Area-Law Entangled Eigenstates from Nullspaces of Local Hamiltonians

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Eigenstate thermalization in quantum many-body systems implies that eigenstates at high energy are similar to random vectors. Identifying systems where at least some eigenstates are nonthermal is an outstanding question. In this Letter we show that interacting quantum models that have a nullspace—a degenerate subspace of eigenstates at zero energy (zero modes), which corresponds to infinite temperature, provide a route to nonthermal eigenstates. We analytically show the existence of a zero mode which can be represented as a matrix product state for a certain class of local Hamiltonians. In the more general case we use a subspace disentangling algorithm to generate an orthogonal basis of zero modes characterized by increasing entanglement entropy. We show evidence for an area-law entanglement scaling of the least-entangled zero mode in the broad parameter regime, leading to a conjecture that all local Hamiltonians with the nullspace feature zero modes with area-law entanglement scaling and, as such, break the strong thermalization hypothesis. Finally, we find zero modes in constrained models and propose a setup for observing their experimental signatures.

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Introduction.—Eigenstate thermalization hypothesis (ETH) [1,2] provides a specific mechanism for thermalization in isolated quantum many-body systems. ETH suggests that the eigenstates of the Hamiltonian at a given energy density are indistinguishable by local measurements and resemble random vectors. A particular consequence of ETH is that highly excited states of quantum systems feature strong entanglement. Numerical studies demonstrated that ETH can describe the vast majority of quantum systems [3]. At the same time, possible mechanisms leading to violations of ETH are a subject of active research. Typically, ETH can be avoided due to the emergence of additional conserved quantities that may originate from special properties of Hamiltonian in integrable models [4] or from the presence of strong disorder in the many-body localized phase [5–7].

While in integrable and localized systems all eigenstates disobey ETH, recently the focus shifted to systems with weak ergodicity breaking, which have a small number of weakly entangled eigenstates coexisting with the bulk of “thermal” eigenstates that obey ETH. These weakly entangled and thus nonthermal eigenstates were dubbed quantum many-body scars (QMBS) and were reported in a number of different models [8–16] (see also Ref. [17] for a recent review). Interestingly, a large fraction of scarred

systems features an exponentially large in system size nullspace which is protected by the symmetries of the model [18–21]. The relevance of such nullspaces to the weak ergodicity breaking was suggested by Ref. [22] which analytically constructed a particular eigenstate from the nullspace (zero mode) of the so-called PXP model [19,23,24] as a matrix product state (MPS). Similar zero modes were also discovered in two-dimensional models [25,26] and models with larger blockades [27], while Ref. [28] proposed a systematic way of constructing a parent Hamiltonian for MPS zero modes. The MPS form of these zero modes implies an area-law scaling of entanglement. Thus, such zero modes can be regarded as QMBS and provide an example of weak ergodicity breakdown. Moreover, in some cases they could be utilized as a “vacuum” for the construction of other QMBS states outside of the nullspace [22,29]. However, although weakly entangled zero modes were established for certain models and in many-body localized systems [30], the general conditions for their existence remain unclear.

In this Letter we explore the structure of the exponentially degenerate nullspaces in a large class of spin chains. We analytically construct an MPS zero mode for a broad class of two-local Hamiltonians with symmetry-protected nullspace. For more generic Hamiltonians, we use a numerical algorithm to construct a basis in the nullspace that is ordered according to entanglement entropy [31]. We define a notion of a least-entangled zero mode, that is shown to obey area-law entanglement scaling in a family of generic Hamiltonians, even though the majority of states in this basis features volume-law entanglement scaling, signaling thermalization [20]. Thus, we conjecture that all local

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Hamiltonians with an exponentially degenerate nullspace feature a zero mode with area-law scaling of entanglement entropy, establishing a generic route to QMBS and weak ergodicity breaking. Finally, we find the MPS zero modes in a kinetically constrained Hamiltonian and propose an experimental scheme to observe their effects in Rydberg atom arrays [32].

