Infinite-size Density Matrix Renormalization Group with Parallel Hida’s Algorithm

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In this study, we report a parallel algorithm for the infinite-size density matrix renormalization group (iDMRG) that is applicable to one-dimensional (1D) quantum systems with \( \ell \)-site periods, where \( \ell \) is an even number. It combines Hida’s iDMRG applied to random 1D spin systems with a variant of McCulloch’s wavefunction prediction. This allows us to apply \( \ell/2 \) times of computational power to accelerate the investigation of multi-leg frustrated quantum systems in the thermodynamic limit, which is a challenging simulation. We performed benchmark calculations for a spin-1/2 Heisenberg model on a Kagome cylinder YC8 using the parallel iDMRG, and found that the proposed iDMRG was efficiently parallelized for shared memory and distributed memory systems, and provided such bulk physical quantities as total energy, bond strength on nearest neighbor spins, and spin-spin correlation functions and their correlation lengths without finite-size effects. Moreover, the variant of the wavefunction prediction sped up Lanczos methods in the parallel iDMRG by approximately three times.

1. Introduction

Quantum spin systems on low-dimensional lattices with geometrical frustrations, which are beyond the reach of quantum Monte Carlo simulations, are a fascinating subject of study in condensed matter physics because a variety of non-trivial quantum phases can emerge due to the coexistence of geometrical frustration and quantum fluctuation. The density matrix renormalization group (DMRG) proposed by White is a powerful tool to analyze low-energy states of such systems.1 In particular, the infinite-size DMRG (iDMRG) can directly tackle position-dependent Hamiltonians was proposed by Hida17) and has been extensively studied in condensed matter physics.2,3) The iDMRG has recently been applied as a useful detector for finding symmetry-protected topological phases in 1D systems, and this has enhanced its importance.4–7) Therefore, the sophistication of numerical algorithms for iDMRG also becomes important.

One of goals of iDMRG is to obtain a wavefunction represented by a translationally invariant matrix product state (MPS) with a unit cell. To achieve this, two algorithm are typically used to accelerate the iDMRG, the product wavefunction renormalization group (PWFRG)12–14) and McCulloch’s wavefunction prediction,15,16) when the translationally invariant MPS has a finite size. On the contrary, a generalization of the iDMRG for position-dependent Hamiltonians was proposed by Hida17) and applied to the analysis of 1D quantum random systems.18–20) It has been claimed17) that Hida’s iDMRG is useful for studying systems with large unit cells, and can be accelerated by wavefunction prediction methods.12) However, we still cannot implement it on multi-leg, typically more than 10 legs, ladder/cylinder systems, which have recently become the typical target of the DMRG.21)

In this article, we propose an extension of the iDMRG with a variant of McCulloch’s wavefunction prediction, which can be applied to quantum systems with large (\( \ell \)-site) unit cells. We show that our algorithm is efficiently parallelizable for both shared memory and distributed memory systems, and the wavefunction predictions reduces the number of Lanczos iterations to approximately a third of that without the predictions. Moreover, this method is compatible with the subtraction method21) and can easily obtain the total energy in the bulk limit under a fixed \( m \), the number of states maintained for block-spin variables. The numerical accuracy of the iDMRG can be considered by using the truncation error or discarded weight \( \epsilon \) as a function of \( m \),1) where the results of the iDMRG on multi-leg systems are strongly dependent on \( \epsilon \). The error \( \epsilon \) is not given uniquely in the MPS with multi-site unit cells, and we succeeded in finding an appropriate \( \epsilon \) for our parallel iDMRG that significantly suppresses higher-order terms of \( \epsilon \) in bulk energy with respect to \( \epsilon \). We can apply \( \ell/2 \) times computational power to challenging simulations, thus accelerating the examination of multi-leg frustrated quantum systems in the thermodynamic limit through our parallel algorithm. We applied them to the spin-1/2 Heisenberg model on a Kagome cylinder YC8,22) which can be mapped to 1D quantum systems with a 12-site unit cell.

