

Quantum Circuits for Matrix-Product Unitaries

Georgios Styliaris¹,* Rahul Trivedi²,* and J. Ignacio Cirac¹

*Max Planck Institute of Quantum Optics, Hans-Kopfermann-Straße 1, Garching 85748, Germany
and Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, 80799 München, Germany*

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Matrix-product unitaries (MPUs) are many-body unitary operators that, as a consequence of their tensor-network structure, preserve the entanglement area law in 1D systems. However, it is unknown how to implement an MPU as a quantum circuit since the individual tensors describing the MPU are not unitary. In this Letter, we show that a large class of MPUs can be implemented with a polynomial-depth quantum circuit. For an N -site MPU built from a repeated bulk tensor with open boundary, we explicitly construct a quantum circuit of polynomial depth $T = O(N^\alpha)$ realizing the MPU, where the constant α depends only on the bulk and boundary tensor and not the system size N . We show that this class includes nontrivial unitaries that generate long-range entanglement and, in particular, contains a large class of unitaries constructed from representations of C^* -weak Hopf algebras. Furthermore, we also adapt our construction to nonuniform translationally varying MPUs and show that they can be implemented by a circuit of depth $O(N^\beta \text{poly} D)$ where $\beta \leq 1 + \log_2 \sqrt{D}/s_{\min}$, with D being the bond dimension and $s_{\min}$ the smallest nonzero Schmidt value of the normalized Choi state corresponding to the MPU.

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Introduction—The entanglement area law is a hallmark of many-body quantum systems with local interactions [1]. It captures the observation that in many physical quantum states, only degrees of freedom near the boundary of a region contribute significantly to its entanglement with the rest [2–6]. On the level of quantum operations, it is thus a fundamental task to characterize unitaries that *preserve* the area law. Perhaps the most natural class with this property are unitaries admitting a tensor-network representation, which inherently ensures the preservation of the area law [7].

In one spatial dimension, the corresponding tensor-network class is that of matrix-product unitaries (MPUs) [7]. In addition to describing discrete time evolution, MPUs capture families of exactly solvable quantum circuits [8], describe unitary symmetries of 1D systems [9,10], and have been useful to characterize Floquet phases in 2D via their boundary dynamics [11]. A well-understood subclass of MPUs is one-dimensional quantum cellular automata (QCA) [12], which coincide with MPUs formed by a single repeated tensor [13–15]. This subfamily, which includes finite-depth quantum circuits, is characterized by a strict causal cone, and thus, preserves the phase of

matter of the input state. This is, however, not a universal property: certain MPUs, such as sequential quantum circuits [16], fermionic MPUs [17], or MPUs with open boundaries [18], can change the underlying phase, as they can generate long-range entanglement.

Although the tensor-network form of MPUs has the advantage of automatically enforcing the preservation of the area law, the individual tensors do not inherently correspond to unitary or other physical processes. This poses a challenge for translating the tensor-network description into implementable quantum circuits. While it is well known that every matrix-product state (MPS) can be prepared by a sequential (linear-depth) circuit acting on a product state [19], no general framework exists for efficiently implementing MPUs as circuits beyond the limited case of QCA [13,14]. The present Letter addresses this gap (Fig. 1).

The problem of efficiently realizing MPUs as quantum circuits plays a key role in quantum computation. Hybrid schemes that combine finite-depth local circuits with measurements and feedback allow implementing certain global unitaries with substantial speedups compared to purely unitary algorithms [20–26], including experimental realizations [27–30]. Yet, only a few isolated examples are currently understood, e.g., those exploiting measurements to parallelize Clifford unitaries [31–34]. In one dimension, all unitaries achievable by such finite-depth circuits with measurements are, by construction, MPUs. It is, therefore, natural to study MPUs in full generality, both to systematically devise a general theory of hybrid protocols and to understand the fundamental limits of measurement-assisted speedups.

*These authors contributed equally to this work.

