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Classical simulation of quantum many-body systems with a tree tensor network

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We show how to efficiently simulate a quantum many-body system with tree structure when its entanglement (Schmidt number) is small for any bipartite split along an edge of the tree. As an application, we show that any one-way quantum computation on a tree graph can be efficiently simulated with a classical computer.

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I. INTRODUCTION

Developing fast classical algorithms to simulate quantum many-body systems is important for understanding the underlying physical principles, as well as the limitations of quantum computation. Furthermore, it provides powerful tools for the analysis and engineering of quantum-information-processing components. However, efficient simulation is in general very difficult, due to the fundamental difference between quantum and classical physical laws. Fortunately, if the quantum evolution has certain restrictions, an efficient classical simulation may be possible [1–8].

Indeed, efficient simulation algorithms are known for several restricted quantum circuit models [1,2], while a general connection between entanglement and the classical simulatability of quantum lattice models has been unveiled [3–5]. In one spatial dimension (1D), for instance, the state of a quantum chain with a limited amount of entanglement between any bipartition along the chain can be efficiently described using a matrix product state (MPS) [9]. This is exploited by the density matrix renormalization group algorithm [10] to find the ground state of the chain and by the time-evolving block decimation (TEBD) method [4] to simulate an evolution in time. Furthermore, projected entangled-pair states (PEPSs) have been introduced as an extension of MPSs to simulate two–dimensional (2D) systems [6].

In this work we consider the simulation of quantum many-body systems with a restricted amount of entanglement according to a tree structure. As in the 1D and 2D approaches mentioned above, we express the d^n complex amplitudes $c_{i_1\cdots i_n}$ of the state $|\Psi\rangle$ of n qudits (or d-level quantum systems),

$$|\Psi\rangle = \sum_{i_1=1}^{d} \cdots \sum_{i_n=1}^{d} c_{i_1\cdots i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle, \qquad (1)$$

in terms of a network of tensors [11], but specialize to the case where this tensor network (TN) has a tree structure. Given a tree TN, we explain (i) how to simulate the response of the system to local operations and classical communication (LOCC), that is, to generic manipulation of individual qudits, including adaptive unitary transformations and measurements, and (ii) how to simulate time evolution. The latter is achieved by extending the TEBD algorithm [4], originally proposed to simulate 1D quantum lattices, so that it applies to a much broader class of states and physical situations. As in the 1D case, the key to an efficient simulation is that the amount of entanglement in the system remains sufficiently bounded during the time evolution.

From the perspective of theoretical computer science, our results imply that one-way quantum computation with a tree-graph cluster state can be efficiently simulated with a classical computer. One-way quantum computation with cluster states [12], an interesting alternative to the quantum circuit model, had previously been shown to be universal for quantum computation in a 2D lattice [13] but classically simulatable in a 1D lattice [14]. By extending the classical simulatability result to tree cluster states, we further sharpen the boundary between the complexities for classical and quantum computation.

From the perspective of computational physics, our results provide an algorithm both to find the ground state and to simulate time evolution in complex quantum systems with tree structure (see also [15]), such as dendrimers—a class of highly branched polymers [16]. This algorithm, based solely on tensor multiplications and singular value decompositions, offers additional ways to simulate 1D systems with long-range interactions.

II. CANONICAL FORM OF A TREE TN

We use a TN with n open indices and tree structure (see Fig. 1), to express the d^n complex coefficients of the n-qudit

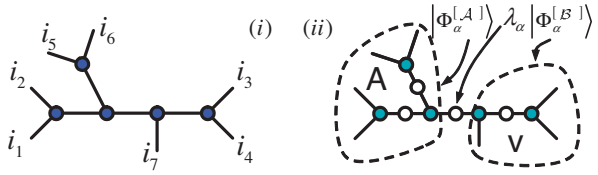

FIG. 1. (Color online) (i) A tree TN for state $|\Psi\rangle$ of $n=7$ qudits. Each open index labels an orthonormal single-qudit basis [see Eq. (1)]. Each vertex has three edges and corresponds to a tensor with three indices. Pairs of tensors are connected in the network through a shared index, over which there is an implicit summation. (ii) Canonical form of the previous tree TN. For each bipartition, subtrees $\mathcal{A}$ and $\mathcal{B}$ describe Schmidt bases [see Eq. (2)]. An empty circle on top of an edge represents a set of Schmidt coefficients weighting the corresponding index.

state $|\Psi\rangle$. More specifically, we consider a tree network made of tensors with only three indices each [17], the network therefore containing $n-2$ tensors. An index connecting two tensors divides the network into two subtrees $\mathcal{A}$ and $\mathcal{B}$ and the n qudits into two disjoint sets. We use the term *bipartition* to refer only to such divisions. The rank of an index is the number of values it takes. In what follows, χ denotes the largest rank among all indices in the network. Notice that the tree TN depends on $O(n\chi^3)$ complex coefficients.

