Local Characterization of Global Tensor Network Eigenstates

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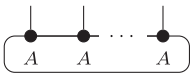
We study the conditions under which matrix product states (MPSs) or matrix product operators are exact eigenvectors of an extensive local operator such as a Hamiltonian. By suitably choosing the local operator, this covers a wide range of settings: exact eigenstates of Hamiltonians, including scar states; exact MPS trajectories for driven quantum systems; steady states of local Lindbladians; generalized symmetries of either Hamiltonians or density matrices; and many more. Our key result is that a local, fixed-size equation —namely, how a single term in the operator acts on a block of tensors—provides a necessary and sufficient condition for exact solutions. This local characterization allows us to obtain the full space of MPS solutions to all of the aforementioned problems; in particular, we exemplify the power of our results by recovering the quantum group symmetries of the XXZ model. We also discuss applications to numerical algorithms with MPSs and the generalization of our results to 2D, i.e., projected entangled pair states.

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Introduction—Understanding the spectrum and the eigenstates of quantum systems is fundamental to condensed matter physics and quantum information. A central question is how to characterize the eigenstates of Hamiltonians that appear in nature: those consisting of local interactions (given by a sum of local terms).

The characterization of the eigenstates in these systems, both ground states and excited states, is essential because they provide direct access to observable physical properties and enable the classification of quantum phases. Yet solving eigenvalue problems for local Hamiltonians in general is computationally difficult—already determining the ground state energy is QMA hard [1]—and a direct solution becomes intractable for large systems.

Given this computational difficulty, physicists have long sought systematic methods to find exact eigenstates by assuming they belong to a restricted class of states with some inherent structure. The arguably most successful such class is matrix product states (MPSs), where the many-body wave function coefficients are constructed as a trace over a product of matrices, $\langle i_1 \cdots i_N | \psi_N \rangle = \mathrm{Tr}(A^{i_1} \cdots A^{i_N})$, where A^i is a $D \times D$ matrix for every $i = 1, \ldots, d$ of the local Hilbert space [2]. The matrix indices are denoted by Greek letters $(\alpha, \beta, \cdots)$ and are dubbed *virtual* indices. Graphically, the state can be represented as

$|\psi_N\rangle =$ 

,

where lines denote indices, and connected lines are summed over (contracted). This *Ansatz* is remarkably powerful for several reasons. First, gapped ground states of local Hamiltonians in one dimension (1D) satisfy an area law for the entanglement entropy, meaning their entanglement scales with the boundary of a region rather than its volume [3]: in 1D, this results in a constant entanglement entropy. MPSs naturally respect this area law and provide efficient representations of area law states [4,5]. Second, the MPS *Ansatz* forms the foundation of the highly successful density matrix renormalization group (RG) algorithm [6], which has become the standard numerical tool for studying 1D quantum systems. Third, many relevant models—such as the Affleck–Kennedy–Lieb–Tasaki model and its generalizations—have ground states that admit exact MPS representations with small bond dimensions, providing paradigmatic examples.

The defining advantage of the MPS *Ansatz* is that the global properties of a many-body state—even those in the thermodynamic limit—are encoded within the structure of its individual, local tensors. This local encoding [7,8] has been the cornerstone for classifying symmetry protected topological phases [9,10], describing topologically ordered

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states [11], understanding density matrix RG fixed points [12], and many other applications [2]. It has long been "folklore" not only that local and global symmetries can be represented by local constraints, but also whether an MPS is an eigenstate of a local operator (as in Baxter's work [13] for tensor product states). This has been used, for example, to find symmetries in spin chains [14–17] and in non-equilibrium statistical physics [18,19], even if the MPSs involved there have infinite bond dimensions; to uncover duality transformations [20]; in finding scar states [21–23]; as well as in many other examples. Despite this, a rigorous proof of necessity—i.e., that any symmetry can be represented locally—has been missing. Establishing a complete, "if and only if" local characterization of symmetries is essential to transform MPSs from a successful numerical tool into a robust analytical framework for exploring and characterizing such scenarios in quantum many-body spin systems.

