Plaquette Renormalization Scheme for Tensor Network States

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We present a method for contracting a square-lattice tensor network in two dimensions, based on auxiliary tensors accomplishing successive truncations (renormalization) of 8-index tensors for $2 \times 2$ plaquettes into 4-index tensors. The scheme is variational, and thus the tensors can be optimized by minimizing the energy. Test results for the quantum phase transition of the transverse-field Ising model confirm that even the smallest possible tensors (two values for each tensor index at each renormalization level) produce much better results than the simple product (mean-field) state.

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Tensor network states (TNSs) are emerging as a promising route toward unbiased modeling of challenging quantum many-body systems, such as frustrated spins. These correlated states are higher-dimensional generalizations of matrix product states (MPSs), which are implicitly produced in density matrix renormalization group (DMRG) calculations and are known to faithfully represent ground states of one-dimensional (1D) hamiltonians with short-range interactions. The matrix size $m$ has to increase at most polynomially with the system size $N$, which underlies the success of the DMRG method in 1D. For 2D and 3D systems, correlations are not reproduced properly by MPSs due to the inherently 1D nature of the local quantum entanglement in these states (although improved schemes can restore 2D or 3D uniformity), and $m$ then has to grow exponentially with $N$. In the TNSs, the matrices are replaced by tensors of rank corresponding to the coordination number of the lattice, e.g., on a 2D square lattice the tensors have four indices, in addition to their physical index (here spin $z$-component), as illustrated in Fig. 1. While it is believed, based on entanglement entropy considerations, that TNSs can represent ground states of short-range 2D and 3D hamiltonians, a serious problem in practice is that contracting the tensors is, in general, an NP hard problem. To overcome this challenge, approximate ways to compute the contraction have been proposed. Another approach is to use tree-tensor networks or more sophisticated extensions of these which can be efficiently contracted. Promising results based on TNSs have already been reported for several quantum spin models, but further reduction of the computational complexity, while maintaining the ability of the TNSs to properly account for entanglement, will still be necessary before the most challenging systems can be studied reliably.

In this paper, we introduce a plaquette renormalization scheme for 2D TNSs inspired by recent work of Levin and Nave. They suggested to replace the effective tensors for $2 \times 2$ plaquettes on the square lattice, which have $m^8$ elements, by some “renormalized” tensors with $m_{\text{cut}}^4$ elements, as illustrated in Fig. 2(a). This is exact, corresponding just to a regrouping of indices, if $m_{\text{cut}} = m^2$, and may be a good approximation even if $m_{\text{cut}} \sim m$. For a square $L \times L$ lattice, the new tensors describing $2 \times 2$ spins should be contracted on a new lattice of length $L/2$. If the original $L$ is a power of 2, this decimation can be continued until there is a single tensor left, which is then contracted with itself (under periodic boundary conditions) to give the wave function. One can also carry out this kind of renormalization of the “double tensors” obtained when the physical spins are traced out first. The full contraction of the double-tensor network, illustrated in Figs. 1(b,c), is the norm $\langle \Psi | \Psi \rangle$ of the wave function. A matrix element $\langle \Psi | A | \Psi \rangle$ of some operator involving one or several sites can be treated in a similar way. In practice, in most TNS approaches, one would first construct the double tensors and then compute the full contraction in some approximate way. A plaquette renormalization with double tensors is depicted in Fig. 2(b). This may be a good approximation for some judiciously chosen renormalized tensor, but how to find the best one is an open question. Gu, Levin, and Wen implemented a singular value decomposition (SVD) scheme for the double tensors, and a similar method was proposed by Jiang, Weng, and Xiang. In our scheme, the renormalization is instead accomplished with the aid of auxiliary 3-index tensors $S_{s}^{abc}$, which transform and truncate pairs of indices of the plaquette tensors in the wave function, as shown in Fig. 3.