The Schmidt decomposition of $|\Psi\rangle$ according to bipartition $\mathcal{A}:\mathcal{B}$ reads

$$|\Psi\rangle = \sum_{\alpha=1}^{\chi_{(\mathcal{A}:\mathcal{B})}} \lambda_\alpha |\Phi_\alpha^{[\mathcal{A}]}\rangle \otimes |\Phi_\alpha^{[\mathcal{B}]}\rangle, \tag{2}$$

where $\langle\Phi_\alpha^{[\mathcal{A}]}|\Phi_{\alpha'}^{[\mathcal{A}]}\rangle = \langle\Phi_\alpha^{[\mathcal{B}]}|\Phi_{\alpha'}^{[\mathcal{B}]}\rangle = \delta_{\alpha\alpha'}$, $\Sigma_\alpha(\lambda_\alpha)^2 = 1$, and the Schmidt rank satisfies $\chi_{(\mathcal{A}:\mathcal{B})} \leqslant \chi$. We next introduce the canonical form of a tree TN, which also consists of tensors with three indices but where each index α shared by two tensors carries weights (see Fig. 1).

Definition. A tree TN is in the canonical form for bipartition $\mathcal{A}:\mathcal{B}$ if (i) the weights on the connecting index α correspond to the Schmidt coefficients $\{\lambda_\alpha\}$ and (ii) the subtrees $\mathcal{A}$ and $\mathcal{B}$ describe a set of Schmidt bases $\{|\Phi_\alpha^{[\mathcal{A}]}\rangle\}$ and $\{|\Phi_\alpha^{[\mathcal{B}]}\rangle\}$. A tree TN is in the canonical form if it is so for all bipartitions.

Theorem 1. The canonical form of an n-qudit tree TN n can be obtained with $O(n\chi^4)$ basic operations.

Proof. Given a bipartition $\mathcal{A}:\mathcal{B}$, $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \sum_\alpha |\phi_\alpha^{[\mathcal{A}]}\rangle \otimes |\phi_\alpha^{[\mathcal{B}]}\rangle, \tag{3}$$

where the sets of states $\{|\phi_\mu^{[\mathcal{A}]}\rangle\}$ and $\{|\phi_\mu^{[\mathcal{B}]}\rangle\}$ for subtrees $\mathcal{A}$ and $\mathcal{B}$ may not be orthonormal. Our goal is to turn Eq. (3) into the Schmidt decomposition (2). Let

$$M = \tilde{X} D \tilde{X}^\dagger, \quad M_{\alpha\alpha'} \equiv \langle\phi_{\alpha'}^{[\mathcal{A}]}|\phi_\alpha^{[\mathcal{A}]}\rangle \tag{4}$$

be the spectral decomposition of the matrix M of scalar products in $\mathcal{A}$, where $\tilde{X}^\dagger\tilde{X} = \tilde{X}\tilde{X}^\dagger = I$, and $D_{\tau\tau'} = \delta_{\tau\tau'} d_\tau$. Then the vectors

$$|\hat{e}_\tau\rangle \equiv \frac{1}{\sqrt{d_\tau}} \sum_\alpha (\tilde{X}^\dagger)_{\tau\alpha} |\phi_\alpha^{[\mathcal{A}]}\rangle, \quad d_\tau > 0, \tag{5}$$

form an orthonormal set. We define $X \equiv \tilde{X}\sqrt{D}$. Analogous considerations in $\mathcal{B}$ lead to an orthonormal set $\{|\hat{f}_\eta\rangle\}$ and a matrix Y. Equation (3) can be rewritten as

$$|\Psi\rangle = \sum_{\tau\eta} (X^T Y)_{\tau\eta} |\hat{e}_\tau\rangle \otimes |\hat{f}_\eta\rangle. \tag{6}$$