The remainder of this article is organized as follows: In the next section, we recall the algorithm for Hida’s iDMRG in terms of the formalism of the matrix product. In Section 3, we introduce our proposed algorithm for parallel iDMRG. We test the performance of the iDMRG in Section 4, where we show the effectiveness of a variant of wavefunction predictions3) to reduce the number of Lanczos iterations in the parallel iDMRG, and introduce an appropriate value of \( \epsilon \) for extrapolations to estimate the bulk energy of the Kagome cylinder YC8. We also discuss the bond strength of nearest neighbor spins, and a spin-spin correlation function and its correlation length. We summarize our conclusions in the final section, where we state the relation between Hida’s iDMRG and the real-space parallel DMRG.23)

2. Hida’s iDMRG from the Perspective of Matrix Product Formalism

In this section, we review the algorithm of Hida’s iDMRG17) in terms of a matrix product formalism. This algorithm targets \( \ell \)-site systems represented by position-dependent Hamiltonians, where \( \ell \) is an even number. Using
the formalism of the matrix product operator (MPO),\textsuperscript{15} we can express a position-dependent Hamiltonian as

\[ h_{\sigma \sigma'} = L_{1}^{\sigma \sigma'} \left[ \prod_{i=2}^{\ell-1} W_{i}^{\sigma \sigma'} \right] R_{\ell}^{\sigma \sigma'}, \]  

(1)

where \( \sigma = (\sigma_1, \ldots, \sigma_\ell) \), and \( W_{i}^{\sigma \sigma'} \) is a lower-triangular matrix defined for the outer product of local states \( |\sigma_i\rangle \langle \sigma'_{i}| \) for the \( i \)th site. The left and right boundary vectors, \( L_{1}^{\sigma \sigma'} \) and \( R_{\ell}^{\sigma \sigma'} \), are identical to the last row and the first column of the matrix \( W_{i}^{\sigma \sigma'} \), respectively. Hereinafter, unless otherwise noted, we abbreviate the subscripts in \( \sigma \) for the sake of simplicity. Figure 1 shows a graphical representation of \( W_{i}^{\sigma \sigma'}, L_{i}^{\sigma \sigma'} \), and \( R_{i}^{\sigma \sigma'} \).

[Fig. 1. Graphical representations of \( W_{i}^{\sigma \sigma'}, L_{i}^{\sigma \sigma'} \), and \( R_{i}^{\sigma \sigma'} \), where vertical and horizontal lines emerging from rounded squares represent physical and auxiliary variables, respectively. Integer \( a_{i} \) represents the number of rows (columns) of \( W_{i}^{\sigma \sigma'} \) (\( R_{i}^{\sigma \sigma'} \)). The number of lines without indices of states represents the rank of the tensor, which means that \( W_{i}^{\sigma \sigma'} \) is a matrix, and \( L_{i}^{\sigma \sigma'} \) and \( R_{i}^{\sigma \sigma'} \) are row and column vectors, respectively.

Hida’s iDMRG proceeds as follows:

(1) Give \( W_{i}^{\sigma \sigma'} \) in Eq. (1) and prepare pairs of blocks, \( L_{2i-1}^{(0)} = L_{2i-1} \) and \( R_{2i}^{(0)} = R_{2i} \), where \( 1 \leq i \leq \ell/2 \). Then, set the number of iterations \( n = 1 \).

(2) Expand each pair of blocks as follows:

\[ L_{2i-1}^{(n)} \cdot W_{2i}^{\sigma \sigma'} \cdot R_{2i}^{(n)} = \sum_{\sigma \sigma'} L_{2i-1}^{(n-1)\sigma \sigma'} W_{2i}^{\sigma \sigma'} R_{2i}^{(n-1)\sigma \sigma'}, \]  

(2)

where \( 1 \leq i \leq \ell/2 - n \) and \( 1 \leq \alpha \leq \min[d_{\sigma_{i}} m] \), where \( d \) is the number of degrees of freedom of the local state [Fig. 2(a)].

