Symmetric cluster expansions with tensor networks

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Cluster expansions for the exponential of local operators are constructed using tensor networks. In contrast to other approaches, the cluster expansion does not break any spatial or internal symmetries and exhibits a very favorable prefactor to the error scaling versus bond dimension. This is illustrated by time evolving a matrix product state using very large time steps, and by constructing a robust algorithm for finding ground states of two-dimensional Hamiltonians using projected entangled pair states as fixed points of two-dimensional transfer matrices.

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1. INTRODUCTION

The Trotter-Suzuki expansion [1,2] plays a ubiquitous role in theoretical physics as it relates quantum-mechanical problems in $d$ spatial dimensions to statistical-mechanical problems in $d + 1$ dimensions. It is also a preferred tool for simulating the time-dependent Schrödinger equation on a computer, as it allows one to split a continuous differential equation into smaller steps $dt$ that can be integrated exactly; the corresponding error scales as $c_d dt^{n+1}$ for an $n$th-order expansion, with $c_d$ a prefactor that can be optimized [3]. This Trotter-Suzuki expansion forms the basis for the time-evolving block decimation algorithms [4] for simulating quantum spin chains, and has been used extensively in that context for finding ground states (imaginary-time evolution) and for simulating real-time dynamics. The success of this method follows to a large extent from the fact that Trotter-Suzuki expansions are size extensive: they scale well in the thermodynamic limit. A very important drawback however is the fact that they always break spatial and/or internal symmetries of the underlying quantum system. A different approach which preserves the symmetries of the Hamiltonian is the cluster expansion, widely used in the form of series-expansion methods in quantum Monte Carlo [5]. Such methods are however not size extensive, as they involve a power series of the Hamiltonian terms outside of the cluster are ignored. The idea is to grow a matrix product operator which captures more and more terms in the perturbative expansion, but in such a way that the results in a given cluster are exact if Hamiltonian terms outside of the cluster are ignored.

The first nonzero element in the MPO tensor encodes the action of the unit operator, i.e., we set

$$\exp \left( t \sum_i h_{i,i+1} \right) \approx \ldots \circ \circ \circ \circ \ldots$$

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The first nonzero element in the MPO tensor encodes the action of the unit operator, i.e., we set

$$\circ \ldots \circ = \mathbb{I},$$

where the label “0” denotes the first entry of the virtual legs. The first nontrivial cluster is of size 2, and is obtained by exponentiating the nearest-neighbor interaction term and subtracting the unit that we have already incorporated. This cluster is encoded in the MPO by introducing a new virtual
level in the MPO denoted by label “1” and with degeneracy depending on the Schmidt decomposition of the exponential of the local Hamiltonian under consideration. By performing a singular-value decomposition of this exponential minus the identity operator, we get two new tensor elements $O'_{01}$ and $O'_{10}$ such that

$$
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\rightarrow
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}.
$$

We add these elements to the MPO, so $O \rightarrow O + O'$. Note that this cluster contains two-site terms of all orders and the extensivity property of the ensuing MPO is of crucial importance: the MPO contains an extensive number of terms with multiple nonoverlapping clusters such as

$$
\begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 0 \\
0 & 0 & 1
\end{pmatrix}.
$$

The MPO does not contain overlapping terms, however, and therefore we have to introduce three-site cluster terms. We obtain these by exponentiating the terms of the Hamiltonian that act nontrivially on three sites, and subtract what was already contained in the two-site cluster terms. Again, we can introduce a new element in the MPO tensor for capturing these terms:

$$
\begin{pmatrix}
0 & 1 & 1 & 1 \\
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\frac{1}{\sqrt{h_{12}h_{13}}} & 0 \\
0 & \frac{1}{\sqrt{h_{12}h_{13}}}
\end{pmatrix}
\begin{pmatrix}
0 & 1 & 1 \\
1 & 0 & 0 \\
0 & 0 & 1
\end{pmatrix},
$$

where on the right-hand side we sum over the unlabeled legs. We compute this tensor element $O'_{22}$ by applying the inverses of the $O_{10}$ and $O_{01}$ elements to the right-hand side, and as such we do not have to increase the bond dimension of the MPO to achieve this. Adding this tensor element to the MPO, $O \rightarrow O + O'$ then encodes an extensive number of two- and three-site cluster terms.

