Reconstructing Entanglement Hamiltonian via Entanglement Eigenstates

W. Zhu,1,* Zhoushen Huang,1,† and Yin-Chen He2,3,‡

1Theoretical Division, T-4, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
2Department of Physics, Harvard University, Cambridge MA 02138
3Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada

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The entanglement Hamiltonian $H_E$, defined through the reduced density matrix of a subsystem $\rho_A = \exp(-H_E)$, is an important concept in understanding the nature of quantum entanglement in many-body systems and quantum field theories. In this work, we explore a numerical scheme which explicitly reconstructs the entanglement Hamiltonian using one entangled mode (i.e., an eigenstate) of $\rho_A$. We demonstrate and benchmark this scheme on quantum spin lattice models. The resulting $H_E$ bears a form similar to a physical Hamiltonian with spatially varying couplings, which allows us to make quantitative comparison with perturbation theory and conformal field theory.

Introduction.—Entanglement-based analysis has brought new insights into the study of condensed matter systems, particularly those with strong interactions [1–3], where the understanding of ground state correlations is of central importance. Given a pure state $|\psi\rangle$, the entanglement between two complementary parts ($A$ and $B$) can be extracted from the reduced density matrix of (say) part $A$, $\rho_A = \text{Tr}_B|\psi\rangle\langle\psi|$. The entanglement entropy is $S = -\text{Tr}(\rho_A \ln \rho_A)$ and has been extensively used to identify quantum criticality [4, 5] and intrinsic topological orders [6, 7]. Following Li and Haldane [8], more recent developments have gone beyond the single number $S$, and invoked the full spectrum $\{\rho_n\}$ of $\rho_A$, i.e., the entanglement spectrum (ES), as more fine-grained “fingerprints” to distinguish between various topological orders [8–11], symmetry protected phases [12, 13], symmetry broken phases [14, 15], quantum criticality [16–21], to name a few.

The reduced density matrix can be formally written as $\rho_A = e^{-H_E}$, and regarded as a thermal density matrix with “Hamiltonian” $H_E$ (or entanglement Hamiltonian EH) at inverse temperature $\beta = 1$. Knowledge of $H_E$ in terms of its operator content could then offer an alternative picture of how subsystem $A$ behaves, by appealing to our intuition of thermodynamics. Specifically, a concrete form of $H_E$ may provide insight for interesting problem such as bulk-edge correspondence [8, 22] and physics of thermalization in the non-equilibrium dynamics [23–25]. From an information extraction point of view, both the entropy and the ES represent ways of reducing the full information content in $\rho_A$ to more manageable forms. The reconstruction of the EH, if achievable, points to a different reduction scheme, whereby the exponentially many complex-valued matrix elements in $\rho_A$ are compressed into a handful of coupling constants in $H_E$. In a limited number of tractable cases, $H_E$ has been explicitly obtained either exactly [26–30] or perturbatively [31]. To date, however, there is no generic recipe to derive $H_E$ in such a compact form in strongly-correlated systems.

In this work, we present a systematic strategy to obtain $H_E$. Instead of evaluating $-\log \rho_A$ directly, we construct $H_E$ from an eigenstate (practically chosen as the highest weight one) of $\rho_A$. We consider an ansatz $H_P = \sum_n w_n L_n$, which is a weighted sum of a prescribed set of physically motivated local operators $\{L_n\}$. Examples of such operators include spin-spin interactions, fermion hoppings, etc. The coefficients $\{w_n\}$ will be determined by demanding the highest weight eigenstate of $\rho_A$ (i.e., the entanglement ground state) to be an (approximate) eigenstate of $H_P$, which leverages a method reported in recent works on parent Hamiltonian construction [32–34] (see [35] for an alternative perspective). Generically, the EH $H_E$ should be a function of $H_P$, $H_E = f(H_P)$. In many physical interesting situations, however, $H_E$ is believed to contain only local terms. In those cases, one can always choose the local operators $\{L_n\}$ properly such that $H_P$ is the EH (with a proper rescaling). We demonstrate our method using two exemplary spin-$\frac{1}{2}$ models (see Fig. 1). In both models, we obtain numerically exact EHs, which also converge to analytical forms, if obtainable in the corresponding conformal field theory (CFT) or perturbatively around exactly solvable points. Toward the end, we will briefly discuss its implications in Haldane conjecture and non-equilibrium statistical mechanics.

Method.—Our aim is to obtain the EH, $H_E = -\log \rho_A$, explicitly in terms of intelligible operators. This problem is in general analytically intractable due to the difficulty in evaluating the log. Below, we will instead (1) Confine ourselves to a restricted operator space $\mathcal{L}$ consisting of linear combinations of a prescribed set of basis operators, $\mathcal{L} = \text{Span}\{L_n\}$, and then (2) Construct an operator $H_P \in \mathcal{L}$, such that it (approximately) shares one eigenstate with $\rho_A$ (the highest weight state). In principle, $H_P$ thus constructed may not be $H_E$, instead it could be a certain function of $H_E$. However, the EH obtained from the groundstate of a local Hamiltonian is itself believed to be local. Thus as long as one chooses the operators $\{L_n\}$ properly (e.g. by including enough local operators), $H_P$ and $H_E$ should be equivalent up to a proper rescale. We find this is indeed the case in the two examples to be discussed later.
To obtain $H_P$, we use a recently reported method [32–34] which takes as input a state $|\xi\rangle$ and a set of basis operators $\{L_a\}$, and returns a set of weights $\{w_a\}$, such that $H_P = \sum_a w_a L_a$ has $|\xi\rangle$ as an (approximate) eigenstate. Specifically, we take $|\xi\rangle$ as the entanglement ground state, and compute the correlation matrix

$$G_{ab} = \langle \xi | L_a L_b | \xi \rangle - \langle \xi | L_a | \xi \rangle \langle \xi | L_b | \xi \rangle .$$

(1)

Note that $G$ is positive-semidefinite [35]. The desired weights are given by the eigenvector of the matrix $G$ with the lowest eigenvalue $g_0 \geq 0$, \begin{equation}
\{w_a\} : \sum_b G_{ab} w_b = g_0 w_a , \quad g_0 = \min \{\text{Spec}(G)\} \geq 0 \tag{2}
\end{equation}

\begin{equation}
H_P = \sum_a w_a L_a . \tag{3}
\end{equation}

One can easily verify that $g_0 = \langle \xi | H_P^2 | \xi \rangle - \langle \xi | H_P | \xi \rangle^2$, i.e., $g_0$ is the “energy fluctuation” of the state $|\xi\rangle$ under “Hamiltonian” $H_P$. $|\xi\rangle$ becomes an exact eigenstate of $H_P$ if $g_0 = 0$. For small but nonvanishing $g_0$, $H_P$ is the best approximate parent “Hamiltonian” of $|\xi\rangle$ [36].

Although the above construction formally only ensures that $H_P$ and $E_P$ (approximately) share one eigenstate $|\xi\rangle$, we found in our study that the remainder of the eigenbasis also match well whenever $g_0$ is small, which we will quantify in the examples later. Note also that there is no a priori relation between the spectra of $H_P$ and $E_P$ even when the eigenbases match exactly, this is why we take the more general form $H_P = f(E_P)$.