From the singular value decomposition (SVD) of $X^T Y$,

$$(X^T Y) = U \Lambda V, \tag{7}$$

where $U^\dagger U = V V^\dagger = I$ and Λ is a diagonal matrix, we obtain the Schmidt coefficients $\lambda_\alpha = \Lambda_{\alpha\alpha}$ and bases

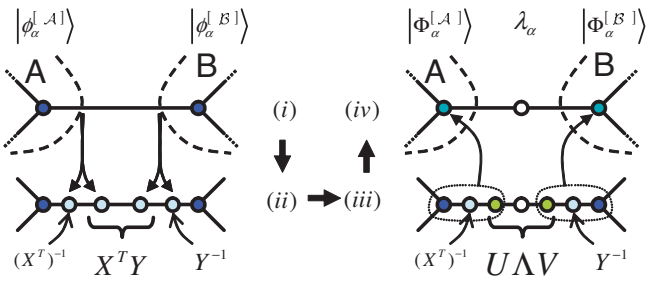

FIG. 2. (Color online) (i) Initial decomposition Eq. (3). (ii) Insertion of $(X^T)^{-1}X^T$ and YY^{-1}, projectors onto the subspaces generated by $\{|\hat{e}_\tau\rangle\}$ and $\{|\hat{f}_\eta\rangle\}$. (iii) $X^T Y$ is replaced with its singular value decomposition $U\Lambda V$, computed in $O(\chi^3)$ time. (iv) The Schmidt decomposition Eq. (2) is obtained after contracting some indices [$O(\chi^4)$ time].

$$|\Phi_\alpha^{[\mathcal{A}]}\rangle = \sum_\tau (U^T)_{\alpha\tau} |\hat{e}_\tau\rangle, \quad |\Phi_\alpha^{[\mathcal{B}]}\rangle = \sum_\eta V_{\alpha\eta} |\hat{f}_\eta\rangle. \tag{8}$$

All the above steps, summarized in Fig. 2, take $O(\chi^4)$ time and are repeated for each of the $n-3$ bipartitions of the tree TN. It is not hard to see that the scalar product matrices M for all edges can be computed sequentially in an appropriate order also in time $O(n\chi^4)$.

III. MANIPULATING A TREE TN

We now describe some basic tasks involving a tree TN, that is assumed to be in the canonical form. First, we can compute the reduced density matrix for just one or two qudits. Figure 3 shows how to proceed for one qudit.

Theorem 2. A two-qudit reduced density matrix can be computed with $O(md^2\chi^4)$ basic operations, where m is the number of tensors in the path that connects the two qudits in the tree TN (see Fig. 4).

Second, we can arbitrarily relocate a qudit within the tree TN. This is achieved by swapping the index corresponding to this qudit with other indices in the tree.

Theorem 3. Swapping a qudit index of a tensor with an

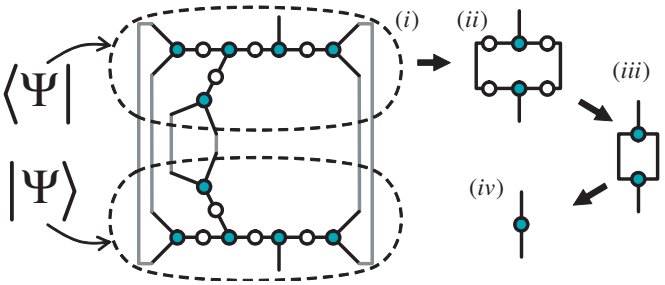

FIG. 3. (Color online) A single-qudit reduced density matrix is computed by contracting the TN in (i), which represents $|\Psi\rangle\langle\Psi|$ with a partial trace over all qudits but one. This TN reduces to the TN in (ii) thanks to the orthogonality of the Schmidt bases. In (iii) the weights have been absorbed into the three-index tensors [$O(d\chi^2)$ operations] and in (iv) the remaining shared indices have been contracted [$O(d^2\chi^2)$ operations].