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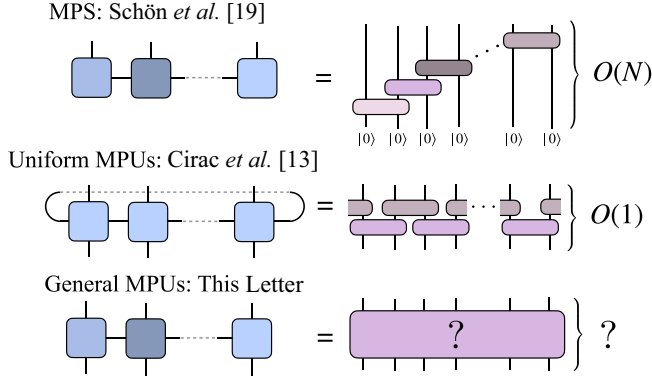


FIG. 1. MPS over N sites admit a sequential circuit decomposition with depth $O(N \text{poly} D)$, where D is the bond dimension [19]. How can MPUs be implemented as quantum circuits, and what is the corresponding depth? The answer is known only for the case of MPUs with uniform bulk and periodic boundary, which correspond to QCA [13]. Here, we introduce a circuit decomposition of $\text{poly}(N)$ depth for arbitrary MPUs when they are well conditioned. We show this holds (i) for MPUs with uniform bulk and open boundary and (ii) for arbitrary MPUs when $\sqrt{D}/s_{\min} = O(1)$ ($s_{\min}$: smallest nonzero singular value of the MPU Choi state).

The problem of implementing an MPU as a quantum circuit is fundamentally more challenging than MPS preparation, which is far better understood [19,33,35–39]. Unlike MPSs, only a subclass of MPUs can be implemented by sequential circuits [18]. This may at first seem surprising, given that sequential circuits are sufficient to map any given initial MPS to any other target MPS. However, certain MPUs, such as the multicontrolled NOT gate, can provably not be implemented by sequential circuits, since they noncausally propagate correlations [18].

An arguably obvious strategy to implement an MPU by exploiting its tensor network structure would be to start from its Choi state [40], which is automatically an MPS and thus efficiently preparable. However, while such a Choi MPS can be physically prepared with a linear-depth circuit [19], this does not necessarily imply that the associated unitary can be efficiently applied to an unknown input state. Given $2N$ qubits initialized in the Choi state of the N -qubit unitary, the only general-purpose strategy to apply the unitary on an input state is via N joint measurements (e.g., Bell measurements) between the input state and the Choi state [20,41,42] followed by a postselection on the N measurement outcomes. However, such a strategy will typically incur an exponential cost due to the postselection, rendering it inefficient.

Alternatively, one could consider formulating this question within the oracle model. Since the MPU structure guarantees that individual matrix elements of the unitary can be efficiently classically computed [7], a quantum oracle accessing the MPU elements can be implemented in polynomial time. However, there is no general-purpose

strategy to, given such an oracle for the unitary elements, apply the unitary onto an input state. Using state-preparation strategies given oracles for computing the vector elements of the state [43] can, again, allow us to prepare only the Choi state of such a unitary efficiently. Consequently, to obtain an efficient circuit implementation of an MPU, we need to identify and exploit the structure beyond the fact that it has an MPS Choi state or efficiently computable matrix elements.

In this Letter, we present a systematic and efficient quantum circuit decomposition of MPUs starting from their tensor-network representation. The resulting circuit, under the assumption that the bond dimension cannot be further reduced, has depth $O(\text{poly} N)$ for N -site MPUs consisting of a repeated bulk tensor and open boundary. This class goes beyond QCA—moreover, we provide a systematic construction of nontrivial MPUs arising from C^* -weak Hopf algebras [44–46], which are in this class. Furthermore, we consider nontranslation-invariant MPUs. Our algorithm gives a circuit decomposition with polynomial depth, provided a spectral condition is satisfied.