(3) Solve an eigenvalue problem for each superblock Hamiltonian \( H_{2i}^{(n)} = \left( \sum_{\sigma \sigma'} L_{2i-1}^{(n-1)\sigma \sigma'} W_{2i}^{\sigma \sigma'} R_{2i}^{(n-1)\sigma \sigma'} \right) \) as \( H_{2i}^{(n)} \mathbf{v}_{i}^{(n)} \) by the iteration method—for example, Lanczos, Jacobi–Davidson, etc., where the ground state energy and a corresponding eigenvector are represented by \( \mathbf{v}_{i}^{(n)} \) and \( \mathbf{v}_{i}^{(n)} \) respectively [Fig. 2(b)]. An initial vector \( \mathbf{v}_{i}^{(0)} \) is required to start the iteration method, which is often given randomly.

(4) Apply singular value decomposition (SVD) to \( \mathbf{v}_{i}^{(n)} \) to \( \mathbf{u}_{i}^{(n)} \otimes \mathbf{v}_{i}^{(n)} \), where \( \mathbf{u}_{i}^{(n)} \) and \( \mathbf{v}_{i}^{(n)} \) with \( 1 \leq \gamma \leq \min[d_{\sigma_{i}} m] \) are unitary matrices. The diagonal matrix \( \Lambda_{i}^{(n)} = \text{diag}(\mathbf{u}_{i}^{(n)} \otimes \mathbf{v}_{i}^{(n)}) \) contains singular values, and is normalized as \( \sum_{\gamma} \Lambda_{i}^{(n)} \) is one, where \( \Lambda_{i}^{(n)} \leq \Lambda_{i}^{(n)} \leq \cdots, \) because \( \mathbf{v}_{i}^{(n)} \) is \( \ell/4 \) [Fig. 2(c)].

(5) If \( n = \ell/2 - 1 \), complete the calculations.

(6) Apply block-spin transformations, as depicted in Fig. 2(d), to each expanded block as follows:

\[ L_{2i-1}^{(n)} = \sum_{\sigma \sigma'} u_{L_{2i-1}, \sigma \sigma'}^{(n)} L_{2i-1, \sigma \sigma'}^{(n)} u_{R_{2i}, \sigma \sigma'}^{(n)} R_{2i, \sigma \sigma'}, \]  

(4)

where \( 1 \leq \beta \leq \min[d_{\sigma_{i}} m] \). The truncation of the number of degrees of freedom of the blocks can be introduced in this step.

(7) Set \( n + 1 \rightarrow n \), and go to Step 2.

Through these processes, we obtain a variational/exact ground state \( \Psi = |\psi_{\sigma}\rangle \) of the original Hamiltonian as follows:

\[ \psi_{\sigma} = \mathbf{u}_{1, \sigma_{1}}^{(1)} \mathbf{u}_{2, \sigma_{2}}^{(2)} \cdots \mathbf{u}_{(\ell/2 - 1), \sigma_{(\ell/2 - 1)}}^{(\ell/2 - 1)} \mathbf{v}_{(\ell/2 - 1), \sigma_{(\ell/2 - 1)}}^{(\ell/2 - 1)} \mathbf{v}_{(\ell/2 - 1), \sigma_{(\ell/2 - 1)}}^{(\ell/2 - 1)}, \]  

(6)

where \( \mathbf{u}_{i, \sigma_{i}} = [u_{(i-1), \sigma_{i} \sigma_{i+1}}] \) and \( \mathbf{v}_{i, \sigma_{i}} = [v_{(i-1), \sigma_{i} \sigma_{i+1}}] \) are matrices defined for the local state \( |\sigma_{i}\rangle \). In Eq. (6), \( \mathbf{u}_{i, \sigma_{i} \sigma_{i+1}} = [u_{(i-1), \sigma_{i} \sigma_{i+1}}] \) and \( \mathbf{v}_{i, \sigma_{i} \sigma_{i+1}} = [v_{(i-1), \sigma_{i} \sigma_{i+1}}] \) are column and row vectors defined for \( |\sigma_{i+1} \rangle \) and \( |\sigma_{i-1} \rangle \), respectively [Fig. 2(c)].