With $H_P$ fixed, we can determine the best $f$, in principle, by maximizing the density matrix fidelity [37] between the original $\rho_A$ and its reconstruction $\varrho = e^{-f(H_P)}$,

$$F(\rho_A, \varrho) = \text{Tr} \sqrt{\sqrt{\rho_A} \varrho \sqrt{\rho_A}} . \tag{4}
$$

We write the eigen-decomposition of $\varrho$ as

$$\varrho(q) = \sum_n q_n |\phi_n\rangle \langle \phi_n| , \tag{5}
$$

where $q = (q_1, q_2, \cdots)$, $q_n = e^{-f(e_n)}$, and $|\phi_n\rangle$ and $e_n$ are the $n$th eigenstate and eigenvalue of $H_P$, respectively. In SM [35], we show that maximizing $F(\rho_A, \varrho)$ leads to a self-consistent equation of $q$. Its solution implicitly defines the $f$ function through $f(e_n) = -\log q_n$. When the eigenbasis $\{ |\phi_n\rangle \}$ of $H_P$ matches well with the entanglement states $\{ |\xi_n\rangle \}$, the optimal $q$ can be approximated by (see [35])

$$q_n \simeq \langle \phi_n | \rho_A | \phi_n \rangle \quad \forall n . \tag{6}
$$

In other words, under this approximation, $\varrho$ describes the diagonal ensemble of $\rho_A$ in the reconstructed $\{|\phi_n\rangle\}$ basis.

Before going into examples, we remark that the EH can in principle be calculated by numerically evaluating $-\log \rho_A$ using exact diagonalization. Such calculations, however, require keeping track of the coefficients of exponentially many operators $|n\rangle\langle n'|$ in a manybody complete basis $\{|n\rangle\}$. Our method is numerically more efficient although it needs extra input regarding the physical properties of the system (reflected in the choice of $\{L_a\}$). More importantly, our method applies to situations (e.g. in simulations using matrix product state) where $-\log \rho_A$ is hard to calculate numerically.

**One-dimensional chain.**—As a first case example, we study the EH of bipartition of a one dimensional spin–1/2 chain model (as shown in Fig. 1(a)):

$$H = \sum_{n=1}^{2L} \hat{h}_{n,n+1} = \sum_{n=1}^{2L} S_n^x \sigma_{n+1}^x + S_n^y v n + \Delta S_n^z \sigma_{n+1}^z .$$

For $|\Delta| \leq 1$, the ground state can be effectively described by a gapless Luttinger liquid. Importantly, this phase is an example of quantum critical phase with conformal invariance, governed by a (1+1) conformal field theory (CFT). As a benefit of the conformal invariance, the EH can be directly mapped out [23, 38–41]:

$$H_E^{\text{CFT}} = \sum_{n=1}^{L} f_{\text{env}}(\tilde{n}) \hat{h}_{n,n+1} , \tag{7}
$$

where $f_{\text{env}}(\tilde{n}) = \tilde{n}(1 - \tilde{n})$ is the envelope function and $\tilde{n} = (n + \frac{1}{2})/L$.

By implementing the numerical scheme discussed in the method section, we search for a parent Hamiltonian with the form $H_P = \sum_n J_{n,n+1} \hat{h}_{n,n+1}$ on modest partition sizes. First of all, we identify one exact zero eigenvalue ($g_0 < 10^{-13}$) in the spectrum of correlation matrix (Tab. 1). The coefficients $J_{n,n+1}$ in $H_P$ can be obtained from the corresponding eigenvector. Since subsystems A and B both have open boundaries after bipartition (Fig. 1(b)), translation symmetry is broken and $J_{n,n+1}$ is expected to be spatially dependent. In Fig. 2(a), we show the spatial dependence of $J_{n,n+1}$ on $n$ (the distance from the bound-
TABLE I. Lowest eigenvalue $g_0$ of correlation matrix $G$, and density matrix fidelity $F(ρ_A, 0)$ obtained on different system sizes $L$. Here we set $Δ = 0$ in one-dimension spin–1/2 chain model.

| $2 \times L$ | 20   | 24   | 28   | 32   |
|--------------|------|------|------|------|
| $g_0$        | 2.9 × 10$^{-14}$ | 1.4 × 10$^{-13}$ | 1.2 × 10$^{-13}$ | 9.4 × 10$^{-15}$ |
| $F(ρ_A, 0)$  | 0.99999 | 0.99998 | 0.99996 | 0.99991 |

ary) matches the CFT predicted envelope function $f_{\text{env}}$ (black dashed line).

The agreement between $J_{n,n+1}$ and $f_{\text{env}}(\tilde{n})$ suggests that for this model, $H_P$ and $H_E$ are equivalent up to shift and rescaling, $H_E = f(H_P) = a + bH_P$. To verify, we first compare the ES $\{-\log p_n\}$ and the eigenvalues $\{\varepsilon_n\}$ of $H_P$. As shown in Fig. 2(b), down to order $10^{-7}$, the ES is extremely well captured by $\{\varepsilon_n\}$ through a simple linear fit, $-\log p_n = a + b\varepsilon_n$. Using the fitted $a$ and $b$, we compute the fidelity between the original and reconstructed RDMs, $F(ρ_A, 0)$ where $0 = e^{-(a + bH_P)}$. As shown in Tab. I, $F(ρ_A, 0) > 0.9999$ for all system sizes tested. We thus conclude that $H_P$ and $H_E$ are indeed equivalent.

Spin ladder model.—We turn to study a two-leg spin–1/2 ladder Hamiltonian (as shown in Fig. 1(b)):

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB}$$

$$\hat{H}_{A(B)} = J_\perp \sum_{i \in (ij)} [S_{i,α}^x S_{j,α}'^x + S_{i,α}^y S_{j,α}'^y + ΔS_{i,α}^z S_{j,α}'^z]$$

$$\hat{H}_{AB} = J_\parallel \sum_i [S_{i,A}^x S_{i,B}^x + S_{i,A}^y S_{i,B}^y + ΔS_{i,A}^z S_{i,B}^z].$$

where $J\parallel = \cos \theta$ describes the nearest-neighbor exchange interaction in each chain, and $J_\perp = \sin \theta$ is “rung” exchange coupling between two chains. Below, we focus on the isotropic case $Δ = 1$ and antiferromagnetic intra-chain coupling $J_\parallel > 0$ (see [35] for the anisotropic $Δ > 1$). The nature of the ground state depends on the sign of $J_\perp$. For antiferromagnetic $J_\perp > 0$, spin singlets form on the rungs and the ground state can be viewed as the product of rung singlets [42]. For ferromagnetic $J_\perp < 0$, the ladder system can be effectively mapped onto a spin–1 chain, thus the ground state is in the “Haldane” phase [43, 44].

We now reconstruct the EH $H_E$ on chain $A$ using translationally invariant Heisenberg couplings,

$$H_E = \sum_{n=1}^{N_L} J_n \hat{h}_n, \quad \hat{h}_n = \sum_{i=1}^{L} S_i \cdot S_{i+n},$$

where $\hat{h}_n$ is the $n$-th neighbor coupling, and $N_L$ is long-range interaction cut-off. As before, the coefficients $J_n$ are obtained through diagonalization of correlation matrix $G$. We identify one approximate zero mode in the correlation spectrum. Tab. II shows one typical example of the corresponding coupling constants in the EH.