We can continue this procedure, and incorporate four- and five-site clusters with an extra virtual level “2” and three new tensor elements $O'_{12}$, $O'_{21}$, and, in a next step, $O'_{22}$:

$$
\begin{pmatrix}
0 & 1 & 1 & 2 & 1 \\
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}.
$$

This construction provides us with a MPO representation for cluster expansion of the exponentiated Hamiltonian, which conserves all spatial symmetries such as translation invariance and reflection symmetry. Thanks to the extensivity property, the MPO works directly in the thermodynamic limit as well as for finite systems—for periodic boundary conditions one closes the MPO to a loop, and for open boundary conditions one projects the boundary legs on the “0” space. It is correct up to order $t^{p-1}$, where $p$ is the largest cluster size that is incorporated in the MPO, but, in fact, it captures a large portion of the higher-order terms as well. The terms of order $t^p$ that are lacking from the MPO representation are, indeed, only the $p + 1$ clusters. There are $p!$ such terms in the exponential of size $p$, whereas we can count there are $p^p$ different $O(t^p)$ terms with those same Hamiltonian terms. We thus find that the MPO gets a fraction $p! / p^p$ of the $O(t^p)$ terms wrong, or that the error decreases very quickly as $\epsilon \propto \sqrt{2\pi pe^{-p}}$.

As an example, we use this MPO construction to simulate time evolution for the $XXZ$ model in the thermodynamic limit:

$$
H_{XXZ} = \sum_i (S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1}),
$$

where $S^{\alpha}_i$ denotes the spin-1/2 operators at site $i$ and we choose $\Delta = 1/2$. We use an MPO cluster expansion of the time-evolution operator with time step $dt$ up to clusters of size 5, leading to a bond dimension of $1 + 4 + 16 = 21$ (see
above), and we start our time evolution from the Néel state. We represent the time-evolved state as an MPS with bond dimension $\chi$. In each time step the bond dimension increases by applying the time-evolution MPO, and after a number of time steps we truncate the bond dimension down to $\chi$. We perform this truncation step by a variational optimization of the global overlap of the wave function, which can be done in a way very similar to other variational algorithms for uniform MPSs [13,14].

Our results are presented in Fig. 1. We have chosen to look at the occupation number per site as a function of time, $n = 1/2 + \langle S_z \rangle / 2$, as well as the bipartite entanglement entropy $S$. We compare to simulations with the time-dependent variational principle (TDVP) for uniform MPSs [15]. We observe that the entropy grows linearly up to $t \approx 13$, showing that up to this time the evolution is captured well by a finite-$\chi$ MPS. We see that the MPO cluster expansion produces almost exact results for time steps up to $dt = 2.1$. Given that the error to the MPO goes as $dt^2$, this illustrates that the prefactor to this error is exceedingly small.

We do not see a great decrease in computation time as the time step is increased, because the truncation step gets more time consuming with larger time steps. While this method is competitive with other time-evolution schemes, we believe it is best used in tandem with the TDVP: using the TDVP for the main time evolution, and the cluster expansion MPO to increase the bond dimension. Increasing bond dimension such that spatial symmetries are conserved is nontrivial yet crucial for accurate simulation [16,17], and with a cluster MPO time step one can do just that. Additionally, a large time step allows for a more accurate bond dimension increase than several bond increases with small time steps, as must be done in most time-evolution schemes. This holds true in infinite but also finite systems.

### III. CONSTRUCTION IN TWO DIMENSIONS

The above construction for the MPO cluster expansion is generic, and can be applied to more general cases in higher dimensions. Here, we illustrate how the construction generalizes to the case of a projected entangled pair operator (PEPO) representation for an exponentiated nearest-neighbor Hamiltonian on a square lattice:

$$\exp \left( t \sum_{(ij)} h_{ij} \right) \approx \frac{\chi}{\chi - 1} \left[ \begin{array}{cccc}
-\chi & \chi \gamma_{1} & \ldots & \chi \\
\chi \gamma_{1} & -2 & \ldots & \chi \\
\vdots & \vdots & \ddots & \vdots \\
\chi & \chi & \ldots & -2
\end{array} \right].$$

In a similar vein as for the MPO case, we incorporate the trivial part of the operator on the first virtual level, labeled “0,” and introduce a virtual level “1” for capturing the two-site clusters with the diagrams

$$\begin{array}{cccc}
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}, \quad
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}, \quad
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}.$$

The three-site clusters and some four- and five-site clusters do not require a new virtual level, but can be encoded as

$$\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}, \quad
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}, \quad
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}.$$

In contrast to the one-dimensional case, loops will occur for large enough clusters, but this can be straightforwardly incorporated in the PEPO. The simplest loop involves the four-site cluster on a plaquette, which can be encoded by introducing a new virtual level “2”:

$$\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}, \quad
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}, \quad
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}.$$

This virtual level “2” must always appear in right angles to ensure it is part of a loop. More complicated clusters may be incorporated by building upon this basic construction, adding another virtual level whenever necessary.