MPUs with uniform bulk—MPUs are defined via rank-4 tensors, graphically represented as

$$A_{mn}^{ij} = m \begin{array}{c} i \\ \downarrow \\ \boxed{A} \\ \uparrow \\ j \end{array} n = \left(m \begin{array}{c} j \\ \downarrow \\ \boxed{A^\dagger} \\ \uparrow \\ i \end{array} n \right)^* \in \mathbb{C}, \quad (1)$$

where the vertical legs $i, j = 1, \dots, d$ label the physical space and the horizontal ones $m, n = 1, \dots, D$ the auxiliary space, with D the bond dimension. We use arrows to indicate the input-output space of operators, e.g.,

$$\begin{array}{c} \uparrow \\ \boxed{A} \\ \downarrow \end{array} = \sum A_{mn}^{ij} |ij\rangle \langle mn|.$$

We first consider MPUs with uniform bulk and open boundary.

Definition 1 (Uniform-bulk MPU)—The tensor A , together with the boundary vectors l and r , define a *uniform-bulk MPU* if the N -site matrix-product operator (MPO),

$$U_N = l \begin{array}{c} \uparrow \\ \boxed{A} \\ \downarrow \end{array} \cdots \begin{array}{c} \uparrow \\ \boxed{A} \\ \downarrow \end{array} r \quad (2)$$

is unitary for all N .

This open-boundary definition also includes uniform-bulk MPUs with a boundary of the form

$$U_N = b \begin{array}{c} \uparrow \\ \boxed{A} \\ \downarrow \end{array} \cdots \begin{array}{c} \uparrow \\ \boxed{A} \\ \downarrow \end{array} , \quad (3)$$

studied in Ref. [18], by suitably enlarging the bond dimension.

The class of uniform-bulk MPUs includes all (translation-invariant) 1D QCA, that is, unitaries possessing a strict light cone. This is because QCA can be represented as uniform-bulk MPUs with periodic boundary [13,14] ($b = 1$ above), and thus, they also fall in the open boundary setting considered here by increasing the bond dimension from D to D^2 . Beyond QCA, uniform-bulk MPUs encompass multiqutrit control operations with a single target qudit [18], such as the multicontrol Z-gate $U_{C\dots CZ} = \mathbb{1} - 2(|0\rangle\langle 0|)^{\otimes N}$. Unlike QCA, however, such control unitaries can create long-range correlations through a single application. This directly implies that a uniform-bulk representation of long-range entangling unitaries necessitates open boundary conditions [18].

A further example of uniform-bulk MPUs capable of creating long-range correlations is provided by *MPO-projector unitaries*, $U = \sum_{j=1}^{\ell} e^{i\phi_j} P_j$. Here, P_j form a complete set of orthogonal MPO projectors, with a uniform bulk, and ℓ is an N -independent constant. Such projectors have a nontrivial structure and arise naturally in the context of topologically ordered states and anyons [47]. They also contain long-range entangling unitaries. In our setting, this class is useful because it provides nontrivial MPUs specified directly at the tensor-network level rather than through a circuit description. It can be viewed as a broad generalization of the $U_{C\dots CZ}$ gate, in that the resulting unitaries act by applying distinct phase factors to the subspaces defined by the projectors. In Supplemental Material [48], we present a systematic construction of unitaries arising from the input of a C^* -weak Hopf algebra and an associated representation based on the techniques developed in Refs. [45,46]. This MPU class, which includes and generalizes the MPO-projector unitaries, lacks a known quantum circuit implementation.

Main result—We seek an efficient quantum circuit decomposition scheme for MPUs, that is, with the number of gates scaling, at most, polynomially with system size. We begin with the case of uniform-bulk MPUs, which already capture nontrivial examples. We then extend our construction to general, nonuniform MPUs. Throughout, we allow arbitrary two-qudit gates, taking the physical dimension d to be a constant. For our main result, we need the following assumption:

Assumption 1—It holds that

$$\text{rank} \left(\begin{array}{c} \uparrow \\ \textcircled{l} \text{---} \text{A} \text{---} \textcircled{r} \\ \downarrow \end{array} \right) = \text{rank} \left(\begin{array}{c} \uparrow \\ \text{---} \text{A} \text{---} \textcircled{r} \\ \downarrow \end{array} \right) = D. \quad (4)$$

