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FAST TRACK COMMUNICATION

An efficient algorithm for translationally invariant finite-size periodic lattice systems in one spatial dimension

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Abstract

We develop an efficient algorithm to find a matrix product state representation of the ground-state wavefunctions for translationally invariant finite-size periodic lattice systems in one spatial dimension. This is based on the observation that the efficient computation of the ground-state energy per site only needs to retain a certain number of the largest eigenvalues of the transfer matrix for a matrix product state, without any sacrifice of accuracy. The computational cost is independent of the system's size, and scales as χ^3 with χ being the truncation dimension. The algorithm is tested for the critical quantum Ising model in a transverse field on a finite-size lattice, with the size as large as 4800 for the truncation dimension 200.

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(Some figures in this article are in colour only in the electronic version)

Significant advances in classical simulations of quantum many-body lattice systems have been made in the recent decades. Indeed, many powerful numerical methods, such as quantum Monte Carlo (QMC) [1] and the density matrix renormalization group (DMRG) [2], have been developed. Although these methods are able to simulate quantum many-body lattice systems, they do suffer from their respective problems: there is a notorious sign problem with the QMC, whereas the DMRG is mainly limited to quantum lattice systems in one spatial dimension. Therefore, it is highly desirable to develop efficient algorithms to classically simulate quantum many-body systems beyond these limitations. A promising prospect to meet this challenge comes from the tensor network algorithms [3–8], including the matrix product states (MPS) [9] for quantum lattice systems in one spatial dimension, and the projected entangled-pair states (PEPS) [5] for quantum lattice systems in two and higher spatial dimensions.

Specifically, Verstraete, Porras and Cirac [4] devised a variational algorithm to find an MPS representation of low-lying states for finite-size periodic quantum lattice systems in one spatial dimension. The computational cost of the algorithm is roughly proportional to

the lattice size, and also scales as the fifth power with the truncation dimension [4]. This drawback, as shown by Pippan *et al* [8], may be remedied in the improved MPS algorithm. The computational cost of the improved MPS algorithm may be reduced to that comparable to the DMRG. But it is still proportional to the lattice size, namely, simulating a large size quantum system is memory demanding and time consuming. On the other hand, an infinite MPS (iMPS) algorithm has been initiated by Vidal [6], to simulate translationally invariant quantum systems on an infinite-size lattice in one spatial dimension. Thus an interesting question arises as to whether or not it is possible to develop an efficient MPS algorithm for translationally invariant finite-size periodic lattice systems in one spatial dimension, with the computational cost independent of the lattice size.

In this communication, we address this question. It is shown that one may adapt the iMPS algorithm to simulate translationally invariant finite-size periodic lattice systems in one spatial dimension, with the computational cost independent of the lattice size. Moreover, the scaling of the cost with the truncation dimension is comparable to the improved MPS algorithm. This is based on the observation that, not all the eigenvalues and eigenvectors of the transfer matrix for an MPS state contribute significantly to the ground-state energy. This enables us to dramatically reduce the computational cost, since *only* a few largest eigenvalues of the transfer matrix, with the corresponding left and right eigenvectors, need to be retained when the ground-state energy per site is computed.

The algorithm is tested by computing the MPS representation of the ground-state wavefunctions for the quantum Ising model in a transverse field on a finite-size lattice with periodic boundary conditions (PBCs). Since the cost does not depend on the system's size, we are able to compute the ground states for both small and large sizes. For a system with the size ranging from 10 to 100, its ground-state energy per site e_N is computed at criticality. It turns out that it is consistent with the conformal field theory prediction, with the deviation of the predicted central charge from the exact value around 10^{-4}. We also compute the von Neumann entropy, a bipartite entanglement measure, for a system with sizes up to 4800. The discrepancies between the fitted central charges and the exact value are all less than 1.3×10^{-3}.