First of all, we found that the reconstructed EH is dominated by the nearest-neighbor coupling, $J_1 \gg J_{n>1}$. Further-neighbor couplings decay as inter-spin distance increases, and we truncated at $N_L = 4^{th}$ neighbor coupling, which already yields very good reconstruction fidelity of $F(ρ_A, 0) > 0.998$. The vanishingly small long-ranged interactions reflects locality of the EH. We thus conclude that the main feature of the EH is captured by a spin–1/2 chain with nearest neighbor antiferromagnetic Heisenberg couplings. In addition, in Tab. II, we observe an unfrustrated ferromagnetic second-neighbor coupling $J_2 < 0$. The oscillatory nature of interaction couplings, which can be antiferromagnetic or ferromagnetic depending upon the separation, is reminiscent of the Ruderman-Kittel-Kasuya-Yosida interaction from which indirect interaction couplings in subsystem A can be induced through subsystem B.

To further understand the obtained EH, we make a perturbative calculation [35] in the strong inter-chain coupling limit ($J_\parallel / J_\perp \ll 1$). Up to order $O(J_\parallel / J_\perp)^2$, the
EH is

\[ H_E^{\text{per}} \approx J_1^{\text{per}} \sum_i S_i \cdot S_{i+1} - J_2^{\text{per}} \sum_i S_i \cdot S_{i+2}, \]  

where \( J_1^{\text{per}} = 2 \frac{J_1}{J_\perp} \) and \( J_2^{\text{per}} = \frac{1}{2} \left( \frac{J_1}{J_\perp} \right)^2 \). Thus up to \( O(\frac{J_1}{J_\perp})^2 \), subsystem \( A \) behaves effectively as a spin-1/2 chain with first- and second-neighbor couplings. In particular, the second-neighbor coupling is ferromagnetic, consistent with our results in Tab. II. Fig. 3(b) shows quantitative agreement between perturbative and numerical results near \( J_\parallel / J_\perp \to 0 \), where numerics from different system sizes converge to the same perturbation theory values. This agreement not only provides an analytical understanding of the oscillatory nature of interaction couplings, but also validates the accuracy of our numerical results.

One major advantage of our current scheme is its applicability in the whole parameter regime, which is beyond the reach of perturbation-based effective theories. In Fig. 3(a), we show the EH parameters as a function of \( \theta = \tan^{-1}(J_\perp / J_\parallel) \), up to fourth-neighbor couplings. At \( \theta = 0 \), the two chains are effectively decoupled, thus it is reasonable to obtain \( J_n > 1 \) tending to zero. Away from this decoupling point, generally long-ranged interaction terms appear in \( H_E \). We note that the obtained couplings \( J_n / J_\parallel \) show non-monotonic dependence on \( \theta \).

With the reconstructed EH in hand, a natural question is if it belongs in the same class with its physical counterpart \( H_A \). Since the ground state of \( H_E \) can be smoothly and adiabatically connected to that of \( H_A \) without gap closing (Fig. 3(c)), we conclude that \( H_E \) and \( H_A \) are indeed in the same class [45]. Interestingly, even though the whole system experiences a quantum phase transition at \( \theta = 0 \), the EH still faithfully represents the physical Hamiltonian \( H_A \).

**Summary and Discussion.**—We have presented a numerical scheme to reconstruct the entanglement Hamiltonian \( H_E \) based on entangled modes of reduced density matrix, with the help of the recently reported eigenstate-to-Hamiltonian mapping [32–34]. As a proof of principle, we applied this method to two quantum spin lattice models. We found that the reconstructed \( H_E \) accurately recovers the expected results and faithfully captures all features of the reduced density matrices, which are evidenced by direct comparison to analytical theories, the agreement between the original and reconstructed full entanglement spectra, and the close-to-1 density matrix fidelity.

This scalable recipe for constructing the entanglement Hamiltonian opens up a number of directions worthy of further exploration. We explicitly showed in our examples that \( H_E \) bears a similar form as the physical Hamiltonian, which unambiguously supports the conjecture that there exists a deep correspondence between the entanglement Hamiltonian and the physical Hamiltonian with a virtual boundary [8, 22]. Similar numerical calculations may be used to investigate the time evolution of entanglement Hamiltonian after a quantum quench [23–25], which may provide intuitive pictures and additional insights regarding the nature of entanglement propagation and subsystem thermalization. This work also paves the way for future studies of entanglement Hamiltonian in higher dimensions using matrix product state and similar variational ansatz, for which the correlation matrix (Eq. 1) remains accessible at intermediate system sizes.

**Note added.**—At the final stage of preparing this manuscript, we became aware of a different scheme to map out entanglement Hamiltonian [46].

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* weizhu@lanl.gov  
† zsh@lanl.gov  
‡ yinchenghe@perimeterinstitute.ca

[1] L. Amico, R. Fazio, A. Osterloh, and V. Ve...
I. Constructing a parent operator from an eigenstate, a linear dependency perspective

In Ref. 32 (see also Refs. 33 and 34), Qi and Ranard showed that given a many-body wavefunction $|v\rangle$, a (more or less) unique parent Hamiltonian can be constructed in the form

$$H = \sum_i w_i L_i ,$$  \hspace{1cm} (11)

where $\{L_i\}$ is a set of Hermitian operators, if and only if the following “correlation matrix” $M_{ij}^{(v)}$ has a unique zero eigenvalue (with eigenvector $(w_1, w_2, \cdots)$),

$$M_{ij}^{(v)} \equiv \frac{1}{2} \langle v | \{ L_i , L_j \} | v \rangle - \langle v | L_i | v \rangle \langle v | L_j | v \rangle ,$$  \hspace{1cm} (12)

$$\sum_j M_{ij}^{(v)} w_j = 0 .$$  \hspace{1cm} (13)

Restricting $\{L_i\}$ to spatially local operators, the above observation then provides a guiding principle for constructing a local parent Hamiltonian for an arbitrary state $|v\rangle$. Note that $|v\rangle$ is not necessarily the ground state of thus constructed $H$.

We now provide an alternative perspective for the above and other related results, in terms of a linear dependence analysis. A sufficient and necessary condition for a normalized state $|v\rangle$ to be an eigenstate of $H$ is that

$$(I - P_v)H|v\rangle = 0 , \quad P_v \equiv |v\rangle \langle v| ,$$  \hspace{1cm} (14)

where $I$ is identity, and $P_v$ projects onto $|v\rangle$. Consider now a Hamiltonian of the form Eq. 11. Then

$$(I - P_v)H|v\rangle = \sum_i w_i |u_i\rangle , \quad |u_i\rangle \equiv (I - P_v) L_i |v\rangle .$$  \hspace{1cm} (15)

The unnormalized $\{|u_i\rangle\}$ states are generated by first “exciting” $|v\rangle$ by $L_i$, and then projecting out the part parallel to $|v\rangle$. Eq. 14 is equivalent to demanding that the $\{|u_i\rangle\}$ states are linearly dependent,

$$\sum_i w_i |u_i\rangle = 0 .$$  \hspace{1cm} (16)
Linear dependence of a set of vectors can be checked via a principal component analysis, which is mathematically equivalent to a singular value decomposition (SVD). To proceed, we construct a $D \times M$ matrix $A$ by arranging $|u_i\rangle$ as its $i^{th}$ column,

$$A_{D \times M} \equiv (|u_1\rangle, |u_2\rangle, \cdots)$$.