Physically, the assumption implies that the bond dimension cannot be further compressed, i.e., the MPU has only nonzero operator Schmidt values at every bipartition. The condition is automatically satisfied if A , viewed as an MPS tensor, is injective. More generally, it remains valid if A in Eq. (3) is in block-diagonal canonical form [52], with linearly independent blocks, and the boundary operator b is

full rank [48]. This set of assumptions is usually taken as a starting point [45,47]. This class includes, beyond the trivial case of QCA, the MPO-projector unitaries introduced previously. Our main result is as follows:

Theorem 1—Uniform-bulk MPUs satisfying Assumption 1 can be implemented with a quantum circuit of $O(\text{poly}N)$ depth and $O(N)$ auxiliary qudits.

We note that, in general, a polynomially scaling circuit depth is necessary to implement the MPUs covered by Theorem 1 using geometrically local gates and local auxiliary qudits. This is because the family includes unitaries capable of generating long-range correlations, such as the multicontrol Z gate, which require at least linear depth.

Tree implementation of MPUs—The key idea behind the algorithm in Theorem 1 is to first implement small disjoint local unitaries and then to successively merge them in a tree scheme (see Fig. 2). However, individual MPU tensors do not, in general, correspond to unitary operators. Nevertheless, for a uniform-bulk MPU, any segment of n consecutive bulk tensors can be turned into an *isometry*. More specifically, we define

$$V_n^{[L,R]} := \begin{array}{c} \uparrow \quad \uparrow \\ \textcircled{L} \text{---} \text{A} \text{---} \dots \text{---} \text{A} \text{---} \textcircled{R} \\ \downarrow \quad \downarrow \end{array}, \quad (5)$$

where L, R can be operators or vectors and, by definition, $U_N = V_N^{[L,R]}$. In the End Matter, we show explicitly construct tensors $L, R \in \mathcal{M}(\mathbb{C}^D)$, independent of n , such that $V_n^{[L,R]}$ is an isometry for all n , i.e., $V_n^{[L,R]\dagger} V_n^{[L,R]} = \mathbb{1}$. Furthermore, the isometry property is retained at the boundary; i.e., $V_n^{[L,R]}$, $V_n^{[L,R]}$ are also isometries. Moreover, using Assumption 1, introduced earlier, we can guarantee that L, R can be chosen to be *full rank*—the importance of this will be clear shortly.

Since the isometry property of $V_n^{[L,R]}$ holds for arbitrary n , it naturally motivates a recursive circuit decomposition for uniform-bulk MPUs. In particular, neighboring isometries are successively merged following a treelike structure (Fig. 2). To illustrate the idea, suppose, for the moment, that we have an implementation of $V_n^{[L,R]}$ and $V_m^{[L,R]}$ in terms of 2-qudit gates (recall that an isometry corresponds to a unitary with a partially fixed input). Then, the larger isometry $V_{n+m}^{[L,R]}$ can be realized by merging the two via the action of the operator

$$M := |00\rangle\langle 11| (R^{-1} \otimes L^{-1}) = \begin{array}{c} \uparrow \quad \uparrow \\ |0\rangle \quad |0\rangle \\ \text{---} \text{---} \\ \textcircled{R^{-1}} \text{---} \textcircled{L^{-1}} \\ \downarrow \quad \downarrow \end{array}. \quad (6)$$