This is precisely what we achieve in this work. We derive a necessary and sufficient local equation—a "complete characterization"—that describes how a k-local Hamiltonian acts on a block of k adjacent MPS tensors. This result provides a unified framework that covers a remarkably diverse range of physical scenarios. Beyond simply identifying ground states, our characterization allows for the systematic discovery of exact quantum many-body scars, the determination of steady states in dissipative Lindbladian dynamics, and the identification of all generalized matrix product operator (MPO) symmetries for a given Hamiltonian. By reducing a complex global problem to a simple local identity, our framework provides a rigorous foundation for existing numerical methods and offers a powerful new tool for discovering exact solutions in both 1D and 2D quantum systems.

Injective MPSs—Our result applies to *injective* MPSs [24], a central object in the theory of tensor networks. Their importance is highlighted by the following facts. (1) Any MPS, after blocking, decomposes into a sum of injective MPSs. (2) Injective MPSs are orthogonal to each other in the thermodynamic limit. (3) Injective MPSs are unique ground states of local, gapped Hamiltonians. (4) An injective MPS is normalizable in the thermodynamic limit; this distinguishes it from almost all "excited" states that are non-normalizable plane waves of quasiparticles (with the exception of scar states). An MPS is injective, with injectivity length L, if there is a left inverse of A: a tensor $\tilde{A}$ on L sites defined by the matrices $\tilde{A}^{i_1\cdots i_L}$ such that $\sum_i \tilde{A}^{i_1\cdots i_L}_{\gamma\epsilon} \cdot (A^{i_1}\ldots A^{i_L})_{\alpha\beta} = \delta_{\alpha\gamma}\cdot\delta_{\beta\epsilon}$ [2].

Our key result is the characterization of injective MPSs that are eigenstates of local operators.

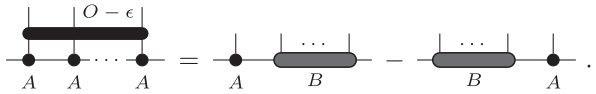
Main theorem—Let $\mathcal{O}_N$ be an operator acting on N particles that is the sum of all translations of a k-local operator $O_{[i]}$ acting on sites from i to $i+k-1$, $\mathcal{O}_N = \sum_{i=1}^{N} O_{[i]}$. An injective MPS $|\psi_N\rangle$ on N sites defined by the matrices A^i with injectivity length L such that $N \geq 2L+2k-1$ is an exact eigenstate of $\mathcal{O}_N$,

$$\mathcal{O}_N|\psi_N\rangle = E_N|\psi_N\rangle, \tag{1}$$

if and only if there exist (d^k of size $D\times D$) matrices $B^{i_1\cdots i_k}$ such that

$$\sum_{j\gamma}(O^{i_1\cdots i_k}_{j_1\cdots j_k} - \epsilon)A^{j_1}_{\alpha\gamma_1}\cdots A^{j_k}_{\gamma_k\beta} = \sum_{\gamma} A^{i_1}_{\alpha\gamma}B^{i_2\cdots i_k}_{\gamma\beta} - \sum_{\gamma} B^{i_1\cdots i_{k-1}}_{\alpha\gamma}A^{i_k}_{\gamma\beta}, \tag{2}$$