(17)

Here $D$ is the full Hilbert space dimension, and $M$ is the rank of the operator set $\{L_a\}$, $a = 1, 2, \cdots, M$. The linear dependence condition Eq. 16 is formally equivalent to demanding that $A$ has at least one zero singular value (a more detailed discussion of the related SVD will be provided below). Equivalently, the overlap matrix $G_{ij} = (A^\dagger A)_{ij} = \langle u_i|u_j\rangle$ should have at least one zero eigenvalue, with the coefficients $\{w_i\}$ given by the corresponding eigenvector,

$$G_{ij} = \langle u_i|u_j\rangle = \langle v|L_iL_j|v\rangle - \langle v|L_i|v\rangle \langle v|L_j|v\rangle,$$

(18)

$$\sum_j G_{ij} w_j = 0.$$

(19)

Note that Qi and Ranard’s correlation matrix $M$ is the real part of the hermitian $G$ matrix. Replacing $G$ with $M$ is equivalent to enforcing real-valuedness of the resulting coefficients $\{w_i\}$, as required by the Hermiticity of $H = \sum w_i L_i$. A non-Hermitian parent operator $H$ can be viewed as an annihilator of the state $|v\rangle$, as discussed in Ref. 34.

1. Principal component analysis of the states $\{L_i|v\rangle\}$

In practice, the choice of the basis operators $\{L_i\}$ is often based on physical intuition, so for efficiency reasons one may start with a relatively small set of $\{L_i\}$, and gradually add in more operators (e.g., in increasing order of spatial span or other physical preferences), until the lowest singular value of $A$ (or eigenvalue of $G = A^\dagger A$) converges toward zero. A natural question therefore concerns the meaning of the SVD of $A$, which we now address. The SVD reads

$$A_{D \times M} = L A R^\dagger = \sum_{i=1}^M \lambda_i |l_i\rangle \langle r_i|,$$

$$\Lambda = \text{Diag}(\lambda_1, \lambda_2, \cdots, \lambda_M),$$

$$L_{D \times M} = (|l_1\rangle, |l_2\rangle, \cdots, |l_M\rangle),$$

$$R_{M \times M} = (|r_1\rangle, |r_2\rangle, \cdots, |r_M\rangle).$$

(20)

(21)

The columns of $L$ and $R$ are the left and right singular vectors, respectively, and are denoted as $|l_i\rangle$ and $|r_i\rangle$. Note that the right singular vectors (which are the eigenvectors of $G$) are $M$-dimensional. Vectors in the right singular space $\text{Span}\{|r_i\rangle\}$ represent operators in the operator space $\text{Span}\{L_i\}$: Writing the $i^{th}$ right singular vector as

$$|r_i\rangle = (r_i^{(1)}, r_i^{(2)}, \cdots, r_i^{(M)})^t,$$

then the corresponding “Hamiltonian” is

$$H^{(i)} \equiv \sum_j L_j r_j^{(i)} = (L_1, L_2, \cdots, L_M)|r_i\rangle,$$

(22)

(23)

similar in spirit to writing polarized spin operators as $\sigma_b = b \cdot \sigma$. One can then verify that

$$(\mathbb{I} - P_v)H^{(i)}|v\rangle = A|r_i\rangle = \lambda_i |l_i\rangle.$$ 

(24)

The first equality follows from Eq. 17, and the second one follows from Eq. 20. Note that $\langle v|l_i\rangle = 0 \forall i$, which can be checked by left multiplying $|v\rangle$ to the above equation. In words, this equation means that the action of $H^{(i)}$ on $|v\rangle$ generates a deviation, perpendicular to $|v\rangle$, as given by the corresponding left singular vector $|l_i\rangle$, with weight $\lambda_i$ (the singular value). In particular, if $\lambda_i = 0$, then one recovers Eq. 14, and $|v\rangle$ becomes an eigenstate of $H^{(i)}$. Thinking of $H^{(i)} = i \partial_t$ as a time evolution generator, then the LHS is the covariant time derivative $iD_t$. The $i^{th}$ left singular vector $|l_i\rangle$ is thus the normalized tangent vector generated by $H^{(i)}$, and the corresponding singular value is related to the Fubini-Study metric in the time direction, $\lambda_i^2 = \langle v|D_t^2|v\rangle$, which is also the energy fluctuation,

$$\lambda_i^2 = \langle v|H^{(i)}(\mathbb{I} - P_v)H^{(i)}|v\rangle = \langle H^{(i)}|^2 v - \langle H^{(i)}|^2 v.$$ 

(25)
2. In what sense is the reconstructed parent operator optimal?

The right singular vectors satisfy orthonormality $\langle r_i | r_j \rangle = \delta_{ij}$. What does it entail for their operator counterparts $H^{(i)}$ (Eq. 23)? In order to carry this over to the operator space, one should additionally require the operators $\{L_i\}$ to satisfy certain operator orthonormality, which, up until now, we have not enforced. Following Qi and Ranard [32], we use the Hilbert-Schmidt inner product for operators,

$$\langle A, B \rangle \equiv \frac{1}{Tr\mathbb{I}} Tr(A^\dagger B) ,$$

where $Tr\mathbb{I} = D$ is the full Hilbert space dimension. An orthonormal operator basis $\{L_i\}$ satisfies

$$\langle L_i, L_j \rangle \equiv \delta_{ij} .$$

Then “Hamiltonians” corresponding to different right singular vectors also satisfy orthonormality,

$$\langle H^{(i)}, H^{(j)} \rangle = \sum_{i',j'} r_i^{(i')} r_j^{(j')} \langle L^{(i')}, L^{(j')} \rangle = \langle r_i | r_j \rangle = \delta_{ij} .$$

In other words, these “eigen-Hamiltonians” $\{H^{(i)}\}$ form an orthonormal basis for the operator space spanned by $\{L_i\}$. A normalized traceless “Hamiltonian” $H$ simply means its spectrum has unit variance, $Tr(H^2)/Tr(\mathbb{I}) = 1$.

Using orthonormal $\{L_i\}$, in situations where an exact zero eigenvalue does not exist for $G$ (Eq. 18), the parent operator $H^{(i_{min})}$ corresponding to the lowest eigenvalue of $G$ is an “optimal” approximate parent Hamiltonian, in the sense that out of all normalized operators in the space of $\text{Span}\{L_i\}$, $H^{(i_{min})}$ generates the lowest energy fluctuation on $|v\rangle$, or equivalently the least deviation of $H|v\rangle$ from $|v\rangle$.

II. Quantifying the quality of the reconstructed basis using IPR

The method described in the text is based on the ansatz that the RDM $\rho_A$ can be written as a scalar function $y$ of a local operator $H_P$, and $H_P$ itself is to be (approximately) constructed, from an exact eigenstate $|\xi\rangle$ of $\rho_A$, in the space of $\mathcal{L} \equiv \text{Span}\{L_i\}$,

$$\rho_A \overset{?}{=} y(H_P) , \quad H_P \in \mathcal{L} .$$

The construction scheme for $H_P$, however, only guarantees that $H_P$ and $\rho_A$ (approximately) share one eigenstate $|\xi\rangle$, with no constraint on the remainder of the eigenbasis. Therefore, to claim that one has successfully reconstructed $\rho_A$ in terms of $\{L_i\}$, one needs to verify that the entire eigenbasis of $H_P$ approximately matches that of $\rho_A$.

A simple way to quantify the quality of one set of basis states $\{|\phi_n\rangle\}$ in terms of their similarity to a reference basis $\Psi \equiv \{|\psi_n\rangle\}$, is to use the inverse participation ratio,

$$\text{IPR}(\phi_n|\Psi) = \frac{1}{\sum_{m=1}^{N} |\langle \phi_n | \psi_m \rangle|^4} \in [1, N] .$$

The IPR measures effectively how many basis states in $\Psi$ one needs to span a particular $|\phi_n\rangle$. It is 1 if $\langle \phi_n | \psi_m \rangle = \delta_{m,n}$, and saturates to $N$ if $|\langle \phi_n | \psi_m \rangle| = 1/\sqrt{N} \forall m$. In the context of RDM reconstruction, one would compute the IPR for each of the eigenstates of $H_P$ in the exact eigenbasis of $\rho_A$; if all of them are close to 1, then $H_P$ and $\rho_A$ approximately share the same set of basis states.