More explicitly, acting with M on the intermediate bond legs gives

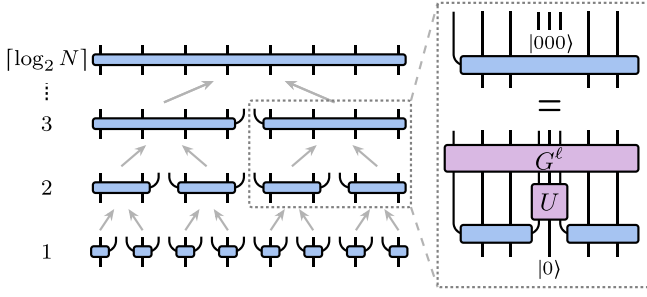
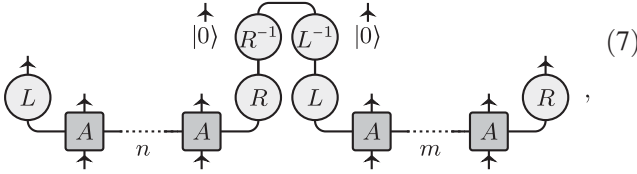


FIG. 2. The MPU implementation algorithm proceeds by first realizing small local isometries, and then, recursively merging them in a treelike structure, here indicated by arrows. After $\lceil \log_2 N \rceil$ layers of merging, the global MPU is obtained (left). Each individual merging step is performed deterministically using an amplitude amplification technique (right).

$$M(V_n^{[L,R]} \otimes V_m^{[L,R]}) = |00\rangle \otimes V_{n+m}^{[L,R]} =$$



thereby merging the two isometries into a single one over a larger region. Recall that, importantly, L, R are full rank.

These observations give rise to the following implementation strategy for a uniform-bulk MPU (Fig. 2).

- (i) Implement $V_1^{[L,R]} \otimes (V_1^{[L,R]})^{\otimes N-2} \otimes V_1^{[L,R]}$ in parallel. This requires $O(1)$ depth and $O(N)$ auxiliary qudits.
- (ii) Merge neighboring isometries via applying M in a tree fashion, as in Fig. 2, until the full MPU is obtained.

While M correctly implements the desired merging between two neighboring isometries, it is itself not unitary. Consequently, each application of M must be interpreted as a generalized measurement necessitating postselection. However, this postselection is generally infeasible, as its success probability decays exponentially with the system size [53].

To bypass the postselection problem, we will instead employ a *unitary* subroutine that merges neighboring isometries. Specifically, we will show that if a unitary realizing the isometry $V_n^{[x,R]} \otimes V_m^{[L,y]}$ ($x \in \{l, L\}, y \in \{r, R\}$) can be implemented in depth $T(V_n^{[x,R]} \otimes V_m^{[L,y]})$, then

$$T(V_{n+m}^{[x,y]}) \leq 2q_{\text{unif}} T(V_n^{[x,R]} \otimes V_m^{[L,y]}) + O(n+m) \quad (8)$$

using $O(1)$ additional auxiliary qudits. The constant q_{unif} , which we refer to as the *MPU conditioning number*, is defined for the uniform case as

$$q_{\text{unif}}(R, L) := \sqrt{\text{tr}[R^{-2}(L^{-2})^T]}. \quad (9)$$

We note that q_{unif} is independent of the system size N , since R, L are system size independent operators. The total cost of implementing the MPU, starting from $V_1^{[\cdot, \cdot]}$, can be bounded from Eq. (8), leading to a depth

$$T(U_N) = O(N^{1+\log_2 q_{\text{unif}}}), \quad (10)$$

which is $O(\text{poly}N)$, as claimed in Theorem 1. The degree of the polynomial is governed by the MPU conditioning number q_{unif} , which can be optimized by the choice of L, R satisfying Eq. (5) (see End Matter).

Merging isometries without postselection—Now, we explain how the merging of neighboring isometries in Eq. (7) can be performed unitarily. In general terms, the problem we need to solve is as follows: Implement

$$MV = \begin{array}{c} \uparrow \uparrow \uparrow \uparrow \\ \boxed{M} \\ \uparrow \uparrow \uparrow \uparrow \\ \boxed{V} \\ \uparrow \uparrow \uparrow \uparrow \end{array} \in \text{isometry} \quad (11)$$