where $\epsilon = E_N/N$. In graphical notation [2],

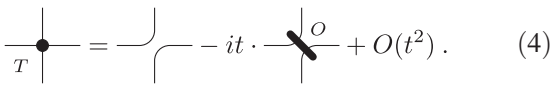


Let us emphasize some facets of this theorem. First, it is enough to assume that Eq. (1) holds for *one* given system size to conclude that Eq. (2) holds. Then, as Eq. (2) is independent of N, the MPS is an eigenstate for any other system size: $\mathcal{O}_K|\psi_K\rangle = E_K|\psi_K\rangle$, $\forall\ K$, where $E_K = \epsilon\cdot K$. Second, $\mathcal{O}$ does not need to be Hermitian, and E_N does not need to be its smallest (or largest) eigenvalue. Moreover, we do not assume that $|\psi_N\rangle$ is the unique eigenstate with eigenvalue E_N. Third, we note that neither the MPS nor the local operator needs to be translation invariant; the exact statement is presented below. Fourth, the tensor B is not unique: any tensor of the form $B^{i_1\cdots i_k} + \lambda A^{i_1}\cdots A^{i_k}$ satisfies Eq. (2), and this is the only ambiguity in B [see the Supplemental Material (SM) [25]]. Fifth, we note that in most applications, O is given, and the equation provides solutions for A and B. Sixth, the result is also valid for a one-body local operator, in which case B is just a virtual matrix; see SM [25]. Finally, the action of $\mathcal{O}$ in a region Λ at the physical boundary is

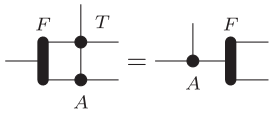
$$\left(\sum_{i\in\Lambda} O_{[i]} - \epsilon|\Lambda|\right)|\psi_N\rangle = (Q_{[i]} - Q_{[i+|\Lambda|]})|\psi_N\rangle, \tag{3}$$

where $\langle l|Q|j\rangle = \sum_{\alpha,\beta} B^l_{\alpha\beta}\tilde{A}^j_{\alpha\beta}$, assuming $L = 1 = k-1$ for simplicity. This form (local boundary action) has been used to classify Hamiltonian types in quantum many-body scar systems [26].

A simple proof—A rigorous proof of the previous theorem can be found in the SM [25]. Here, we provide a simplified and more intuitive argument (restricting for simplicity to the translation invariant case with $k=2$). The operator $e^{-i\mathcal{O}t}\cdot S$, where S is the shift operator and t is small, has an MPO description with the following MPO tensor T:

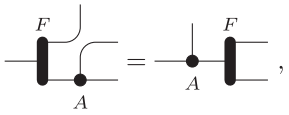


As the MPS in the theorem is translation invariant and (after shifting by ϵ) an eigenstate with eigenvalue zero of $\mathcal{O}$, $e^{-i\mathcal{O}t} \cdot S|\psi_N\rangle = |\psi_N\rangle$. This equality between MPSs can be characterized locally by using the "fundamental theorem" of MPS [2] that implies the existence of a rank-three fusion tensor F such that [27]

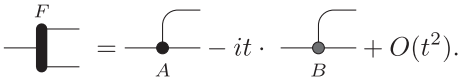


(5)

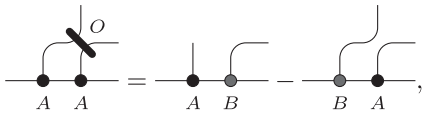
Let us expand Eq. (5) in orders of t using the decomposition of Eq. (4). In zeroth order, we obtain that



and thus, by injectivity, in zeroth order, the fusion tensor is nothing but the MPS tensor. We can, thus, write



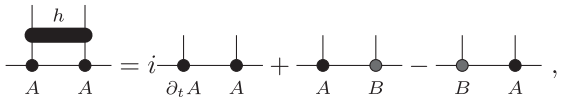
Plugging this back into Eq. (5), expanding in t again, and considering the first order terms, we obtain that



which is the desired equation.

Different applications—Our main theorem has a plethora of applications, some of which are already used in the literature, where the central principle of telescopic sums has been applied to great success. In these applications, Eq. (2) is used as an *ad hoc Ansatz*; that is, only the implication Eq. (2) $\Rightarrow$ Eq. (1) is used. The result presented in this Letter provides the formal justification of these applications by showing that this indeed presents the most general MPS solution to such an eigenvalue equation. At the same time, our result provides a unified framework that allows one to treat these problems as well as others, which we now present.