1. Generalized IPR in the presence of degeneracy

When $H_P$ has degeneracy, there is a $U(M)$ indeterminacy in an $M$-fold degenerate subspace $\mathcal{M}$. Then taking a single numerically obtained eigenstate out of this $M$-dimensional subspace may yield a “broadened” IPR (i.e., one $> 1$), even if upon a $U(M)$ transformation, each of the $M$ (transformed) states could have a perfectly sharp IPR (i.e.,
FIG. 4. Inverse participation ratio of eigenstates of parent Hamiltonian $H_P$.

= 1). To fix this, we generalize the notion of IPR to a degenerate subspace. Denote the projection operator of this subspace and a corresponding density operator as

$$P_M = \sum_{n=1}^{N_M} |\phi_n\rangle\langle\phi_n|, \quad \rho_M = P_M/\text{Tr}P_M.$$  

The generalized IPR is defined as the exponentiated 2nd Renyi entropy, $e^{S_2}$, of the diagonal ensemble in the $\Psi$ basis,

$$\text{IPR}(P_M|\Psi) = \frac{1}{\sum_{m=1}^{N_M} \langle\psi_m|\rho_M|\psi_m\rangle^2}.$$  

One can verify that the generalized IPR reduces to the standard one when there is no degeneracy ($M \rightarrow 1$). Note that if $P_M$ exactly matches an equal-dimensional subspace in the $\Psi$ basis, $P_M = \sum_{n=1}^{N_M} |\phi_n\rangle\langle\phi_n|$, then $\langle\psi_m|\rho_M|\psi_m\rangle = \frac{1}{M}$, hence $\text{IPR}(P_M|\Psi) = M$. In other words, in the perfect match case, the generalized IPR is given by the dimension of the degenerate subspace $M$. On the other hand, if each of the degenerate $|\phi_n\rangle$ still satisfies $|\langle\phi_n|\psi_m\rangle| = \frac{1}{\sqrt{N}} \forall m$, then $\langle\psi_m|\rho_M|\psi_m\rangle = \frac{1}{N}$, hence $\text{IPR} = N$. The generalized IPR thus reflects the notion of effective number of $|\psi\rangle$ states needed to span the subspace $P_M$.

2. Direct comparison the eigenstates of entanglement Hamiltonian and those of parent Hamiltonian using IPR

In this section, we explicitly show the comparison of eigenstates of $H_P$ with those of $H_E$ using IPR. We take the 1D spin chain as example again. Since the reconstructed $H_E$ has degeneracy, we use the generalized IPR introduced in Eq. 32 when appropriate. In Fig. 4, we show the IPR of eigenstates of $H_P$ as labeled by their (renormalized) weight $\epsilon_n$. It is found $\text{IPR}_n \approx 1$ for all of eigenstates with weight $\epsilon_n > 10^{-6}$, showing that each eigenstate of $H_E$ is identical to the eigenstate of $H_P$. Please note that, for worst case, if the eigenstates of $H_P$ and that of $H_E$ are totally independent, it should be expected maximum value of $\text{IPR} \sim N \sim 2^{L/2}$ ($L$ total system size) which is exponential growing with $L$. In Fig. 4, $\text{IPR}_n$ are all close to 1 show that the eigenstates of $H_P$ has well captured the eigenstates of $H_E$.

In the main text, we have demonstrated that the eigenvalue of parent Hamiltonian $H_P$ has one-to-one correspondence with the entanglement spectra of reduced density matrix. Here, we further show that each eigenstate of $H_P$ can be captured by the eigenstate of $H_E$. Taking into account that density matrix fidelity $F(\rho_A, \varrho) = \text{Tr}\sqrt{\sqrt{\rho_A}\varrho\sqrt{\rho_A}}$ itself reveals the weighted averaged wavefunction overlap between the eigenstates of $H_P$ and that of $H_E$, we now can understand very large value of density matrix fidelity as shown in the main text. In conclusion, the very large density matrix fidelity unambiguously sets up the equivalence between $H_P$ and entanglement Hamiltonian $H_E$. 

III. Optimizing RDM reconstruction fidelity

Under the ansatz Eq. 29, if the eigenbasis of the constructed \( H_P \) matches exactly with that of the target RDM \( \rho_A \), then the scalar function \( y \) is implicitly determined through the map between their spectra, \( y(\varepsilon_n) = p_n \), where \( \varepsilon_n \) and \( p_n \) are the eigenvalue of \( H_P \) and \( \rho_A \), respectively, associated with their common eigenvector \( |\psi_n\rangle \). When the basis reconstruction is only approximate, the best \( y \) function can be determined in principle by maximizing the fidelity between the original and reconstructed RDMs. For clarity, in this section we will drop the subscript \( A \) and denote the target RDM as \( \rho \). Its eigen decomposition is

\[
\rho = \sum_n p_n |\psi_n\rangle \langle \psi_n| .
\]

The reconstructed density matrix is \( \varrho = y(H_P) \) with as of yet unknown \( y \), where \( H_P = \sum_n \varepsilon_n |\phi_n\rangle \langle \phi_n| \) is the reconstructed parent operator. The eigen decomposition of \( \varrho \) is therefore

\[
\varrho = \sum_n q_n |\phi_n\rangle \langle \phi_n| ,
\]

where \( q_n = y(\varepsilon_n) \). The fidelity between the original and the reconstructed RDMs is defined as

\[
F(\rho, \varrho) = \text{Tr} \hat{F}(\rho, \varrho) , \quad \hat{F}(\rho, \varrho) = \sqrt{\rho} \varrho \sqrt{\rho} .
\]

It will be useful to note that the operator \( \hat{F}(\rho, \varrho) \) arises from the following polar decomposition,

\[
\sqrt{\rho_1 \sqrt{\rho_2}} = \hat{F}(\rho_1, \rho_2) U(\rho_1, \rho_2) , \quad U(\rho_1, \rho_2)^\dagger U(\rho_2, \rho_1) ,
\]

where the unitary \( U(\rho_1, \rho_2) \), although not of our concern in the present context, is related to Uhlmann’s parallel transport of density matrices [37]. The maximization of \( F \) can be viewed as a variational problem in the space of normalized distributions \( \{q_n\} \), and once the optimal weights are obtained, \( y \) can be determined (or defined) through \( y(\varepsilon_n) = q_n \).