The description of the algorithm

Consider a translationally invariant quantum system on a finite-size periodic lattice in one spatial dimension. Suppose each site is endowed with a local Hilbert space of d dimension, that is $\mathcal{H}^{[i]} \cong C^d$, so that the Hilbert space of the system is $\mathcal{H} = \otimes_{i=1}^{N} \mathcal{H}^{[i]}$. We restrict ourselves to study quantum lattice models consisting of the nearest-neighbor interactions, characterized by a Hamiltonian $H = \sum_{i=1}^{N} h^{[i,i+1]}$. As is well known, the ground-state wavefunction is generated via an imaginary time evolution, with a randomly chosen state as an initial state $|\psi_0\rangle$:

$$|\psi_\tau\rangle = \frac{\exp(-H\tau)|\psi_0\rangle}{\|\exp(-H\tau)|\psi_0\rangle\|}, \tag{1}$$

when $\tau \to \infty$, as long as the initial state is not orthogonal to the genuine ground state.

Let us now introduce an MPS representation of a quantum state wavefunction translationally invariant under two-site shifts $|\psi\rangle$. It may be represented in terms of an MPS in the form: $|\psi\rangle = \sum_{s_1,\ldots,s_N} \mathrm{tr}\big[\Gamma_A^{s_1}\lambda_A\Gamma_B^{s_2}\lambda_B\cdots\Gamma_A^{s_{N-1}}\lambda_A\Gamma_B^{s_N}\lambda_B\big]|s_1,\ldots,s_N\rangle$, where s_i is the physical index, $s_i = 1,\ldots,d$, and $\Gamma_A^{s_i}$ and $\Gamma_B^{s_i}$ are $\chi \times \chi$ matrices for a given s_i, with χ being the truncation dimension and λ_A, λ_B are singular value matrices. Here, we have assumed that N is even. Note that the entries of $\Gamma_A^{s_i}$ and $\Gamma_B^{s_i}$ are labeled by the inner indices α and β, which take values from 1 to χ. In other words, the matrices $\Gamma_A^{s_i}$ and $\Gamma_B^{s_i}$ may be regarded

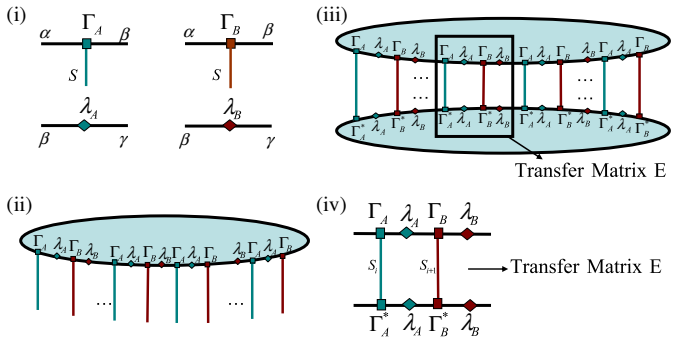

Figure 1. (i) Two three-index tensors $\Gamma^{s}_{A\alpha\beta}$ and $\Gamma^{s}_{B\alpha\beta}$, together with singular value matrices λ_A and λ_B, used to make up the MPS representation of the ground-state wavefunctions for a translationally invariant periodic finite-size system, with s being the physical index, and α, β, γ denoting the inner indices. (ii) The pictorial representation of an MPS $|\psi\rangle$. (iii) The norm $\langle\psi|\psi\rangle$, which is the trace of the power $N/2$ of the transfer matrix E, with N being the system's size. Here, we have assumed that N is even. (iv) The $\chi^2 \times \chi^2$ transfer matrix E.

as three-index tensors: $\Gamma^{s_i}_{A\alpha\beta}$ and $\Gamma^{s_i}_{B\alpha\beta}$, as visualized in figure 1(i). For a quantum state $|\psi\rangle$ translationally invariant under two-site shifts, they are the building blocks to make up an MPS representation, a visualization of which is presented in figure 1(ii). One of the advantages for an MPS representation of a quantum state is that it is straightforward to compute physical quantities. For example, if one intends to compute the norm for the quantum state $|\psi\rangle$, all needed to be done is to contract the corresponding physical indices s_i for their MPS representations, as seen in figure 1(iii). Here, the basic building block is the so-called $\chi^2 \times \chi^2$ transfer matrix E, which is indicated in figure 1(iv). In passing, we point out that an MPS with the truncation dimension χ satisfies the area law, i.e., the entanglement across each bond is bounded by $\log \chi$. It is efficient to approximate ground states for a gapped local Hamiltonian.