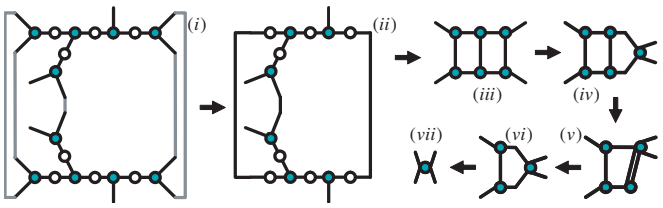

FIG. 4. (Color online) The reduced density matrix for two qudits separated by $m=3$ tensors is computed by contracting the TN in (i). This reduces to the TN in (ii) thanks to the orthogonality of the Schmidt bases. In (iii) the Schmidt weights have been absorbed into the tensors [$O(d\chi^2)$ operations], which in turn are reorganized on a line made of $m=3$ columns. Networks (iv)–(vi) illustrate how to reduce by one the number of columns [$O(d^2\chi^4)$ operations]. By iteration, a single tensor (vii) with four open indices is obtained.

index of a neighboring tensor can be achieved with $O(d^2\chi^4)$ basic operations (see Fig. 5).

Third, we can update the tree TN after a unitary gate U has acted either on one qudit or on two neighboring qudits. Unitarity preserves the orthogonality of the Schmidt bases for most bipartitions, and as a result the update process involves changing only one or two tensors. When U acts on one qudit or on two qudits that are connected to the same three-legged tensor, that tensor simply absorbs the gate through index contraction.

Theorem 4. Consider a two-qudit gate U acting on a pair of open indices of two tensors that are nearest neighbors in the network. The tree TN can be updated by replacing these two tensors, at a cost of $O(d^3\chi^3)$ basic operations (see Fig. 6).

IV. EFFICIENT SIMULATION WITH A TREE TN

All the above manipulations require computational time (and space as well) that scales at most linearly in the number of qudits n and as a small power of the maximal Schmidt rank χ. Therefore, in those systems where the amount of entanglement across all relevant bipartitions, as characterized by χ, scales at most polynomially in n, such manipulations can be implemented efficiently. This opens up a number of simulation possibilities.

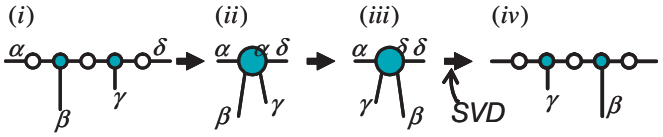

FIG. 5. (Color online) In order to exchange the positions of indices β and γ in (i), we contract the corresponding tensors (including all neighboring weights) into the four-legged tensor in (ii). After swapping the two indices, we split the resulting tensor (iii) through a SVD (of a matrix of the dimension $d\chi\times d\chi$ or $d\chi\times\chi^2$) that costs $O(d^2\chi^4)$ basic operations. The singular values define the new weights of the central index, whose initial rank χ may have increased to at most $d\chi$. The old weights for lateral indices are detached from the two tensors to leave the resulting tree TN in the canonical form.

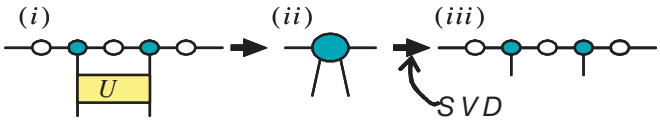

FIG. 6. (Color online) The tensor subnetwork in (i) is contracted into the four-legged tensor in (ii), which is then decomposed into (iii) by using a SVD (of a $d\chi\times d\chi$ matrix) that takes $O(d^3\chi^3)$ basic operations. Notice that, as in Fig. 5, special attention is paid to first absorbing and then detaching the weights of the lateral indices. This guarantees that the resulting tree TN is in its canonical form.

For instance, we can simulate the response of the system to arbitrary local manipulation. Recall that LOCC manipulation can be decomposed as an adaptive sequence of generalized local measurements mapping pure states into pure states. Let $\mathcal{E}$ denote one such measurement on a qudit, as characterized by a set of operators $\{E_r\}$, where r labels the measurement outcome. Outcome r occurs with probability $p_r=\langle\Psi|E_r^\dagger E_r|\Psi\rangle$, in which case the state of the system becomes $|\Psi_r\rangle=E_r|\Psi\rangle/\sqrt{p_r}$. To simulate $\mathcal{E}$, first we randomly draw an outcome r according to the probability $p_r=\mathrm{tr}[E_r\rho^{(1)}E_r^\dagger]$, computed from the reduced density matrix $\rho^{(1)}$ of the qudit to be measured. Then a tree TN for $|\Psi_r\rangle$ is obtained from that of $|\Psi\rangle$ by simply absorbing operator E_r into it. The new maximal Schmidt rank χ_r satisfies $\chi_r\leq\chi$.