FIG. 1: (a) For each site $s$ on an $N$-site square lattice, there is a 4-index tensor $T_{ijkl}^{s}(\sigma_{s})$, where $\sigma_{s}$ is the physical index (here a spin $\sigma_{s}^{z} = \pm 1$) and $i, j, k, l \in \{1, \ldots, N\}$. The wave function $\Psi(\sigma_{1}, \ldots, \sigma_{N})$ is the $N$-tensor product (contraction) defined as a summation over all shared indices on the links. (b) The norm $\langle \Psi | \Psi \rangle$ is obtained by contracting also the physical indices, which is normally done by first summing $T_{ijkl}^{2}(\sigma_{s})T_{kjl}^{1}(\sigma_{s})$ over $\sigma_{s}$, giving double tensors (c).

FIG. 2: (a) The norm $\langle \Psi | A | \Psi \rangle$ of some operator involving one or several sites can be treated in a similar way. In practice, in most TNS approaches, one would first construct the double tensors and then compute the full contraction in some approximate way.
a, . . . , h

 FIG. 2: (a) Truncation (renormalization) of an 8-index plaquette tensor into an effective 4-index tensor. The indices a, . . . , h ∈ \{1, . . . , m\} and i, j, k, l ∈ \{1, . . . , m_{\text{cut}}\}. The diagonal lines indicate physical indices, which for an $S = \frac{1}{2}$ spin system can take two values before the renormalization and 16 values after (and is further multiplied by 16 after each successive renormalization). In (b) the physical indices are traced out first, leading to double tensors. To stay with the same level of truncation as in (a), the indices after the renormalization should then take values i, j, k, l ∈ \{1, . . . , m_{\text{cut}}\}.

izations effectively corresponds to a new tensor network, which is illustrated in the case of the wave function on an $8 \times 8$ lattice in Fig. 4.

Here we will apply this scheme to the transverse-field Ising model (which has become the bench-mark of choice for initial tests within TNS approaches):

$$H = -J \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x - h \sum_i \sigma_i^z,$$

where $\sigma_i^x$ and $\sigma_i^z$ are standard Pauli matrices and $\langle ij \rangle$ denotes nearest-neighbor site pairs on a 2D square $L \times L$ lattice with periodic boundary conditions. The ground-state wave function of this system is translationally invariant and positive-definite. We can then take the original tensors to be site-independent, i.e., there are just two tensors $T_{ijkl}(\sigma_s = \pm 1)$ and the tensors $S^n$ are the same for all plaquettes on a given renormalization level $n = 1, ..., \log_2(L) - 1$. At the last level, four tensors remain (see Fig. 4), which we contract directly. The problem is now to optimize the elements of the $T$ and $S$ tensors, to minimize the energy. Before proceeding to calculations, several comments are in order.

It is clear from Fig. 4 that the plaquette renormalization (no matter how it is accomplished) breaks translational symmetry, which, in the optimized state, should gradually be restored with increasing $m$. A way to restore the symmetry for finite $m_{\text{cut}}$ is to sum over all (here four) symmetrically non-equivalent ways of arranging the plaquettes on the lattice at each level. In a similar way, one can also ensure that the wave function is symmetric under other lattice transformations (rotations and reflections) for arbitrary $T$ and $S^n$ (as an alternative to enforcing these symmetry in the individual tensors), and spin-inversion symmetry can be implemented in a similar way. These symmetrization procedures (which also enable studies of states with different quantum-numbers of the symmetry operators) can be carried out if the spins are sampled using Monte Carlo simulations but cannot be easily used with the double-tensor network. Here, in this initial test of the scheme, we will trace out the spins exactly and work with the double tensors. When minimizing the energy, it is then important to calculate the full, translationally averaged energy, not just the site and bond energies on a single plaquette (as is done in the SDV scheme of Gu et al.), in order to maintain the variational property of the scheme. No approximations are made when contracting the effective renormalized tensor network, also when using the double tensors. In contrast, the SVD applied to the double-tensor network introduces an approximation due to which the calculated energy becomes non-variational. This can cause problems when optimizing the tensors. Note that in our double-tensor approach, there is a pair of equal $S$ tensors for each plaquette edge (one from $\langle \Psi \rangle$ and one from $\langle \overline{\Psi} \rangle$) and one cannot combine these into arbitrary tensors, which would make the scheme non-variational.

