse that couples two hyperfine states. Such optical manipulation of a single site in optical lattices has been realized in experiments (for example, in [14–16]). We give a explicit example for the operator \(\hat{\sigma}_x^1 \hat{\sigma}_2^z\). By tuning the relative phase between Raman laser, we choose the coupling between two hyperfine states on the first site as \(\delta \hat{H} = \Omega \hat{\sigma}_y^1\). We consider applying a \(\pi/2\) pulse, which leads to an unitary evolution denoted by \(\hat{U}\). Using the fact that \(\hat{\sigma}_x^1 = -\hat{U}^\dagger \hat{\sigma}_x^1 \hat{U}\), we have

\[
\langle \psi | \hat{\sigma}_x^1 \hat{\sigma}_2^z | \psi \rangle = -\langle \psi | \hat{U}^\dagger \hat{\sigma}_1^x \hat{\sigma}_2^z \hat{U} | \psi \rangle. \tag{S4}
\]

As a result, after applying the \(\pi/2\) pulse, the experimental protocol to measure \(\hat{\sigma}_x^1 \hat{\sigma}_2^z\) directly follows the protocol of measuring \(\hat{\sigma}_x^1 \hat{\sigma}_2^z\). Other operators can be measured in the same spirit, and the generalization to \(k\)-local operators is straightforward.

### Table I. Optimization results of entanglement entropy upper bounds of scar states (with eigenstate index \(n\)) of the PXP model in the zero momentum and inversion even sector.

<table>
<thead>
<tr>
<th>(k)</th>
<th>(n = 1)</th>
<th>(n = 2)</th>
<th>(n = 7)</th>
<th>(n = 30)</th>
<th>(n = 102)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.4038</td>
<td>1.6391</td>
<td>2.1314</td>
<td>2.6668</td>
<td>2.2858</td>
</tr>
<tr>
<td>4</td>
<td>0.4031</td>
<td>1.5718</td>
<td>2.0201</td>
<td>2.0227</td>
<td>1.9797</td>
</tr>
<tr>
<td>5</td>
<td>0.3868</td>
<td>1.4835</td>
<td>1.9588</td>
<td>2.0090</td>
<td>1.7840</td>
</tr>
</tbody>
</table>

In each cell, the left value is the optimized EE upper bound (rounded with 4 decimal points) and the right number is the corresponding optimal value of \(N_1 - N_0\). Due to the “particle-hole” symmetry of the PXP model [6], results from the only the first half, with eigenstate indices \(n = 1, 2, 7, 30, 102\), of all the scar states are shown.
[5] Our open source code for the program including the original data are freely available at https://github.com/ZhiyuanYao/CorrMat_EE.git.