The imaginary time evolution operator $\exp(-H\tau)$ in equation (1) is realized via many small steps, each of which is represented by $\exp(-H\delta\tau)$, with $\tau = M\delta\tau$. As observed by Vidal [6], $\exp(-H\delta\tau)$ is split into two kinds of gates U^{AB} and U^{BA}:

$$U^{AB} \equiv \bigotimes_m U^{2m,2m+1}, \qquad U^{BA} \equiv \bigotimes_m U^{2m-1,2m}, \tag{2}$$

with the two-site gate defined by

$$U^{i,i+1} \equiv \exp(-h^{[i,i+1]}\delta\tau), \qquad \delta\tau \ll 1. \tag{3}$$

We stress that this is a consequence of the Suzuki–Trotter decomposition [10]. A peculiar feature of such a decomposition is that all the two-site gates in U^{AB} and U^{BA} are commutative with each other.

Now the problem to implement the imaginary time evolution is reduced to how to update the MPS tensors Γ^{s}_{A}, λ_A, Γ^{s}_{B} and λ_B under the action of a two-site gate $U^{[i,i+1]}$. This can be done by adapting the strategy used in the iMPS algorithm [6]. Here, we need to complete two tasks: first, absorb the action of a two-site gate $U^{[i,i+1]}$ on an MPS, thus resulting in updated MPS tensors; second, develop an efficient way to compute the ground-state energy per site.

(i) *Updating of the MPS representation.* Due to the fact that all the two-site gates in U_{AB} and U_{BA} are commutative, an evolution $\exp(-H\delta\tau)$ over a small time step can be achieved by successively applying the two-site gates $\exp(-h^{[i,i+1]}\delta\tau)$ on the tensors $\Gamma^{s}_{A\alpha\beta}$, $\Gamma^{s}_{B\alpha\beta}$ and a singular value matrix λ_A, respectively. The translational invariance under two-site

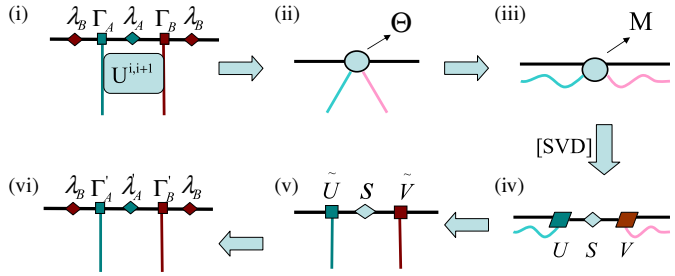

Figure 2. The procedure to update the MPS tensors Γ_A and Γ_B and the singular value matrix λ_A via absorbing the action of a two-site gate $U^{i,i+1}$. (i) The gate $U^{i,i+1} = \exp(-h^{i,i+1}\delta\tau)$ is applied onto the MPS. (ii) A single tensor Θ is formed by contracting the tensors Γ_A, λ_A, Γ_B and λ_B and the gate $U^{i,i+1}$. (iii) Reshape the tensor Θ into a matrix M. (iv) A singular value decomposition (SVD) is performed for the matrix M, followed by a truncation, with only the χ largest singular values retained in the updated singular matrix λ'_A. (v) Reshape the matrices U and V into the tensors $\tilde{U}$ and $\tilde{V}$. (vi) Recover the singular matrix λ_B, and update the tensors Γ_A and λ_A.

shifts makes it possible to focus on two consecutive sites i and $i+1$; once this is done, we simultaneously update all the tensors on the entire lattice. As one may see from figure 2, the updating procedure is formally identical to the infinite-size case, in which the tensors are updated by applying the two-site gate U^{AB}.[1] This consists of a few steps: first, the two-site gate $U^{i,i+1} = \exp(-h^{i,i+1}\delta\tau)$ is applied onto the MPS; second, a single tensor Θ is formed by contracting the tensors Γ_A, λ_A, Γ_B, and λ_B and the gate $U^{i,i+1}$; third, reshape the tensor Θ into a matrix M; fourth, a singular value decomposition (SVD) is performed for the matrix M, followed by a truncation, with only the χ largest singular values retained; fifth, reshape the matrices U and V into the tensors $\tilde{U}$ and $\tilde{V}$; finally, recover the singular value matrix λ_B, and update the tensors Γ_A and Γ_B.