Exponentially degenerate nullspace.—A generic mechanism leading to the exponentially degenerate nullspace of local Hamiltonians is provided by the existence of spatial inversion symmetry and the symmetry of the many-body spectrum around zero energy [19,20]. For concreteness, we consider one-dimensional, inversion-symmetric, spin-1/2 chains with Hamiltonian

$$H_{\text{ZZX}} = \sum_{i=1}^L [X_i + a(Z_i X_{i+1} + X_i Z_{i+1}) + b Z_{i-1} X_i Z_{i+1}], \quad (1)$$

parametrized by two constants a and b . Operators X_i , Y_i , and Z_i correspond to $\sigma_i^{x,y,z}$ Pauli matrices operating on the local Hilbert space of spin i spanned by $\uparrow, \downarrow$ states. We assume L to be even and use periodic boundary conditions identifying spins $L+1$ and 1 . The Hamiltonian (1) anti-commutes with the operator $\Pi = \prod_i^L Z_i$, $\{H_{\text{ZZX}}, \Pi\} = 0$. Π ensures that for each eigenstate $|E\rangle$ at energy E , a partner eigenstate $\Pi|E\rangle = |-E\rangle$ exists at an energy $-E$, resulting in a symmetric energy spectrum around zero energy. We note that this property holds for any Hamiltonian which contains terms with an odd number of X, Y operators and an arbitrary number of Z operators.

The existence of a degenerate nullspace in model (1) and its generalizations is guaranteed by the presence of spectral reflection and inversion symmetries. While this is a basis-independent statement, it is easiest to understand in a computational basis, since product states with an even (odd) number of $\downarrow$ spins correspond to eigenvalues $\Pi = 1$ ($\Pi = -1$). Organizing basis elements into blocks with $\Pi = \pm 1$, the relation $\{H_{\text{ZZX}}, \Pi\} = 0$ implies the block-off-diagonal structure of the Hamiltonian in such a basis. The presence of inversion symmetry leads to a mismatch in the number of basis states between different blocks provided they are restricted to a particular inversion sector, which results in a nonempty kernel. In particular, inversion-symmetric product states necessarily have an even number of $\downarrow$ spins, and there are $2^{L/2}$ such states. An explicit calculation (see Supplemental Material [33]) shows that both inversion-even and -odd sectors feature at least $2^{L/2-1}$ zero modes with an even or odd number of spin $\downarrow$ spins respectively. Summing up these contributions, we obtain a lower bound for the dimension of the nullspace, $\mathcal{D}_0 = \dim(\ker H_{\text{ZZX}}) \geq 2^{L/2}$ [20,23,33].

Analytic MPS zero mode.—We find that all spin-1/2 Hamiltonians of the form $H = \sum_{i=1}^L h_{i,i+1}$, with $h_{i,i+1}$ being a two-site Hermitian operator which is reflection

symmetric and satisfies $\{\Pi, h_{i,i+1}\} = 0$, have exact zero modes which can be represented by MPSs. As a particular example of such a Hamiltonian we use (1) with $b = 0$, while in the Supplementary Material [33] we discuss the more general case.

We search for the zero-energy eigenstate of H_{ZZX} in the MPS form $|\psi\rangle = \sum_{\{a\}, \{s\}} A_{a_L a_1}^{s_1} A_{a_1 a_2}^{s_2} \dots A_{a_{L-1} a_L}^{s_L} |s_1, \dots, s_L\rangle$, where the indices a_i run from 1 to bond dimension χ , while $s_i = \uparrow, \downarrow$ labels the local Hilbert space. The local matrices $A^{\uparrow, \downarrow}$ have dimension $\chi \times \chi$. Because of the translational invariance of H_{ZZX} , a sufficient condition for the state $|\psi\rangle$ to be a zero mode of the full Hamiltonian is the vanishing action of $h_{i,i+1} = (X_i + X_{i+1})/2 + a(Z_i X_{i+1} + X_i Z_{i+1})$ on the corresponding local tensors of the MPS. This condition can be written as $\sum_{s'_i, s'_{i+1}, a_{i+1}} h_{i,i+1}^{s_i s_{i+1}, s'_i s'_{i+1}} A_{a_i a_{i+1}}^{s'_i} A_{a_{i+1} a_{i+2}}^{s'_{i+1}} = 0$. To construct the solution for this equation we use the two-dimensional nullspace of the $h_{i,i+1}$ operator, spanned by a singlet $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ and a state $\theta|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$, where $\theta = (2a-1)/(2a+1)$ for H_{ZZX} with $b = 0$ (see Supplemental Material [33] for more generic Hamiltonians). The following choice of local matrices

$$A^{\uparrow} = \begin{pmatrix} 0 & 1 \\ \theta & 0 \end{pmatrix}, \quad A^{\downarrow} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2)$$

effectively combines these on site nullspaces allowing us to satisfy the condition $h_{i,i+1}|\psi\rangle = 0$ for any i , thus giving an MPS zero mode. The existence of an MPS zero mode for H_{ZZX} with $b = 0$ and its two-spin generalizations that include Y matrices opens the question regarding the fate of zero modes in more general Hamiltonians.