(1) Time evolution: Our theorem can be applied to find MPS solutions of the (time-dependent) Schrödinger equation $H|\psi\rangle = i\partial_t|\psi\rangle$. To see this, note that the time derivative of an MPS can be written as $\partial_t|\psi\rangle = \sum_{j,\{i_k\}} \mathrm{Tr}\,[A^{i_1}\cdots(\partial_t A^{i_j})\cdots A^{i_N}]|i_1\cdots i_N\rangle$. For injective MPS, we can construct a local operator V, $V^i_j = \sum_{\alpha,\beta}(\partial_t A)^i_{\alpha\beta}\tilde{A}^j_{\alpha\beta}$, where $\tilde{A}$ is the left-inverse tensor, such that $\partial_t|\psi\rangle = \sum_j V_{[j]}|\psi\rangle$ [28,29]. Then, the Schrödinger equation reads $(H - i\sum_j V_{[j]})|\psi\rangle = 0$, which is of the form of Eq. (1). Our theorem then implies that the following must be met by any solution (shown here for two-body Hamiltonians):



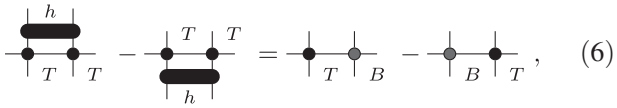
where now A and B (and potentially also h) depend on time. For larger injectivity lengths, the operator V will, correspondingly, act on more sites.

(2) Continuous symmetries of matrix product density operators (MPDOs): Given a unitary symmetry U, a density matrix can be weakly symmetric, i.e., $[U,\rho] = 0$, or strongly symmetric, i.e., $U\rho = \rho$, according to Ref. [30]. Let U be a continuous symmetry generated by 2-local operators, i.e., $U = e^{i\epsilon\sum_i G_{[i,i+1]}}$, and ρ an MPDO, i.e., a density matrix with an MPS form [31,32]. Then, for weak symmetries,

$$\sum_i (G_{[i,i+1]} \otimes \mathrm{Id} - \mathrm{Id} \otimes G^T_{[i,i+1]})|\rho\rangle\!\rangle = 0,$$

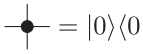
while for strong symmetries, $\sum_i (G_{[i,i+1]} \otimes \mathrm{Id})|\rho\rangle\!\rangle = 0$, where $|\rho\rangle\!\rangle$ denotes the vectorized form, as an MPS, of ρ. Both of these are equations of the form of Eq. (1), and thus, allow for the application of our theorem (the resulting *Ansatz* has, for example, been used *ad hoc* in Ref. [14]).

(3) Matrix product operator symmetries of local Hamiltonians: Let us now consider MPO symmetries O of local Hamiltonians: $[H, O] = 0$ [11,33–35]. By vectorizing the injective MPO into an injective MPS, $O \to |O\rangle\!\rangle$, we can write $\sum_i (h_{[i]} \otimes \mathrm{Id} - \mathrm{Id} \otimes h^T_{[i]})|O\rangle\!\rangle = 0$, whose structure mimics Eq. (1). Our theorem then gives the following local characterization of Hamiltonians with MPO symmetries:



(6)

where T is the tensor of the MPO symmetry O, and B is the auxiliary tensor of Eq. (2). For example, consider the quantum group symmetries of the XXZ model. Let us find MPO symmetries of the XXZ model with the two-body term $h = XX + YY + \Delta ZZ$. We write the MPO tensor T as



$$= |0\rangle\langle 0| \otimes a + |0\rangle\langle 1| \otimes b + |1\rangle\langle 0| \otimes c + |1\rangle\langle 1| \otimes d,$$

where the matrices a, b, c, d act on the virtual degrees of freedom. We express the B tensor in Eq. (6) in a similar form with virtual matrices $\tilde{a}, \tilde{b}, \tilde{c}, \tilde{d}$. The resulting equations coming from Eq. (6) are given in the SM [25]. Special solutions of these equations are given when $\tilde{a} = \tilde{d} = 0$, $\tilde{b} = \lambda b$, $\tilde{c} = -\lambda c$, so that we get