(ii) *Computation of the ground-state energy per site.* Let us turn to the computation of the ground-state energy per site e_N. For a finite-size quantum lattice system with PBCs, the ground-state energy per site e_N takes the form

$$e_N = \frac{1}{N}\sum_{i=1}^{N}\frac{\langle\psi_g|h^{[i,i+1]}|\psi_g\rangle}{\langle\psi_g|\psi_g\rangle}. \tag{4}$$

Here, $|\psi_g\rangle$ is the ground-state wave-function. By taking advantage of the MPS representation, one finds that the expectation value $\langle\psi_g|h^{[i,i+1]}|\psi_g\rangle$ can only take two values, e_{AB} and e_{BA}, respectively, depending on the oddness and evenness of the index i (see figure 3). Therefore, we have $e_N = (e_{AB} + e_{BA})/2$. Since the computation of e_{AB} and e_{BA} is similar, with the only difference in the exchange: $\Gamma_A \leftrightarrow \Gamma_B$ and $\lambda_A \leftrightarrow \lambda_B$, it is enough to focus on the computation of e_{AB}. Denote E as the transfer matrix, $E = \sum_{s_i s_{i+1}} \left(\Gamma_A^{s_i}\lambda_A\Gamma_B^{s_{i+1}}\lambda_B\right) \otimes \left(\Gamma_A^{s_i *}\lambda_A\Gamma_B^{s_{i+1}*}\lambda_B\right)$. Then we have $e_{AB} = \mathrm{Tr}(E^{N/2-1}E')/\mathrm{Tr}(E^{N/2})$, with E' a matrix made of the tensors Γ_A, λ_A, Γ_B and λ_B: $E' = \sum_{s_i s_{i+1} s'_i s'_{i+1}} h^{[i,i+1]}_{s_i s_{i+1} s'_i s'_{i+1}} \left(\Gamma_A^{s_i}\lambda_A\Gamma_B^{s_{i+1}}\lambda_B\right) \otimes \left(\Gamma_A^{s'_i *}\lambda_A\Gamma_B^{s'_{i+1}*}\lambda_B\right)$. The key point is how to tackle the multiplication between two $\chi^2 \times \chi^2$ matrices to compute e_{AB}, since the cost of directly multiplying two $\chi^2 \times \chi^2$ matrices is $O(\chi^6)$. Even if one takes advantage of the tensor product structure of the matrix E, the cost of the matrix multiplication is still

[1] However, we emphasize that the singular value matrices λ_A and λ_B cannot be interpreted as the square root of the eigenvalues of the reduced density matrix for a subsystem on a half chain, in contrast with the infinite-size case.

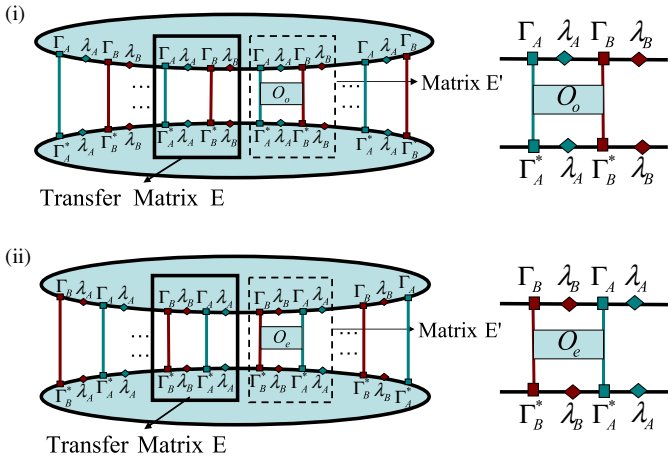

Figure 3. The expectation values e_{AB} and e_{BA} are needed to get the ground-state energy per site for a translationally invariant periodic lattice system in one spatial dimension, with $e_{AB} = \langle\psi_g|O_o|\psi_g\rangle/\langle\psi_g|\psi_g\rangle$ corresponding to an odd site i, and $e_{BA} = \langle\psi_g|O_e|\psi_g\rangle/\langle\psi_g|\psi_g\rangle$ to an even site i. For our specific Hamiltonian H, $O_o \equiv O_e \equiv h^{[i,i+1]}$. Therefore, the $\chi^2 \times \chi^2$ transfer matrix E takes two different forms: E_{AB} and E_{BA}. Similarly, for the matrix E', we have two different types: E'_{AB} and E'_{BA}. This implies that the ground-state energy per site is $e_N = (e_{AB} + e_{BA})/2$.