Let us illustrate the power of this PEPO construction for PEPS ground-state optimization in the thermodynamic limit. The standard method for simulating imaginary-time evolution for PEPSs is the full-update algorithm [18], a method based on Trotter-Suzuki decompositions and local truncation steps. Here we approximate the imaginary-time-evolution operator $e^{-\tau H}$ with a PEPO cluster expansion and find its fixed point variationally using the algorithm in Ref. [19], in such a way that translational invariance and other global symmetries are conserved. In line with existing variational PEPS algorithms [20,21], the present PEPS algorithm performs a variational optimization of the imaginary-time-evolution operator, and therefore the fixed point will converge as $\tau \to 0$ to the optimal PEPS ground-state approximation for the Hamiltonian itself (in contrast to full-update optimization) [20,21]. The computational cost and complexity of the algorithm are significantly smaller than the ones relying on variational optimization of the Hamiltonian itself [20,21].

We consider the Heisenberg Hamiltonian with sublattice rotation:

$$H = \sum_{(ij)} -S_i^z S_j^z + S_i^x S_j^x - S_i^y S_j^y.$$

This particular sublattice rotation ensures that the PEPO is symmetric under reflection and complex conjugation, which simplifies the numerical optimization significantly [19]. We have optimized PEPSs with bond dimensions $D = 3$ and 4 and different $\tau$‘s, and listed the results for the energy in Table I. We observe that we can reach the variational optimum.
as \( \tau \rightarrow 0 \), but already obtain very precise values for the energy for a surprisingly large time step \( \tau = 0.1 \).

**IV. OUTLOOK**

In this paper, we have explained how to construct cluster expansions for exponentiated local operators in quantum lattice systems with tensor networks. We have shown that these cluster expansions are of great practical use. On the one hand, they allow us to simulate time evolution of quantum spin systems with a much larger time step than in traditional approaches [22], and in such a way that symmetries are not broken. This is especially relevant for simulations starting from states with very few entanglements. The large time steps create entanglement very quickly, which has to be contrasted to schemes relying on the time-dependent variational principle [15] which show problems in building up the entanglement.

On the other hand, our cluster expansion provides a systematic scheme for converting the problem of finding ground states of Hamiltonians into one for finding the fixed point of a transfer matrix, which is a much better conditioned problem for two-dimensional problems. In addition, the PEPO inherits all spatial symmetries of the Hamiltonian and we do not introduce an artificial translational symmetry breaking.

In this paper we have restricted ourselves to nearest-neighbor interactions, but our ideas can be applied to generic systems. In particular, it can be applied for simulating time evolution with an MPS on a cylinder [23]. We expect that our PEPO construction will prove crucial for simulating dynamics with PEPSs. On the one hand, one can deduce a PEPS real-time-evolution scheme that does not rely on Trotter-Suzuki decompositions [24,25] for global quantum quenches without breaking any symmetries of the system, and, on the other, the computational cost of evaluating excitation energies with the quasiparticle ansatz [26] can be drastically reduced. Finally, it is clear that the large step sizes enabled by the method are useful for constructing thermal states.

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**TABLE I.** Numerical results for the energy obtained with our variational PEPS algorithm based on the PEPO cluster expansion with imaginary-time step \( \tau \); the PEPO has bond dimension 5.

| Energy, \( D = 3 \) | Energy, \( D = 4 \) |
|-------------------|-------------------|
| PEPO, \( \tau = 0.1 \) | \(-0.6680688\) | \(-0.6689633\) |
| PEPO, \( \tau = 0.0562 \) | \(-0.6680768\) | \(-0.6689645\) |
| PEPO, \( \tau = 0.0316 \) | \(-0.6680797\) | \(-0.6689650\) |
| PEPO, \( \tau = 0.0178 \) | \(-0.6680808\) | \(-0.6689651\) |
| PEPO, \( \tau = 0.01 \) | \(-0.6680810\) | \(-0.6689652\) |
| Variational PEPS [21] | \(-0.6680791\) | \(-0.6689642\) |

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