The renormalization of a plaquette according to Fig. 3 requires 12 internal index summations for each combination of the four external indices of the renormalized tensor, which can be carried out with $\sim m^5$ operations.

FIG. 3: Renormalization of an 8-index plaquette tensor using auxiliary 3-index tensors. The solid circles denote either the original tensors $T = T^0$, which depend on the physical spins (which are not shown here), or tensors $T^n$ arising after $n$ renormalization steps have been carried out (and depend on the $2^{2n}$ spins within the block). The squares denote 3-index tensors $S^n$ by which the external indices are decimated by contracting common $T^{n-1}$ and $S^n$ indices. The remaining four free indices take values 1, . . . , $m_{\text{cut}}$.

FIG. 4: The effective reduced tensor network for an $8 \times 8$ lattice. Here there are two sets of $S$ tensors; $S^1$ and $S^2$, denoted by the smaller and larger squares. The solid circles correspond to the original, spin dependent tensor $T^0$. 

FIG. 5: Steps in the contraction of the renormalized plaquette tensor of Fig. 3. Partial contractions are constructed from left to right. The summations carried out are indicated by Σ and the scaling of each step with \( m \) is shown beneath the diagrams. Each summation and free index contributes a factor \( m \).

(assuming \( m_{\text{cut}} = m \), which we will use here). One example of a sequence of contractions giving this scaling is shown in Fig. 5. When working with double tensors, the scaling becomes \( m^{16} \), since all external and internal indices should then take \( m^2_{\text{cut}} = m^2 \) values. The derivatives of the energy with respect to all the tensor elements, which we use to minimize the energy, can be evaluated with the same scaling in \( m \), using a chain-rule procedure carried out along with the renormalization steps (as we will describe in detail elsewhere).

It should be noted that the optimized \( T \) tensors do not necessarily constitute a good TNS when contracted without the \( S \) tensors, because they are optimized together. On the other hand, it should also be possible to construct special \( S \) tensors that effectively perform something very similar to a SVD (although globally optimized, not locally as in Ref. [13,14]) and then the optimized \( T \) tensors by themselves should also form a good TNS when assembled into a standard 2D tensor network. Here we do not impose any such conditions on the \( S \) tensors.

We now discuss calculations for the hamiltonian \( H \). For \( L \to \infty \), the ground state of this system undergoes a quantum phase transition in the 3D Ising universality class, at a critical field \( h_c/J \approx 3.04 \) determined using quantum Monte Carlo simulations. Here we study the model using the smallest possible tensors and truncation, \( m = m_{\text{cut}} = 2 \), using the double-tensor approach for lattices of size \( L = 4, 8, 16, \) and 32. For the \( T \) tensors, we enforce symmetry with respect to rotations of the indices, for a total of 6 free parameters each for \( T(1) \) and \( T(-1) \). The \( S \) tensors are symmetric in the two indices used in the internal contractions of the plaquettes, and so there are 6 free parameters also for each \( S^n \).

Starting with random tensor elements, we calculate the energy and its derivatives with respect to all the parameters. We then update the parameters based on the derivatives, using a stochastic optimization scheme of the kind discussed in Ref. [15]. The plaquette renormalizations and the derivative calculations are highly parallelizable, which we take advantage of by using a massively parallel computer. In general the method performs very well, although occasionally the energy converges to a local minimum, especially close to the critical point. There can also be problems with the wave-function norm becoming very small, which can be remedied by periodically multiplying the tensors by suitable factors.

The method can produce solutions breaking spin-inversion symmetry, in which case we do not obtain the true ground state for a given system size \( L \), which can have no broken symmetries for finite \( L \). This is to be expected, in analogy with how mean-field theory (corresponding to the \( m = 1 \) simple product state) produces symmetry-broken states for \( h < h_c \). Thus we can simply compute the magnetization \( m_c = \langle \sigma_z \rangle \) (averaged over all sites \( s \)) and study its behavior for increasing \( L \). Note that for fixed \( L \), spin-inversion symmetry should gradually be restored with increasing \( m \), as the optimized state should approach the true finite-\( L \) symmetric ground state. However, for any fixed \( m \), we expect the symmetry to be broken when \( L \to \infty \) for \( h \) below some \( m \)-dependent \( h_c \).