$$ab = q^{-1}ba, \quad ac = q^{-1}ca, \quad bd = q^{-1}db,$$
$$cd = q^{-1}dc, \quad bc = cb, \quad ad - da = -(q - q^{-1})bc,$$

where q and λ satisfy $\Delta = (q + q^{-1})/2$ and $\lambda = q - q^{-1}$. These equations correspond to the matrices defining the matrix quantum group $\mathrm{SL}(2)_q$, whose explicit connection with the quantum group $\mathrm{U}_q(sl_2)$ as symmetries of the XXZ chain and the Pasquier-Saleur Hamiltonian [36] is shown in the SM [25] (see also Ref. [17]). In a similar way, we also show how the (higher) transfer matrices arise from solutions of Eq. (6); see SM [25].

(4) Steady states of local Lindbladians: Let us now consider the problem of finding the steady state, $\mathcal{L}(\rho) = 0$, of a 2-local Lindbladian $\mathcal{L} = \sum_i \mathcal{L}_{[i,i+1]}$. We assume that ρ can be written as an MPDO; see Ref. [37]. An MPDO can be decomposed into injective and locally orthogonal MPDOs $\rho = \sum_a \rho_a$, where we denote the injective tensor of ρ_a by T_a. Then, $\mathcal{L}(\rho) = 0$ if and only if there are MPO tensors M_a for each a such that

$$\sum_{i'j'k'l',\gamma} \mathcal{L}^{ijkl}_{i'j'k'l'} (T_a)^{i'k'}_{\alpha\gamma} (T_a)^{j'l'}_{\gamma\beta} = \sum_{\gamma,\delta} (T_a)^{ik}_{\alpha\gamma} (M_a)^{jl}_{\gamma\beta} - (M_a)^{ik}_{\alpha\delta} (T_a)^{jl}_{\delta\beta}.$$

(5) Local operators and telescopic series: Given a local operator that adds up to zero, $\sum O_{[i,i+1]} = 0$, we can use our result by applying the operator to the identity operator (which is an injective MPO), which yields that $O_{[i,i+1]} = Q_{[i]} \otimes \mathrm{Id}_{[i+1]} - \mathrm{Id}_{[i]} \otimes Q_{[i+1]}$, where Q is a one-body operator; see also Ref. [38].

(6) Numerical applications: variational uniform MPS algorithm (VUMPS). Non-fine-tuned Hamiltonians do not have exact MPS eigenstates, but the success of tensor networks is based on the fact that ground states can be faithfully approximated by MPS [4]. One of the standard algorithms to find those MPS approximations is VUMPS [29,39]. Interestingly, the fixed points of this recursive algorithm can be understood to satisfy a relaxation of the telescopic identity in the main theorem: instead of satisfying this equality exactly, we require it to be satisfied only when projected on the tangent plane; see SM [25]. The two error terms then correspond to the effective Hamiltonian contributions of the left and right part of the chain, respectively. Our central theorem, hence, gives a justification for the working of that algorithm.

Generalizations—The statement of our main theorem can be generalized in a variety of ways. Here, we discuss two possible generalizations: nontranslational systems and two-dimensional systems (which can be combined to state our result for nontranslational two-dimensional systems). (7) Breaking translation invariance: We now assume a setting where both the local terms of the two-body Hamiltonian $H = \sum h_{[n,n+1]}$ and the MPS tensors $A^{[n]}$ depend on the lattice site n. Then, the following holds:

$$\sum_{i'j',\gamma} (h_{[n,n+1]})^{ij}_{i'j'} A^{[n],i'}_{\alpha\gamma} A^{[n+1],j'}_{\gamma\beta} = \sum_{\gamma,\delta} A^{[n],i}_{\alpha\gamma} B^{[n+1],j}_{\gamma\beta} - B^{[n],i}_{\alpha\delta} A^{[n+1],j}_{\delta\beta}.$$

This setting covers two interesting scenarios. The first one is where the MPS is composed of the same tensor everywhere, but a matrix is placed at the virtual indices when closing the boundaries: this class of MPS describes coalgebras; see Ref. [40]. The second case is where translation invariance is broken only inside a bigger unit cell. For example, Ref. [21] constructed scar states with a two-site unit cell for the PXP model.