The stationary condition for extremal \( F \) over the variational space of \( \{q_n\} \) is

\[
\frac{\partial}{\partial q_n} \left[ F - \lambda \left( \sum_m q_m - 1 \right) \right] = 0 ,
\]

where \( \lambda \) is the Lagrangian multiplier for the normalization \( \sum_m q_m = 1 \). Using \( \partial \text{Tr} \sqrt{A} = \frac{i}{2} \text{Tr} (\sqrt{A}^{-1} \partial A) \) for any invertible operator \( A \), Eq. 37 becomes

\[
\frac{\partial F}{\partial q_n} = \frac{1}{2} \langle \phi_n | \hat{Q} | \phi_n \rangle = \lambda \quad \forall n ,
\]

where \( \hat{Q} = \sqrt{\rho} \hat{F}(\rho, \varrho)^{-1} \sqrt{\rho} \). Using Eq. 36, one can show that \( \hat{F}(\rho, \varrho)^{-1} = U(\rho, \varrho) \sqrt{\rho} \sqrt{\varrho} \), thus

\[
\hat{Q} = \sqrt{\rho}^{-1} \hat{F}(\rho, \varrho) \sqrt{\varrho}^{-1} ,
\]

and Eq. 38 becomes \( \langle \phi_n | \hat{F}(\rho, \varrho) | \phi_n \rangle = 2\lambda q_n \forall n \). Note that \( \sum_n q_n = 1 \), thus \( 2\lambda = \sum_n \text{LHS} = \text{Tr} \hat{F}(\rho, \varrho) = F(\rho, \varrho) \), and we finally arrive at a self consistent equation for the weights \( \{q_n\} \),

\[
\frac{\langle \phi_n | \hat{F}(\rho, \varrho) | \phi_n \rangle}{\sum_n \langle \phi_n | \hat{F}(\rho, \varrho) | \phi_n \rangle} = q_n \quad \forall n ,
\]

note that the LHS depends on \( \{q_n\} \) only through \( \rho \).

1. Approximate optimal solution in the high-fidelity limit

When the two bases \( \{|\psi\rangle\} \) and \( \{|\phi\rangle\} \) have a good match, the fidelity operator \( \hat{F} \) (Eq. 35) is dominated by its diagonal line (say, in the \( \{|\phi\rangle\} \) basis). In this case one may adopt the approximation that

\[
\langle \phi_n | \hat{F}^2(\rho, \varrho) | \phi_n \rangle \approx \sqrt{\langle \phi_n | \hat{F}^2(\rho, \varrho) | \phi_n \rangle} = \sqrt{q_n} \sqrt{\langle \phi_n | \rho | \phi_n \rangle} .
\]
Substituting this into Eq. 40, one then obtains
\[ q_n \simeq \langle \phi_n | \rho | \phi_n \rangle , \tag{42} \]
that is, the optimal \( q_n \) is the weight of the reconstructed eigenstate \( | \phi_n \rangle \) in the original (i.e. target) mixed state \( \rho \).

IV. Entanglement Hamiltonian in Strong Inter-chain Coupling Limit

We will derive the entanglement Hamiltonian \( H_E \) in the strong inter-chain coupling limit using perturbation theory. The starting point is the physical Hamiltonian:
\[ \hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB} \]
\[ \hat{H}_{\alpha=A(B)} = J_{\alpha} \sum_{\langle ij \rangle} \left[ S_{i,\alpha}^x S_{j,\alpha}^x + S_{i,\alpha}^y S_{j,\alpha}^y + \Delta S_{i,\alpha}^z S_{j,\alpha}^z \right] \]
\[ \hat{H}_{AB} = J_{\perp} \sum_i \left[ S_{i,A}^x S_{i,B}^x + S_{i,A}^y S_{i,B}^y + \Delta S_{i,A}^z S_{i,B}^z \right]. \tag{43} \]

In the limit of \( J_{\perp} \gg J_{\|} \), we treat \( \hat{H}_{A(B)} \) as the perturbation to \( \hat{H}_{AB} \). Thus the ground state of \( \hat{H}_{AB} \) can be viewed as a product state of spin singlets:
\[ |0\rangle = \prod_i |s_i\rangle , \tag{44} \]
where \( |s_i\rangle \) is the spin singlet living on inter-chain bond:
\[ |s_i\rangle = \frac{1}{\sqrt{2}} (| \uparrow, A \rangle | \downarrow, B \rangle - | \downarrow, A \rangle | \uparrow, B \rangle ) , \quad E_s = \left( -\frac{1}{2} - \frac{\Delta}{4} \right) J_{\perp} \tag{45} \]

On each inter-chain bond, spin excitation state is described by spin triplet excitations:
\[ |t_i^+\rangle = | \uparrow, A \rangle | \uparrow, B \rangle , \quad E_{t^+} = \frac{\Delta}{4} J_{\perp} \]
\[ |t_i^0\rangle = \frac{1}{\sqrt{2}} (| \uparrow, A \rangle | \downarrow, B \rangle + | \downarrow, A \rangle | \uparrow, B \rangle ) , \quad E_{t^0} = \left( \frac{1}{2} - \frac{\Delta}{4} \right) J_{\perp} \]
\[ |t_i^-\rangle = | \downarrow, A \rangle | \downarrow, B \rangle , \quad E_{t^-} = \frac{\Delta}{4} J_{\perp} . \tag{46} \]

At first-order perturbation theory, the first-order correction is
\[ |1\rangle = \sum_i \left[ t_i^+ t_{i+1}^- (t_i^+ t_{i+1}^- | \hat{H}_A + \hat{H}_B | 0 \rangle \right] E_+ + E_- - 2E_s + \frac{t_i^- t_{i+1}^+ (t_i^- t_{i+1}^+ | \hat{H}_A + \hat{H}_B | 0 \rangle \right] E_+ + E_- - 2E_s + \frac{t_i^0 t_{i+1}^0 (t_i^0 t_{i+1}^0 | \hat{H}_A + \hat{H}_B | 0 \rangle \right] 2E_0 - 2E_s }{2E_0 - 2E_s } \]

, where we use the notation:
\[ |t_i^+ t_{i+1}^-\rangle = |s_1\rangle \otimes \ldots |s_{i-1}\rangle |t_i^+\rangle |t_{i+1}^-\rangle \otimes |s_{i+2}\rangle \ldots |s_L\rangle \]
\[ |t_i^- t_{i+1}^+\rangle = |s_1\rangle \otimes \ldots |s_{i-1}\rangle |t_i^-\rangle |t_{i+1}^+\rangle \otimes |s_{i+2}\rangle \ldots |s_L\rangle \]
\[ |t_i^0 t_{i+1}^0\rangle = |s_1\rangle \otimes \ldots |s_{i-1}\rangle |t_i^0\rangle |t_{i+1}^0\rangle \otimes |s_{i+2}\rangle \ldots |s_L\rangle \]

and Hamiltonian elements can be calculated by using:
\[ S_{i,A}^+ S_{i+1,A}^- |s_i\rangle |s_{i+1}\rangle = -\frac{1}{2} (t_i^+ |t_{i+1}^-\rangle ) \]
\[ S_{i,A}^- S_{i+1,A}^+ |s_i\rangle |s_{i+1}\rangle = -\frac{1}{2} (t_i^- |t_{i+1}^+\rangle ) \]
\[ S_{i,A}^z S_{i+1,A}^z |s_i\rangle |s_{i+1}\rangle = \frac{1}{4} (t_i^0 |t_{i+1}^0\rangle ) \]
The reduced density matrix can be obtained by (within first-order perturbation approximation):

\[
\rho_A = Tr_B [\ket{\psi}\bra{\psi}] = Tr_B [(\ket{0} + \ket{1})(\bra{0} + \bra{1})]
\]

First we get

\[
Tr_B |0\rangle \langle 0| = \prod_i Tr_B |s_i\rangle \langle s_i| = \prod_i [\langle t^B_i |s_i\rangle \langle t^A_i | + \langle t^A_i |s_i\rangle \langle t^B_i |] = \frac{1}{2L}
\]