An implication of the above result is that one-way quantum computation on a tree can be efficiently simulated. This follows from two simple facts: (i) a tree-graph cluster state has a very simple tree TN representation, with $\chi=2$, that can be obtained by simulating its preparation, namely, a series of two-qubit gates (according to the tree-graph pattern) applied

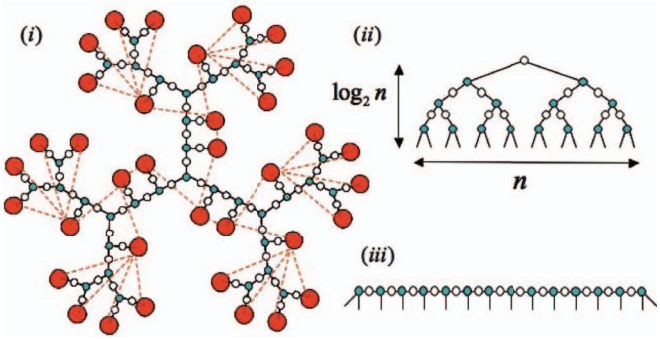

FIG. 7. (Color online) (i) Tree TN for a system with a genuine tree structure, such as a dendrimer. The red circles represent atoms, whose interaction pattern has a tree structure, represented by the red dotted lines. (ii), (iii) Two random qudits in a binary tree TN are connected through $O(\log(n))$ tensors, while in a linear TN (or MPS) they are connected through $O(n)$ tensors. Therefore, the time required to simulate a gate between two qudits is on average a factor $\log(n)/n$ lower when using a tree TN. This is a substantial gain in simulations involving long-range interactions. On the other hand, a generic binary tree TN with rank χ can be replaced with a MPS with a Schmidt rank $\chi'=O(\chi^{\log(n)})=O(n^{\log(\chi)})$. Thus, for constant χ (independent of n) the use of the binary tree TN is markedly more convenient. For $\chi=\mathrm{poly}(n)$, using the binary tree TN requires polynomial resources, while the cost of using a MPS is superpolynomial, namely, $O(n^{\log(n)})$.

to an initial product state; (ii) the manipulations involved in a one-way computation consists of LOCC.

The simulation of a time evolution according to a two-body Hamiltonian $H=\Sigma_{i,j}h_{ij}$ is also possible. As in the case of a 1D system [4], we expand the evolution operator $V=\exp(-iHt)$ into a series of two-qudit unitary gates U using a Suzuki-Trotter expansion. But now, for each of these gates, we first bring the indices of the two qudits together using Theorem 3, then absorb U into the tree TN using Theorem 4, and finally bring the qudit indices back into their initial position. This generalizes the TEBD algorithm [4] from 1D systems to a generic tree TN. With minimal modifications to deal with nonunitary gates, the TEBD algorithm can also be used to simulate an evolution in imaginary time according to $V'=\exp(-Ht)$. In this way we can compute the ground state of H, provided H has a finite gap $\Delta>0$ in its spectrum. Recall that the expectation value of local observables, such as the energy $E=\langle\Psi|H|\Psi\rangle$ or two-point correlators, can be computed from two-qubit reduced density matrices, which follow from Theorem 2.

A tree TN may be used to simulate a many-body system with a genuine tree structure (determined, e.g., by the interaction pattern) as is the case of dendrimers [16]. But it can also be used to simulate a 1D system with long-range interactions, including periodic boundary conditions (see Fig. 7). In a realistic simulation, the tree TN will often be an approximate representation of $|\Psi\rangle$ [18].

We conclude by noticing that in this paper we have explored the most general extension of the TEBD algorithm. Indeed, it appears that a tree TN—not having closed loops—is the most general TN to which we can associate a Schmidt decomposition to each of its indices, a fundamental ingredient of the simulation algorithm.

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[17] A tensor with more than three indices can be decomposed into a tree TN made of tensors with three indices each (for instance, through a sequence of Singular Value Decompositions).

[18] As discussed in [4] for a MPS, the use of a canonical form related to the Schmidt decomposition plays an important role in a simulation where χ is too large, provided that $|\Psi\rangle$ may be reasonably approximated by a tree TN with a smaller effective $\tilde{\chi}$. For a given bipartition $\mathcal{A}:\mathcal{B}$, the best approximation to $|\Psi\rangle$ is obtained by truncating decomposition (2) so as to retain only the $\tilde{\chi}$ terms with greatest weight λ_α. Thus, the canonical form of the tree TN is ideal to implement optimal bipartite truncations.