(8) Beyond 1D: Our theorem can be generalized to 2D injective projected entangled pair states (PEPSs); see SM [25] for the proof, in particular for two-body and plaquette local terms on the square lattice and two-body terms on the hexagonal lattice. These results are summarized in Fig. 1.

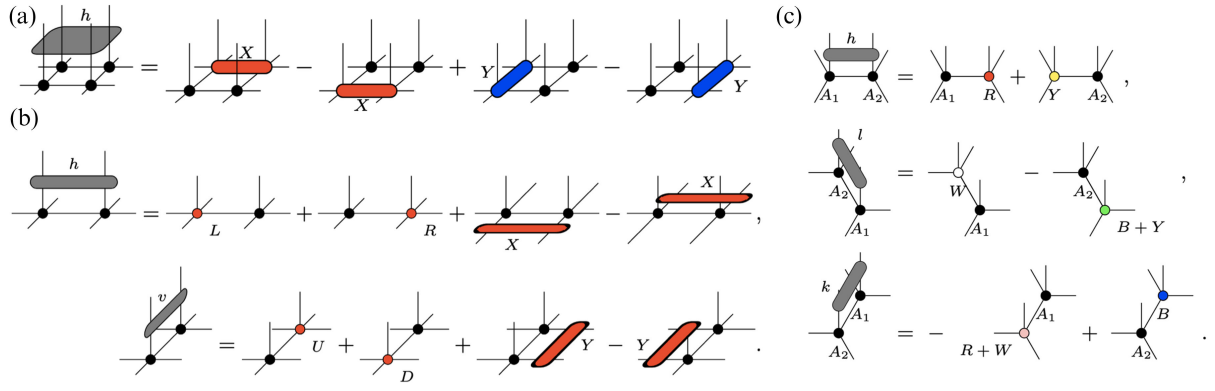


FIG. 1. 2D local Hamiltonian terms acting on an injective PEPS as its ground state. (a) Plaquette term on square lattice resulting in two virtual tensors, X and Y. (b) Two-body terms on square lattice resulting in four tensors satisfying $R + D + L + U = 0$ and two virtual tensors, X and Y. (c) Two-body terms on hexagonal lattice given by two site tensors A_1 and A_2, resulting in four tensors, R, W, B, Y.

Conclusions and outlook—In this Letter, we have derived a necessary and sufficient local condition for an injective MPS to be an exact eigenstate of a finite-range operator, including local Hamiltonians. The resulting equation is formulated as the action of the k-local Hamiltonian term on a block of k adjacent MPS tensors, which is independent of the system size. It gives rise to a telescopic series and is especially relevant for finding non-frustration-free Hamiltonians (the parent Hamiltonian is always frustration-free).

Our framework unifies several constructions into a single local principle covering the time evolution of MPSs, MPO symmetries, Lindbladian steady states, zero-sum local operators, and giving a conceptual justification of VUMPS. It further extends beyond translationally invariant 1D systems to site-dependent tensors (including PXP scar eigenstates) and to 2D injective PEPSs as ground states of local (plaquette and two-body) Hamiltonians on the square and hexagonal lattices.

An important open direction is to extend these results to more general tensor network structures in two dimensions. In particular, proving analogs of our characterizing equation for generalized-injective [41] and G-injective [42] PEPSs would allow extending our framework to applications in symmetry protected and topologically ordered phases in 2D. From the numerical side, a robust 2D version of our characterization could provide new guidance for designing and diagnosing optimization schemes for PEPSs and related *Ansätze*, potentially addressing some of the core difficulties in variational simulations of two- and higher-dimensional quantum systems.

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Data availability—There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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