Second, we calculate

\[
Tr_B |1\rangle \langle 1| = \frac{J_{||}}{4J_{\perp}} [-\Delta Tr_B |t^0_{i+1}\rangle \langle 0| + \frac{2}{1+\Delta} Tr_B |t^+_i t^0_{i+1}\rangle \langle 0| + \frac{2}{1+\Delta} Tr_B |t^-_i t^0_{i+1}\rangle \langle 0| +
\]

\[
-\Delta Tr_B |t^0_{i+1}\rangle \langle t^0_{i+1}| + \frac{2}{1+\Delta} Tr_B |t^+_i t^0_{i+1}\rangle \langle t^0_{i+1}| + \frac{2}{1+\Delta} Tr_B |t^-_i t^0_{i+1}\rangle \langle t^0_{i+1}| +
\]

\[
= \frac{1}{2L} \frac{J_{||}}{4J_{\perp}} [2\Delta 4S^z_i S^z_{i+1} + \frac{2}{1+\Delta} (S^+_i S^-_{i+1} + h.c.)] = \frac{1}{2L} \frac{J_{||}}{4J_{\perp}} [\frac{1}{2}\Delta (1 + \Delta) S^z_i S^z_{i+1} + \frac{1}{2} (S^+_i S^-_{i+1} + h.c.)]
\]

Here we use the following relations:

\[
Tr_B |t^0_{i+1}\rangle \langle 0| = \frac{1}{2L} \frac{J_{||}}{4J_{\perp}} [\langle \uparrow \downarrow | \uparrow \downarrow | t^0_{i+1}\rangle |s_i\rangle \langle s_{i+1} | \uparrow \downarrow | \downarrow \uparrow | t^0_{i+1}\rangle |s_i\rangle \langle s_{i+1} | + \langle \downarrow \uparrow | \downarrow \uparrow | t^0_{i+1}\rangle |s_i\rangle \langle s_{i+1} | \downarrow \uparrow | \uparrow \downarrow | t^0_{i+1}\rangle |s_i\rangle \langle s_{i+1} | +
\]

\[
= \frac{1}{2L} \frac{J_{||}}{4J_{\perp}} [\langle \uparrow \downarrow A |A_i\rangle \langle A_i | \uparrow \downarrow A_i | + \langle \downarrow \uparrow A_i \rangle \langle A_i | \downarrow \uparrow A_i | - \langle \uparrow \downarrow A_i \rangle \langle A_i | \downarrow \uparrow A_i | - \langle \downarrow \uparrow A_i \rangle \langle A_i | \uparrow \downarrow A_i |]
\]

\[
= \frac{1}{2L} 4S^z_i S^z_{i+1}
\]

and

\[
Tr_B |t^+_i t^-_{i+1}\rangle \langle 0| = \frac{1}{2L} \frac{J_{||}}{4J_{\perp}} [\langle \uparrow \downarrow | \uparrow \downarrow | t^+_i t^-_{i+1}\rangle |s_i\rangle \langle s_{i+1} | \uparrow \downarrow | \downarrow \uparrow | t^+_i t^-_{i+1}\rangle |s_i\rangle \langle s_{i+1} | + \langle \downarrow \uparrow | \downarrow \uparrow | t^+_i t^-_{i+1}\rangle |s_i\rangle \langle s_{i+1} | \downarrow \uparrow | \uparrow \downarrow | t^+_i t^-_{i+1}\rangle |s_i\rangle \langle s_{i+1} | +
\]

\[
= \frac{1}{2L} \frac{J_{||}}{4J_{\perp}} [-2 \langle \uparrow \downarrow A_i A_i \rangle |s_i\rangle \langle s_{i+1} |] = \frac{1}{2L} [-2 S^z_i S^z_{i+1}]
\]
Third, we derive
\[
Tr_B[[1]|1]\rangle = \sum_{ij} \left(\frac{J_{\parallel}}{4J_{\perp}}\right)^2 \frac{2}{1 + \Delta} |t^+_i t^+_j| + \frac{2}{1 + \Delta} \langle t^+_i t^+_j | - \Delta \langle t^+_i t^+_j | + \frac{2}{1 + \Delta} \langle t^-_i t^-_j | - \Delta \langle t^-_i t^-_j |
\]
\[
= \left(\frac{J_{\parallel}}{4J_{\perp}}\right)^2 \sum_i \frac{2^2}{(1 + \Delta)^2} Tr_B|t^+_i t^+_i\rangle \langle t^+_i t^+_i| + \frac{2^2}{(1 + \Delta)^2} Tr_B|t^-_i t^-_i\rangle \langle t^-_i t^-_i| - \frac{2\Delta}{1 + \Delta} Tr_B|t^+_i t^+_i\rangle \langle t^+_i t^+_i| - \frac{2\Delta}{1 + \Delta} Tr_B|t^-_i t^-_i\rangle \langle t^-_i t^-_i|
\]
\[
- \frac{2\Delta}{1 + \Delta} Tr_B|t^+_i t^+_i\rangle \langle t^-_i t^-_i| - \frac{2\Delta}{1 + \Delta} Tr_B|t^-_i t^-_i\rangle \langle t^+_i t^+_i| + \Delta^2 Tr_B|t^+_i t^+_i\rangle \langle t^+_i t^+_i|
\]
\[
+ \left(\frac{J_{\parallel}}{4J_{\perp}}\right)^2 \sum_i \frac{2^2}{(1 + \Delta)^2} Tr_B|t^-_i t^-_i\rangle \langle t^+_i t^+_i| + \frac{2^2}{(1 + \Delta)^2} Tr_B|t^-_i t^-_i\rangle \langle t^-_i t^-_i| - \frac{2\Delta}{1 + \Delta} Tr_B|t^-_i t^-_i\rangle \langle t^-_i t^-_i| - \frac{2\Delta}{1 + \Delta} Tr_B|t^+_i t^+_i\rangle \langle t^-_i t^-_i|
\]
\[
- \frac{2\Delta}{1 + \Delta} Tr_B|t^-_i t^-_i\rangle \langle t^+_i t^+_i| + \Delta^2 Tr_B|t^-_i t^-_i\rangle \langle t^-_i t^-_i|
\]
\[
= \frac{1}{2L^3} \left(\frac{J_{\parallel}}{4J_{\perp}}\right)^2 \sum_i \frac{2^2}{(1 + \Delta)^2} \frac{1}{2} \langle S^+_i S^-_i + h.c. \rangle + \frac{\Delta^2}{8} \langle 42 S^+_i S^-_i \rangle
\]

And we need the relations:
\[
Tr_B|t^0_0 t^0_1\rangle \langle t^0_1 t^0_1| = \frac{1}{8} 4 S^+_i S^-_i + S^z_i S^z_i
\]
\[
Tr_B|t^+_i t^+_i\rangle \langle t^-_i t^+_i| = \frac{1}{2} \langle 1 - |A|^2 \rangle \langle 1 + |A|^2 \rangle \langle 1 + |A|^2 |A|^2 \rangle
\]
\[
Tr_B|t^-_i t^-_i\rangle \langle t^+_i t^-_i| = \frac{1}{2} \langle 1 - |A|^2 \rangle \langle 1 + |A|^2 \rangle \langle 1 + |A|^2 |A|^2 \rangle
\]
\[
Tr_B|t^+_i t^-_i\rangle \langle t^-_i t^+_i| = \frac{1}{2} \langle 1 - |A|^2 \rangle \langle 1 + |A|^2 \rangle \langle 1 + |A|^2 |A|^2 \rangle
\]
\[
Tr_B|t^-_i t^+_i\rangle \langle t^+_i t^+_i| = \frac{1}{2} \langle 1 - |A|^2 \rangle \langle 1 + |A|^2 \rangle \langle 1 + |A|^2 |A|^2 \rangle
\]