Least-entangled nullspace basis.—A systematic investigation of the nullspace is complicated due to its degeneracy and the absence of a natural basis. In order to overcome this limitation, we use entanglement to construct an unambiguous least-entangled nullspace basis (LENB), in which vectors are ordered according to bipartite entanglement entropy, $S = -\text{Tr}_A \rho_A \ln \rho_A$. The reduced density matrix $\rho_A = \text{Tr}_B |\psi\rangle\langle\psi|$ is obtained by tracing the right half of the chain B . The LENB is constructed in an iterative procedure: first we calculate the least-entangled zero mode (LEZM), i.e., a superposition of all zero modes $|LE_1\rangle = \sum_{n=1}^{\mathcal{D}_0} c_n |n\rangle$, where $\sum_n |c_n|^2 = 1$, that has the least possible amount of entanglement. This is achieved by employing algorithms [31,36] which minimize the entanglement of a vector in a subspace, here chosen to be the nullspace. The resulting state $|LE_1\rangle$ may be viewed as an analog of the ground state in the nullspace. Once obtained, the state $|LE_1\rangle$ is projected out of the nullspace, and the entanglement minimization algorithm is applied again to the remaining states resulting in $|LE_2\rangle$. The iteration of this process results in the LENB, $\{|LE_n\rangle\}$, $n = 1, \dots, \mathcal{D}_0$, in which the states are ordered according to their bipartite entanglement entropy.

FIG. 1. (a) Nullspace basis from exact diagonalization (dark blue) has uniformly high entropy similar to the entropy of the eigenstates with energy near zero (gray) and close to the Page value (dashed line) [37], $S_p = L/2 \ln 2 - 1/2$. The LENB (light blue) reveals low-entangled zero modes. Inset: density of states. Data are for the ZXZ model with $L = 18$ and the parameters denoted by a star in (b). (b) Entanglement of $|LE_1\rangle$ changes smoothly in the broad range of parameters of the ZXZ model with $L = 18$. The dotted lines denote the regions where $|LE_1\rangle$ is a product state. (c) Scaling of entanglement of the LEZM with system size L is consistent with area-law. Data are shown for four different points in parameter space, corresponding to symbols of the same shape in (b).

We numerically construct the LENB for the H_{ZXZ} model (1) at generic values of parameters. Figure 1(a) shows that the ZXZ model for $L = 18$ in the inversion-symmetric sector of zero total momentum has a Gaussian density of states with a small peak at $E = 0$ corresponding to nullspace. We explicitly check that the model is non-integrable and shows Wigner-Dyson level statistics [33]. The initial basis for the nullspace $\{|n\rangle\}$, obtained by an exact diagonalization algorithm, consists of states with approximately the same entropy, and almost coincides with the entropy of finite energy eigenstates [see Fig. 1(a)]. In contrast, the LENB construction results in a small number of weakly entangled states. In what follows we focus on the systematic analysis of LEZM and its entanglement scaling.

LEZM phase diagram.—Figure 1(b) shows the entanglement of the LEZM as a function of the parameters of the ZXZ model (1) for $L = 18$. The parameter space features two special lines $b = -1 \pm 2a$ for which the LEZM is a product state, $|\downarrow\downarrow\ldots\rangle$ and $|\uparrow\uparrow\ldots\rangle$, respectively. These lines include the point $a = b = 1$ which corresponds to the kinetically constrained PXP model [18]. When $b = 0$, the ZXZ model reduces to a sum of two-site operators for which we constructed an MPS zero mode with bond dimension $\chi = 2$ in Eq. (2), thus implying an area-law entanglement bounded as $S \leq \ln 2$. These three lines in parameter space correspond to local minima in the entanglement of the LEZM as constructed by the numerical algorithm. The entropy changes smoothly around these minima which suggest the persistence of area-law entangled zero modes beyond the set of lines where analytical results are available.

We study the scaling of entropy with the system size for a wide range of model parameters in Fig. 1(c). For all simulated parameters the behavior of entanglement entropy is consistent with area-law scaling. In particular for parameters that are close to the special lines in the phase diagram, entanglement does not change significantly with L .