Here we only consider \( m = 2 \). Results for \( m_z \) and the field-induced \( m_x = \langle \sigma_x \rangle \) are shown versus the field \( h/J \) in Fig. 6. The transition point between the magnetic and paramagnetic states moves toward higher fields with increasing \( L \), converging to \( h_c/J \approx 3.33 \) for the largest sizes. This is closer to the unbiased quantum Monte Carlo result \( h_c/J \approx 3.04 \) than the mean-field \( m = 1 \) value \( h_c/J = 4 \). There is some weak finite-size rounding close to the transition for \( h > h_c(L) \), which becomes less pronounced with increasing \( L \). One the other hand, the magnetization curve for \( h < h_c(L) \) becomes less sharp with increasing \( L \). For \( L = 4 \) and 8 the transitions look almost first-order. However, upon closer examination, the curves can be described in a range of fields \( h < h_c \) by a power-law, \( (h_c - h)^\beta \), with the exponent \( \beta \) increasing with \( L \). For \( L = 32 \) and 64, \( \beta = 0.40 \) describes the data well over a wide range of fields, but it is not clear whether this is the true asymptotic value. Including only points very close to \( h_c \), the mean-field exponent \( \beta = 1/2 \) also...
works well. It is thus presently unclear whether our TNS can describe non-mean-field critical correlations for finite \(m = m_{\text{cut}} = 2\), although we expect that such behavior should certainly emerge with increasing \(m = m_{\text{cut}}\).

Fig. 4 shows the spin-spin correlation function \(C(r) = \langle S^z_i S^z_j \rangle\) averaged over all equidistant spins close to \(h=0\). This shows behavior clearly different from a simple \(m = 1\) product state, which only gives a constant \(C(r) = \langle S^z_i \rangle^2\) for \(r > 0\). Characteristic boundary enhancements of the correlations at \(r \approx L/2\) are seen for the smaller sizes.

In summary, we have presented a scheme using auxiliary tensors to renormalize plaquette tensors in a 2D tensor network. The approach can also be regarded as a different tensor network, which can be contracted efficiently. Figs. 3 and 4 summarize the approach pictorially. Using the example of the transverse-field Ising model, we have shown that the scheme produces results far better than mean-field theory, even with the smallest possible non-trivial tensors and truncation \((m = 2)\). The scaling to the thermodynamic limit is well-behaved. Based on these results, we expect a fast convergence to the exact ground state with increasing \(m\). Increasing \(m\) to 3 is already quite challenging within the double-tensor approach that we have employed here, since the scaling is \(m^{16}\). However, in variational Monte Carlo simulations (sampling the spins and optimizing the tensors based on stochastic estimates of the derivatives)\(^{16}\) the scaling is \(m^8\), and it should then be easier to study larger \(m\). Application to other quantum spin systems (and even fermions) is in principle straightforward, although the convergence with \(m\) can of course be expected to be model dependent.

Here we optimized the tensors variationally, which requires the energy averaged over all non-equivalent sites and bonds. The computational effort then scales with the system size as \(L^2 \log(L)\). If we optimize only a local energy, which is not a variational estimate of the total energy but can produce good results in the SVD approach\(^{13}\) (and may work well also in our scheme for some particular classes of \(S\) tensors), the scaling is \(\log(L)\), as in SVD based schemes. It may also be possible to use imaginary-time evolution (ground-state projection), as is often done in other TNS approaches\(^{20}\).

A technically appealing feature of our scheme is that the plaquette renormalization procedure can be implemented very efficiently on GPUs (graphics processing units, the use of which is emerging as an important trend in high-performance computing\(^{21}\)). The speed-up relative to a standard CPU can be very significant for large tensors. For the spin-dependent tensors we have achieved better than a factor of 150 in efficiency boost when \(m = 6\). We plan to use this approach in future model studies.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7.png}
\caption{(Color on-line) Spin-spin correlation versus separation \(r\) at fields \(h\) close to \(h_c\) such that the long-distance correlations are approximately the same for system sizes \(L = 16, 32,\) and \(64\).}
\end{figure}

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