At last, we sum up all calculations together:
\[
\rho_A = Tr_B[[0|0]) + |1|0]) = \frac{1}{2L} \left[1 - \frac{4J_{\parallel}}{J_{\perp}} (1 + \Delta) \frac{1}{2} \langle S^+_i S^-_i + h.c. \rangle + \frac{2}{1 + \Delta} \langle S^+_i S^-_i + h.c. \rangle + \Delta^2 \langle 42 S^+_i S^-_i \rangle\right]
\]
\[
\approx \frac{1}{2} \exp(-\mathcal{H}_{E}^{per})
\]

, where
\[
\mathcal{H}_{E}^{per} = \tilde{J}_{xy} \sum_{i= \pm 1} \langle S^+_{i+1} S^-_{i+1} + S^z_{i+1} S^z_{i+1}| + \tilde{J}_{zy} \sum_{i= \pm 1} \langle S^+_{i+1} S^-_{i+1} + S^z_{i+1} S^z_{i+1}| - \tilde{J}_{xy} \sum_{i= \pm 1} \langle S^+_{i+1} S^-_{i+1} + S^z_{i+1} S^z_{i+1}| - \tilde{J}_{zy} \sum_{i= \pm 1} \langle S^+_{i+1} S^-_{i+1} + S^z_{i+1} S^z_{i+1}|,
\]

and \(\tilde{J}_{xy} = \frac{4}{\Delta} \frac{J_{\parallel}}{J_{\perp}} \), \(\tilde{J}_{zy} = 2 \Delta \frac{J_{\parallel}}{J_{\perp}} \), \(\tilde{J}_{xy} = \frac{2}{1 + \Delta^2} \langle J_{\parallel} \rangle^2 \) and \(\tilde{J}_{zy} = \frac{\Delta^2}{4} \langle J_{\parallel} \rangle^2 \). Here we only keep the leading term in nearest neighbor and second nearest neighbor couplings. The form that we show in the main text is the case for isotropic case \(\Delta = 1\). The anisotropic form will be discussed in Sec. .

V. Comparison entanglement spectra with eigenvalues spectrum of parent Hamiltonian

The equivalence between the entanglement Hamiltonian \(\mathcal{H}_E\) and parent Hamiltonian \(\mathcal{H}_P\) can be validated through the analysis of universal feature in the entanglement spectra (ES). Here we show the comparison of ES of entanglement
Hamiltonian and eigenvalue spectrum of parent Hamiltonian in spin ladder model (the results for 1D spin chain model has been shown in the main text). Fig. 5 shows typical ES (measured from the minimal value $\xi_0$) plotted as a function of momentum $K = \frac{2\pi k}{L}$ ($k = 0, 1, ..., L - 1$), since the translational symmetry along the chain direction is preserved. For the isotropic case $\Delta = 1$ (Fig. 5(a)), the low-lying excitations of ES form an arch structure, which can be fitted by the des Cloisaux-Pearson dispersion relations $\xi_i - \xi_0 = v|\sin K|$ (red dashed line). It strongly suggests the ES can resemble gapless quantum critical behavior which is intrinsic to the quantum spin–1/2 Heisenberg chain [17, 47]. Importantly, the eigenvalue spectra of obtained $H_P$ shows the very similar features (Fig. 5(b)). As a direct comparison, we plot $\varepsilon_n - \varepsilon_0$ and $\xi_n - \xi_0$ ($\xi_n = -\log p_n$) in Fig. 5(c). It is found that eigenvalue $\varepsilon_n$ has one-to-one correspondence with $\xi_i$, and a linear relationship $\varepsilon_n \propto \xi_n$ can be established (red dashed line). Here, the comparison between entanglement spectra and eigenvalue spectra of $H_P$ clearly establishes the relationship between entanglement Hamiltonian and reduced density matrix: $H_E = f(H_P) \approx H_P$.

![FIG. 5. (a) Entanglement spectra ($\xi_i - \xi_0$), obtained from reduced density matrix, are grouped by total momentum $K$ along the chain direction. (b) Energy spectra ($E_i - E_0$) of reconstructed density matrix. In (a-b), the lowest spectra branch is fitted as $v|\sin K|$ by red dashed line. (c) Direct comparison of entanglement spectra ($\xi_i - \xi_0$) and energy spectra ($E_i - E_0$). All low-lying spectra are computed on $2 \times L$ ladders shown in black circles ($L = 10$), green squares ($L = 12$) and blue diamonds ($L = 14$). Here we set $\theta = \pi/3$ and $\Delta = 1.0$.

### VI. Anisotropic Case

In the main text, we focus on the isotropic Heisenberg model. Here we briefly discuss the anisotropic case ($\Delta > 1$). In our extensive tests, our numerical scheme works well for both isotropic and anisotropic Heisenberg model. For the anisotropic case, we can also map out the entanglement Hamiltonian within the same scheme. Here we show spin ladder model (Fig. 1(b)) and take $J_\perp/J_\parallel = 4$ and $\Delta = 2$ as an example:

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB}$$

$$\hat{H}_{A(\perp)} = J_\perp \sum_{(ij)} [S_{i,\alpha}^x S_{j,\alpha}^x + S_{i,\alpha}^y S_{j,\alpha}^y + \Delta S_{i,\alpha}^z S_{j,\alpha}^z]$$

$$\hat{H}_{AB} = J_\parallel \sum_i [S_{i,A}^x S_{i,B}^x + S_{i,A}^y S_{i,B}^y + \Delta S_{i,A}^z S_{i,B}^z]. \quad (56)$$

The targeting operator space is chosen to be:

$$\hat{H}_E = \sum_{n=1}^{N_\perp} J_{nx}^z \hat{J}_n^z + J_{ny}^z \hat{J}_n^z$$

$$\hat{J}_n^z = \sum_{i=1}^{L} (S_{i}^x S_{i+n}^x + S_{i}^y S_{i+n}^y), \quad \hat{J}_n^z = \sum_{i=1}^{L} S_{i}^z S_{i+n}^z. \quad (57)$$
Within the same scheme shown in the main text, the obtained parameters of entanglement Hamiltonian is shown in Tab. III. As shown in Tab. III, $H_E$ breaks the spin rotation symmetry $J_{xy}^n \neq J_{zz}^n$. We also confirm that the parameters in $H_E$ can be compared with perturbation theory as shown in the Sec. . These facts point to that $H_E$ is effectively described by the XXZ spin chain with spin rotation symmetry breaking. This is not surprising since the parent Hamiltonian breaks spin rotation symmetry explicitly.

TABLE III. Parameters of entanglement Hamiltonian $H_E$ for anisotropic spin ladder model. Here we set $J_\perp / J_\parallel = 4$ and $\Delta = 2$.

| $L$  | $g_0$        | $J_{1,2}^{xy}$ | $J_{1,2}^{zz}$ |
|-----|--------------|----------------|---------------|
| 10  | $1.34 \times 10^{-8}$ | 0.304 | -0.039 | 0.952 | -0.065 |
| 12  | $6.37 \times 10^{-7}$ | 0.299 | -0.039 | 0.951 | -0.061 |
| 14  | $8.89 \times 10^{-7}$ | 0.303 | -0.038 | 0.950 | -0.067 |