For other values of parameters, finite size effects are more pronounced, yet the finite size scaling is consistent with area law and corrections decaying algebraically or exponentially with L [33]. Crucially, for all parameters, the state $|LE_1\rangle$ is locally similar between different system sizes as witnessed by the fidelity between local density matrices, and it features a large entanglement gap in the entanglement spectrum (see Supplemental Material [33]).

The existence of area-law entangled LEZM in a broad parameter regime in the ZXZ model raises the question if it is a simple consequence of the exponentially degenerate nullspace, or if the locality of the Hamiltonian is essential for its existence. This is addressed by comparing our local Hamiltonian with a random matrix Hamiltonian with similar symmetries. In this case, we observe that the least-entangled zero mode follows a volume-law scaling $S \propto L$ (see Supplemental Material [33]). In addition, we show that the distribution of the entanglement spectrum of $|LE_1\rangle$ for a random matrix approaches Marcenko-Pastur distribution [38]. This result suggests that for a random matrix the LENB construction does not lead to states which are qualitatively different from random vectors. The drastic difference in the behavior between random matrices and local Hamiltonians implies that the area-law LEZM is related to the locality of the Hamiltonian.

Eigenstate thermalization in LENB.—We shift the focus from LEZM to characterizing the whole LENB from the perspective of thermalization. We compare the expectation value of the average magnetization, $O = (1/L) \sum_{i=1}^L Z_i$ between the LENB states and nonzero-energy eigenstates of H_{ZXZ} . ETH suggests that expectation values of the operator O in eigenstates $\langle E|O|E\rangle$ are a smooth function of energy up to small fluctuations that are exponentially suppressed with system size [3]. Figure 2(a) shows that as energy E approaches zero, the expectation values of observables in eigenstates concentrate around zero, while entanglement entropy is rapidly increasing. In contrast, the

FIG. 2. (a) Diagonal matrix elements of magnetization O and eigenstates entanglement for $a = -1.3$, $b = -1.7$, and $L = 16$. The color intensity encodes the normalized energy of the eigenstates $\tilde{E} = |E/E_0|$, where E_0 is the ground state energy. (b) Scaling of the entanglement entropy of the LENB with respect to the system size for the same parameters. For $L = 18$ we only calculated the first 20 LEZM states.

states from the LENB defy the expectations from ETH despite having energy $E = 0$: a significant number of states from the LENB have both anomalously large expectation values of magnetization and small values of entanglement.

To understand the difference between zero modes we explore the finite size scaling of entanglement for all LENB states [see Fig. 2(b)]. We observe a two component behavior, where $|LE_n\rangle$ states with small n have a sub-volume-law entanglement scaling, while the rest of the LENB states display a volume-law scaling. This suggests that even though the nullspace as a whole will display a thermal behavior in agreement with previous results [20], it generically hosts a small number of exceptional nonthermal states.

LEZM in PPXPP model.—We illustrate an existence of an area-law zero mode in a constrained spin-1/2 model

$$H_{\text{PPXPP}} = \sum_{i=1}^L P_{i-2} P_{i-1} X_i P_{i+1} P_{i+2}, \quad (3)$$

where $P_i = (1 - Z_i)/2$ is the projector to the $\downarrow$ state and we restrict to the subspace where $\uparrow$ spins are separated by at least two sites. This Hamiltonian corresponds to the idealized description of Rydberg atom chains with range-2 blockade [39]: while in $\downarrow$ environment any given spin performs free Rabi oscillations, the presence of a nearest or next nearest neighbor $\uparrow$ spin arrests the dynamics. As the Hamiltonian has inversion symmetry and anticommutes with operator Π , it features a nullspace as described previously. The entanglement minimization in different momentum sectors reveals a number of low-entangled states in the LENB (see Supplemental Material [33]). A particularly simple LEZM can be written analytically using two-site singlet $|1\rangle_i = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)_{i,i+1}/\sqrt{2}$ and $|2\rangle_i = |\downarrow\downarrow\rangle_{i,i+1}$ states stacked as $|S\rangle = \bigotimes_{k=1}^{L/4} [|1\rangle_{4k} |2\rangle_{4k+2}]$ for mod $(L, 4) = 0$. The state $|S\rangle$,

FIG. 3. (a): Fidelity of the time evolved state quenching from $|S\rangle$ using the Rydberg Hamiltonian with periodic boundary conditions. (b) Dynamics of the local Rydberg densities for the two inequivalent sites of the initial state. Inset: the ladder of Rydberg atoms and its zigzag mapping into a one-dimensional chain.

which was first reported in [27], does not have well-defined momentum; however, appropriate translations of it correspond to LEZMs in different momentum sectors (see Supplemental Material [33]).