$O(\chi^5)$. However, note that, for a large-size quantum lattice system, an approximation can be done to efficiently compute e_{AB}, with the computational cost scaling as χ^3. Meanwhile, this does not affect the accuracy. First, perform a decomposition of the transfer matrix E:

$$E = TST^{-1} = \sum_{i=1}^{\chi^2} u_i s_i v_i. \tag{5}$$

Here, s_i is the ith largest eigenvalue of the transfer matrix E, with u_i and v_i being the corresponding left and right eigenvectors, respectively. When multiplying the E for m times, we get the matrix E^m. Then, for a large m, an approximation of the matrix E^m can be obtained by replacing the matrix E with the k largest eigenvalues and the corresponding eigenvectors. That is,

$$E^m = \sum_{i=1}^{\chi^2} u_i s_i^m v_i \simeq \sum_{i=1}^{k} u_i s_i^m v_i. \tag{6}$$

In other words, for a large size system, only a few largest eigenvalues and the corresponding eigenvectors of the transfer matrix E are needed to approximate $E^{N/2-1}$ and $E^{N/2}$. Moreover, the larger the system's size is, the smaller number k of the eigenvalues of the transfer matrix E one needs to retain within the same accuracy. With such an approximation in mind, and taking account of the tensor product structure of the matrix E', we see that the computational cost of the matrix multiplication between $E^{N/2-1}$ and the matrix E' scales as $O(k\chi^3)$. In addition, computing an eigenvalue and the corresponding (left and right) eigenvectors of the $\chi^2 \times \chi^2$ transfer matrix E costs $O(\chi^3)$.[2] Therefore, the computational cost of e_{AB} scales as $k\chi^3$.

[2] Actually, the left and right eigenvectors of the transfer matrix corresponding to the largest eigenvalues constitute the environment tensors.

Two remarks are in order. First, the update procedure described above is *not* optimal, in the sense that it does not produce the best approximate MPS representation for each imaginary time step during the imaginary time evolution. A consequence of this is that our update procedure is *only* useful to generate the system's ground-state wavefunctions, but *not* for real time evolution from a prescribed initial state, in contrast to the iMPS algorithm [6]. However, a less efficient update procedure is also available to remedy this drawback for translationally invariant finite-size periodic lattice systems, which is *optimal* in the above sense. The procedure is as follows. Form two MPS tensors $A^s \equiv \Gamma^s_A \lambda_A$ and $B^s \equiv \Gamma^s_B \lambda_B$,[3] and construct a transfer matrix $E_{AB} \equiv \sum_{s_i s_{i+1}} (A^{s_i} B^{s_{i+1}}) \otimes (A^{s_i} B^{s_{i+1}})$. In order to absorb a two-site gate, one needs to compute environment tensors, i.e., the left and right eigenvectors (corresponding to a few largest eigenvalues) of the transfer matrix E_{AB} for each two-site non-unitary gate. As such, the update problem is reduced to a two-site sweep procedure consisting of successively solving a set of linear equations [4]. However, this requires updating the environment tensors as we update the tensors A and B in the MPS representation for each two-site non-unitary gate.

Second, although the computational cost of both updating the MPS tensors $\Gamma^s_{A\alpha\beta}$ and $\Gamma^s_{B\alpha\beta}$ under the action of a two-site gate $U^{[i,i+1]}$ and the computation of the ground-state energy per site scales as χ^3, it is more time consuming to get the ground-state energy per site than updating. Therefore, in order to speed up the convergence, it is a good strategy to perform a certain number of updates, followed by the computation of the ground-state energy per site once. This is due to the fact that the number of eigenvectors of the transfer matrix needed to be retained increases with the evolution steps.