if V is an isometry but M is only a linear operator (i.e., not necessarily unitary). For this, the first step is to implement $M = \sum_i c_i W_i$ as a linear combination of unitaries with the aid of an auxiliary system prepared in the state $B|0\rangle_A := (1/C) \sum_i \sqrt{c_i} |i\rangle_A$ (we denote $C := \sum_i c_i$). Concretely, this can be done by applying $U := B^\dagger W^{\text{ctrl}} B$, where $W^{\text{ctrl}} := \sum_i (W_i)_S \otimes |i\rangle_A \langle i|$ is a control unitary and B acts on the ancilla. Indeed, for any $|\psi\rangle_S$ in the image $\mathcal{S} := \text{Im } V$, a direct calculation gives

$$U|\psi\rangle_S |0\rangle_A = \frac{1}{C} |\Phi\rangle + \sqrt{1 - \frac{1}{C^2}} |\Phi^\perp\rangle, \quad (12)$$

where $|\Phi\rangle := (M|\psi\rangle_S)|0\rangle_A$ such that ${}_A\langle 0|\Phi^\perp\rangle = 0$. In conclusion, this shows how postselecting the ancilla in the $|0\rangle_A$ state results in applying M .

At first glance, the above construction appears to offer no advantage, since it again relies on postselection. However, Eq. (12) strongly hints that an amplitude amplification approach could be used to boost the success probability, thus making the scheme deterministic. Unfortunately, standard amplitude amplification [54] is not applicable here, since it requires a reflection about the input state, which is unknown. The setup is instead reminiscent of *oblivious amplitude amplification* [55], where the reflection is independent of the input. However, this method cannot be applied directly, as it requires V to be a unitary, whereas in our case it is merely an isometry. To overcome this, we develop a generalization of the oblivious amplitude amplification scheme applicable to the isometric setting. The method is not strictly oblivious, as the amplitude amplification reflections over the $\{|\Phi\rangle, |\Phi^\perp\rangle\}$ subspace [cf. Eq. (12)] depend on the image of V but, importantly, not on the unknown input state. This modification suffices to keep the circuit implementation efficient. Specifically, we show that

$$G^\ell U(|\psi\rangle_S |0\rangle_A) = (M|\psi\rangle_S) |0\rangle_A, \quad (13)$$

where

$$G := -UR_\Psi U^\dagger R_\Phi \quad (14)$$

corresponds to a single amplitude amplification rotation. The total number of rotations is bounded by $\ell \leq C$, where in our case $C \leq q_{\text{unif}}$ is governed by the MPU conditioning number [48]. The reflections are given by

$$R_\Phi := \mathbb{1}_S \otimes 2|0\rangle_A \langle 0| - \mathbb{1}, \quad (15a)$$

$$R_\Psi := (\mathbb{1}_S \otimes 2|0\rangle_A \langle 0| - \mathbb{1})(\mathbb{1} - P_{S^\perp} \otimes 2|0\rangle_A \langle 0|), \quad (15b)$$

where $P_{S^\perp}$ is the (orthogonal) projector onto the orthogonal complement of S . When S is the entire space, $P_{S^\perp} = 0$, and the standard oblivious amplitude amplification protocol is recovered. Finally, we remark that the projector $P_{S^\perp}$ can be implemented given an implementation of the isometry V —for instance, if V is implemented as a unitary with some auxiliary input qubits set to $|0\rangle$, $P_{S^\perp}$ is equivalent to undoing this unitary, then applying a phase-flip unitary controlled on the auxiliary qubits, and then, applying the unitary.

In summary, a single merging step $V_n^{[x,R]} \otimes V_m^{[L,y]} \mapsto V_{n+m}^{[x,y]}$ can be performed deterministically by applying the unitary $G^\ell U$ (see Fig. 2). Each application of the amplification unitary G requires two evaluations of $V_n^{[x,R]} \otimes V_m^{[L,y]}$, and a total of $\ell \leq q_{\text{unif}}$ repetitions is sufficient. The remaining circuit components contribute a cost of $O(1)$. A detailed counting is provided in [48] and leads to the final bound in Eq. (8).