Experimental signatures of LEZM.—The PPXPP model can be approximately implemented by the triangular ladder of Rydberg atoms (see Fig. 3, inset). Viewing the Rydberg atoms as spin-1/2 degrees of freedom, the system is governed by the Hamiltonian

$$H_{\text{Ry}} = \frac{\omega}{2} \sum_{i=1}^L Z_i + V \sum_{i \neq j} \frac{n_i n_j}{(r_i - r_j)^6}, \quad (4)$$

where $n_i = (1 + Z_i)/2$ projects onto $\uparrow$ that corresponds to the excited state of a Rydberg atom. The long range interactions between excited Rydberg atoms decay with distance, allowing one to find a nearest neighbor atom spacing r , such that $V_{\text{NN}} = V/r^6 \gg \omega$. The zigzag geometry in the Fig. 3 inset leads to the equal strength interaction V_{NN} between atoms i and $i+1$, $i+2$. Therefore, for $V_{\text{NN}} \gg \omega$ the effective range-2 blockade condition emerges, and the Hamiltonian (4) can be transformed into a perturbed PPXPP Hamiltonian using Schrieffer-Wolff transformation (see Supplemental Material [33]).

The perturbations to the H_{PPXPP} include the spin hopping terms and also longer range interaction terms $\delta H = V_3 \sum_{i=1}^L n_i n_{i+3}$. Crucially, these terms do not anticommute with Π (since interaction terms in Eq. (4) contain only n , or equivalently, Z operators), thus lifting the degeneracy of nullspace. While the preparation of $|S\rangle$ is within the limits of current experiments in Rydberg arrays [32], it is an exact eigenstate only for Hamiltonian (3). Thus, while $|S\rangle$

remains invariant under unitary dynamics generated by H_{PPXPP} , we investigate its fate in time evolution under H_{Ry} Hamiltonian.

To this end we use a Trotter-based algorithm to evolve $|S\rangle$ with H_{Ry} for experimentally realistic value $V_{\text{NN}} = 2.5\omega$, leading to a weak but yet considerable range-3 interaction terms $V_3/\omega = 2.5/(\sqrt{3})^6 \approx 0.1$ that cause splitting of the nullspace [32]. Figure 3 shows the evolution of the fidelity $F = |\langle S|e^{-iH_{\text{Ry}}t}|S\rangle|^2$ and local Rydberg excitation densities $\langle n(r) \rangle$ for a 24-atom system within the experimentally accessible timescale. We observe that although fidelity decreases from 1, it remains of the order of 0.5 even at long times. Likewise, the local densities deviate from their original values, but remain far from their equilibrium value according to the microcanonical ensemble. Such dynamics signals that despite the presence of significant perturbations that destroy nullspace, the initialization of the system in the LEZM of the idealized PPXPP model results in a very slow thermalization.

Discussion.—We conjecture the existence of LEZM with area-law entanglement for generic local Hamiltonians with exponentially degenerate nullspace. This conjecture is supported by an analytic construction of an LEZM in the form of an MPS for a particular class of Hamiltonians, and by numerical constructions of LEZM states in the broad parameter regime. Moreover, we demonstrate the existence of LEZMs in kinetically constrained models, whose presence can be probed using Rydberg atom arrays.

These results suggest that slightly entangled zero modes are much more common than previously thought, suggesting that the presence of a nullspace in a local Hamiltonian may be sufficient for the existence of QMBS, thus inviting the systematic studies of nullspaces. It would be interesting to understand the general conditions for the existence of an LEZM that can be represented as a MPS with finite bond dimension, and extend these results to higher dimensions using projected entangled pair states representation [40]. From a numerical perspective, the existence of zero-energy eigenstates with area-law entanglement invites the development of efficient numerical algorithms based on MPS that may be able to find such states for system sizes that are beyond the reach of exact diagonalization, or even directly in the thermodynamic limit. Finally, area-law entangled LEZM may be used as “ground states” for creating anomalous eigenstates outside of the nullspace using local operators [22,29]. Understanding the conditions for a zero mode to provide a vacuum for stable quasiparticles could result in a novel mechanism of thermalization breakdown at finite energies.

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