Example. We consider the quantum spin-1/2 Ising model in a transverse field on a finite-size lattice in one spatial dimension with PBCs. It is described by the Hamiltonian:

$$H = -\sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+1}^x + \lambda \sigma_i^z\right), \tag{7}$$

where σ_α^i ($\alpha = x, z$) are the Pauli spin-1/2 operators at lattice site i, and λ is the transverse magnetic field along the z direction. The model is critical when $\lambda = 1$ in the infinite-size (thermodynamic) limit, with the central charge $c = 1/2$.

Simulation results

First, we test the algorithm by computing the ground-state energy per site e_N for the quantum Ising model in a transverse field with the sizes from 10 to 100. Following the conformal field theory prediction, the ground-state energy per site e_N obeys the universal finite-size corrections: $e_N = e_\infty - \frac{\pi v c}{6N^2}$, where $c = 1/2$ is the central charge and $v = 2$ is the Fermi velocity for the critical quantum Ising model in a transverse field, and e_∞ is the ground-state energy per site in the thermodynamic limit. The least-square fit of the ground-state energy per site e_N, computed from the algorithm, with the system's size N ranging from 10 to 100, yields $e_\infty^{\text{fit}} = -1.273\,238$ and $c = 0.500\,36$, as plotted in figure 4.[4] The relative fitting error for the ground-state energy per site e_N is less than 2.5×10^{-6} (see the inset in figure 4). Here, we should mention that the third-order Suzuki–Trotter decomposition is used to find the best MPS approximation to the ground states during the imaginary time evolution.

[3] For such an update procedure, we only need to use the MPS tensors A and B, without the need to introduce the tensors $\Gamma_{A(B)}$ and $\lambda_{A(B)}$.

[4] Note that the ground-state energy per site e_N, evaluated from the algorithm for $N = 4800$, is 1.273 239 567 31. This is in agreement with the conformal field theory prediction with an error less than 2.0×10^{-10}.

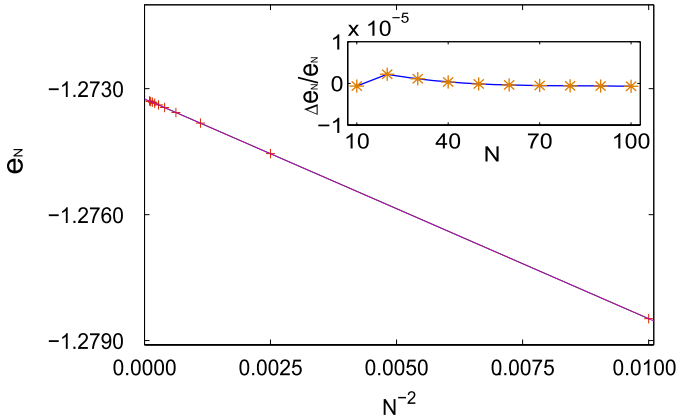

Figure 4. The scaling of the ground-state energy per site e_N with the size N for the critical quantum Ising model in a transverse field with PBCs (main). For sizes N from 10 to 100, the data are fitted to $e_N = e_\infty - \frac{\pi v c}{6N^2}$, with $v = 2$ being the Fermi velocity. The relative fitting errors $|e_N^{\rm fit} - e_N^{\rm algo}|/e_N^{\rm algo}$ are smaller than 2.5×10^{-6}, where $e_N^{\rm fit}$ is extracted from the fit and $e_N^{\rm algo}$ is computed from the algorithm for each N (inset).