Nonuniform MPUs—Our implementation algorithm can be straightforwardly adapted to general, nonuniform MPUs. These are specified by site-dependent tensors $A_1, \dots, A_N$ such that the resulting MPO is unitary. For this case, D denotes the maximum of the local bond dimensions D_k . We take, for convenience, uniform physical dimension d .

The starting point is again a decomposition of the form Eq. (5). However, due to the lack of translational invariance, the corresponding isometries are now site dependent:

$$V_{jk}^{[L_j, R_k]} := \begin{array}{c} \uparrow \\ \textcircled{L_j} \\ \uparrow \\ \boxed{A_j} \cdots \boxed{A_k} \\ \uparrow \quad \uparrow \\ \textcircled{R_k} \\ \uparrow \end{array}. \quad (16)$$

By exploiting the freedom in the representation of the MPU tensors [52], one can bring the MPU into a canonical form, which corresponds to the usual MPS canonical form of its Choi state [18]. In this representation, we can find full-rank operators L_j, R_k that give rise to valid isometries, as in the uniform case, even without the need for Assumption 1, but

with the important difference that they are now site-dependent (see End Matter).

This immediately enables the straightforward application of the tree circuit construction, which relies only on these properties. However, care needs to be taken when calculating the cost of a single merging, since now we need to replace q_{unif} in Eq. (8) with its site-dependent counterpart,

$$q_k := \inf_{R_k, L_{k+1}} \sqrt{\text{tr}[R_k^{-2}(L_{k+1}^{-2})^T]}, \quad (17)$$

where the infimum is taken over valid choices that yield an isometry in Eq. (16). Note that all q_k remain invariant with respect to gauge transformations of the form $(A_k)^{ij} \mapsto X_{k-1}^{-1}(A_k)^{ij}X_k$ for invertible X_k and are, thus, a property of the MPU and not its specific representation. We define the MPU conditioning number for the general case as

$$q := \max_k q_k. \quad (18)$$

Our main result for general, nonuniform MPUs is

Theorem 2—An MPU over N sites can be implemented with a quantum circuit of depth $O(N^{1+\log_2 q} \text{poly} D)$ and $O(N \log D)$ auxiliary qudits.

The complexity is now governed by the scaling of the MPU conditioning number q . A practical upper bound on q can be obtained from the operator Schmidt values of the MPU. Specifically, consider its (properly normalized) Choi state $|U_N\rangle$. Unitarity ensures that $\langle U_N | U_N \rangle = \sum_i s_{k,i}^2 = d^{-N} \text{Tr}(U_N^\dagger U_N) = 1$ where $s_{k,i}$ are the Schmidt values at bipartition $[1, \dots, k; k+1, \dots, N]$. Define the smallest non-zero Schmidt value as

$$s_{\min} := \min_{k,i} \{s_{k,i} : s_{k,i} \neq 0\}. \quad (19)$$

In the End Matter, we construct an explicit choice for L_k, R_k , for which the MPU conditioning number can be related to the MPU Schmidt values, yielding

$$q \leq \sqrt{D}/s_{\min}. \quad (20)$$

This gives a general and efficient criterion to verify polynomial circuit complexity for an arbitrary MPU.

Outlook—We have addressed the question of how to implement MPUs as quantum circuits, providing an explicit construction of polynomial depth for MPUs built from a repeated bulk tensor with open boundary. Our method extends to general MPUs under a mild spectral condition, expressed in terms of the bond dimension and smallest nonzero Schmidt value of the Choi state. More broadly, our results show how the representation of unitaries as tensor networks, a form that constrains their entanglement structure, implies their efficient physical realization. It remains open to optimize the circuit depth of our algorithm using

measurements and (global) feedforward, which could result in speedups. For projected entangled-pair unitaries (PEPUs) in higher spatial dimensions, our algorithm remains applicable provided the boundary state of local regions factories, an analog of the uncorrelated L , R condition that holds automatically in 1D. In this setting, additional care is required, as the corresponding conditioning parameter q may increase as the merging step in higher dimensions involves regions with growing boundary size. It remains an interesting direction for future work to identify and characterize subclasses of two-dimensional PEPUs that can be efficiently implemented using such methods.

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Data availability—No data were created or analyzed in this study.

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End Matter

Local isometries: Uniform bulk—Here, we show that the operators of Eq. (5) are indeed isometries satisfying the properties mentioned in the main text. Consider the $N = 3$ site MPU and σ, τ arbitrary single-site density operators. Then, from unitarity $U^\dagger U = \mathbb{1}$, it is immediately apparent that

$$\text{Tr}_{1,3}[(\sigma \otimes \mathbb{1} \otimes \tau)U^\dagger U] = \mathbb{1}. \quad (\text{A1})$$

In graphical representation,

$$\text{Diagram: A loop with two boxes labeled } A \text{ and } A^\dagger \text{ connected by a vertical line. The left leg is labeled } L^2 \text{ and the right leg is labeled } R^2. \text{ This is equal to a vertical line with an arrow pointing up.} \quad (\text{A2})$$

where

$$L^2 := \text{Diagram}, \quad R^2 := \text{Diagram}. \quad (\text{A3})$$

Note that both L^2, R^2 are positive-semidefinite; thus, their square roots L, R are well defined. Equation (A2) thus establishes $V_1^{[L,R]^\dagger} V_1^{[L,R]} = \mathbb{1}$. Repeating the same argument for $N = n + 2$ and tracing out the first and last sites establishes that $V_n^{[L,R]^\dagger} V_n^{[L,R]} = \mathbb{1}$ while clearly, L, R are independent of N and n . The same argument applies for tracing only the first or last site, thus yielding that $V_n^{[L,R]^\dagger}, V_n^{[L,R]}$ are also isometries. The resulting L, R depend on the choice of σ, τ and their support, which could be an arbitrary number of sites instead of a single site as considered previously. This freedom can be used to optimize the constant q_{unif} that governs the degree of the polynomial in the uniform-bulk MPU circuit [Eq. (10)].

It remains only to show that there exists a full-rank choice of L, R . This is equivalent to Assumption 1. To see this, first notice that $\text{rank}[L(\sigma)] \leq \text{rank}[L(\mathbb{1})]$ for all states σ . This is because, for any matrix X and positive-semidefinite σ , $\text{rank}(X^\dagger \sigma X) \leq \text{rank}(X^\dagger X)$ with equality if σ is full rank. Thus, if a full-rank L exists, it is obtained for $\sigma \propto \mathbb{1}$. Assumption 1 states $\text{rank}[L(\mathbb{1})] = D$, i.e., it is full rank. A similar argument applies for R .

Local isometries: General MPUs—We now consider the nonuniform case [Eq. (16)] with a similar derivation. Consider σ, τ arbitrary density operators supported over

sites $1, \dots, j-1$ and $k+1, \dots, N$, respectively. From unitarity,

$$\text{Diagram} = \text{Diagram}, \quad (\text{B1})$$

where

$$L_j^2 := \text{Diagram}, \quad R_k^2 := \text{Diagram}. \quad (\text{B2})$$

Note that both operators are again positive-definite by construction, and thus, their square roots are well defined, implying $V_{jk}^\dagger V_{jk} = \mathbb{1}$ as claimed. Since L_j and R_k depend on the choices of σ and τ , one can optimize over this choice, as in Eq. (17).

It remains to show that there is a choice with L_k, R_k full rank. This is true by bringing, without loss of generality, the MPU into a canonical form, which corresponds to the usual MPS canonical form of its Choi state [18]. In this representation, by choosing σ and τ maximally mixed states, we get [18]

$$L_k = \mathbb{1}, \quad R_k = \text{diag}(s_{k,1}, \dots, s_{k,D_k}) \quad \forall k, \quad (\text{B3})$$

where the $s_{k,i}$ are *strictly positive*, and they exactly correspond to the nonzero Schmidt values of the Choi state $|U_N\rangle$ for the bipartition $[1, \dots, k : k+1, \dots, N]$.