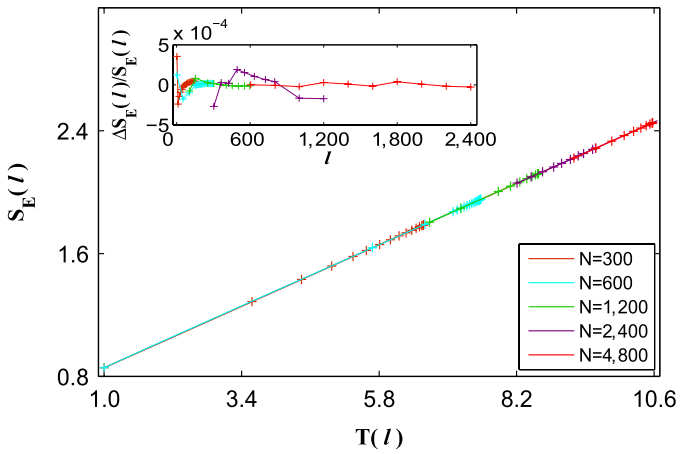

Figure 5. The scaling relation between the von Neumann entropy S_E and the block size $T(l) \equiv \log_2(N/\pi \sin(\pi l/N))$ for the critical quantum Ising model in a transverse field with PBCs (main). For sizes N from 300 to 4800, the data are fitted to $S_E(l) = \frac{c}{3} T(l) + a$. The relative fitting errors $|S_E^{\rm fit}(l) - S_E^{\rm algo}(l)|/S_E^{\rm algo}(l)$ are always smaller than 3.6×10^{-4}, where $S_E^{\rm fit}(l)$ is the value extracted from the fit and $S_E^{\rm algo}(l)$ is the value computed from the algorithm for each l (inset).

For larger sizes, we compute the entanglement entropy, i.e., the von Neumann entropy, for the critical quantum Ising model in a transverse field with the system's size ranging from 300 to 4800. For a system partitioned into two subsystems S_A and S_B, the von Neumann entropy is defined as $S_E \equiv -{\rm Tr}_A \rho_A \log_2 \rho_A = -\sum_i \lambda_i \log_2 \lambda_i$, where ρ_A is the reduced density matrix for the subsystem S_A, and λ_i is the ith eigenvalue of ρ_A. For a critical system, the conformal field theory predicts that the von Neumann entropy follows the universal logarithmic scaling with the subsystem size l: $S_E(l) = c/3 \log_2(N/\pi \sin(\pi l/N)) + a$, where a is a model-dependent constant [11–15]. In figure 5, we show the scaling relation between the von

Neumann entropy and $T(l) \equiv \log_2(N/\pi \sin(\pi l/N))$. The central charge $c_N^{\rm fit}$ and $a_N^{\rm fit}$ are fitted for different sizes. It yields that $c_{300}^{\rm fit} = 0.500\,36$, $a_{300}^{\rm fit} = 0.689\,56$; $c_{600}^{\rm fit} = 0.500\,32$, $a_{600}^{\rm fit} = 0.689\,39$; $c_{1,200}^{\rm fit} = 0.499\,57$, $a_{1,200}^{\rm fit} = 0.691\,59$; $c_{2,400}^{\rm fit} = 0.498\,96$, $a_{2,400}^{\rm fit} = 0.693\,09$; $c_{4,800}^{\rm fit} = 0.500\,14$, $a_{4,800}^{\rm fit} = 0.688\,12$. Note that the relative errors are less than 3.6×10^{-4} for the von Neumann entropy.

Conclusion

For quantum systems on a finite-size lattice in one spatial dimension, we have developed an efficient MPS algorithm to find a matrix product state representation of the ground-state wavefunctions, with the computational cost independent of the lattice size. Moreover, the scaling of the cost with the truncation dimension is comparable to the improved MPS algorithm [8]. The independence of the computational cost on the system's size enables us to simulate the quantum spin-1/2 Ising model in a transverse field on a finite-size lattice in one spatial dimension with PBCs, up to the size as large as 4800 for the truncation dimension 200.[5] Moreover, the algorithm we developed requires the storage of only two tensors A and B. That is, the total number of parameters to represent a quantum state in terms of an MPS is $O(d\chi^2)$, thus more states can be kept during the imaginary time evolution. In other words, larger χ can be taken to achieve higher precision, compared to the improved MPS algorithm.

Finally, we point out that similar ideas are applicable to develop an efficient PEPS algorithm to investigate quantum translationally invariant systems on a finite-size lattice in two spatial dimensions, with the computational cost independent of the system's size.

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[5] We have also checked the validity and efficiency of the algorithm for the Heisenberg chain up to 1200 with the truncation dimension $\chi = 100$, with a relative error less than 10^{-7}.

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