For the overall picture of Hida’s iDMRG, we show a schematic procedure for \( \ell = 10 \) in Fig. 3. Critical to this algorithm are preparing and growing to \( (\ell/2 - 1) \) pairs of blocks \( L_{2i-1}^{(n)} \) and \( R_{2i}^{(n)} \) to provide a proper environment in each position-dependent DMRG calculation. Because of this careful treatment, this infinite-size algorithm can be effectively applied to analyze the ground states of random quantum 1D systems.
the previous section to the following procedures, respectively:

Moreover, the process of expanding and block-spin transformations for each pair of $R_{2i}$ and $R_{2i+1}$ can be parallelized easily. One-to-one communications between nearest neighbor nodes are required for $R_{2i+1}$ in Eq. (3), and the cost per node is constant irrespective of $\ell$. This property is suitable for message passing interface (MPI) programming.

3. Parallel iDMRG Algorithm for Systems with $\ell$-site Period Structure

In this section, we describe a combination of Hida’s iDMRG\(^\text{(7)}\) with a variant of McCulloch’s wavefunction prediction.\(^\text{15, 16}\) A target Hamiltonian containing $\ell k$ ($k \gg 1$) sites can be represented by an MPO as

$$h_{0,\sigma} = \sum_{j=1}^{\ell} W_{\ell,\sigma}^j U_{\ell,\sigma}^j \cdots U_{1,\sigma}.\ (7)$$

We can construct a parallel iDMRG with wavefunction predictions by replacing Steps 2, 3, and 5 of Hida’s iDMRG in the previous section to the following procedures, respectively:

2. Expand each pair of blocks as

$$L_{2i-1,2i} = \sum_{j=1}^{\ell} W_{\ell,\sigma}^j U_{\ell,\sigma}^j \cdots U_{1,\sigma}.\ (8)$$

3. An initial vector $\tilde{\psi}_i^{(0)}$ is given by the wavefunction prediction methods\(^\text{15, 16}\) as follows:

$$\tilde{\psi}_i^{(0)} = \left\{ \begin{array}{ll} 0 & (\lambda_i^{(n-1)} = 0) \\
\sum_{\beta} u_{i,\beta}^{(n-1)} v_{i,\beta}^{(n-2)} & (\lambda_i^{(n-1)} > 0)
\end{array} \right.,\ (9)$$

Using $\tilde{\psi}_i^{(0)}$, solve an eigenvalue problem of the Hamiltonian of each superblock.

5. If mod[$n + 1, \ell$] = 0, estimate the ground state energy per site as $e_g^{(n)} = (e_1^{(n)} - e_1^{(n-1)})/2\ell$ to subtract boundary effects,\(^\text{21}\) where $e_1^{(n)}$ converges with respect to $n$, complete the iDMRG calculation.

As shown in Fig. 5, this parallel iDMRG for systems with $\ell$-site periods can be implemented by introducing slight modifications to the Hida’s iDMRG for $\ell + 2$-site stems.

Following the calculations, we obtain an MPS for the ground state of the original Hamiltonian using the wavefunction prediction method iteratively; namely,

$$\psi_{\phi_i^{(\ell)}} = \tilde{\psi}_i^{(1)} \cdot \tilde{\psi}_i^{(2)} \cdot \tilde{\psi}_i^{(3)} \cdot \cdots \tilde{\psi}_i^{(\ell)} \cdot \Lambda_i^{(n)}\ (10)$$

where $\tilde{\psi}_i^{(n)} = U_{i,\sigma}^{(n)}$ and $\tilde{\psi}_i^{(n)} = U_{i,\sigma}^{(n)}$.\ [Fig. 6].

4. Benchmark Calculations

To test the numerical performance of our parallel iDMRG, we estimate the total energy, bond strength on nearest neighbor spins, spin-spin correlation functions, and correlation effects,\(^\text{21}\)

$$\left(\lambda_{n+1,\beta}^{(n-2)}\right)^{-1} \delta_{g\alpha}^{(n)} = \beta_{(n-2)}^{(n)} \psi_1^{(n)} = \left\{ \begin{array}{ll} 0 & (\lambda_i^{(n-2)} = 0) \\
\sum_{\beta} u_{i,\beta}^{(n-1)} v_{i,\beta}^{(n-2)} & (\lambda_i^{(n-2)} > 0)
\end{array} \right..\ (11)$$

Fig. 4. Graphical representations of tensor contractions in Eq. (10).

Fig. 5. (Color online) Schematic procedure of the parallel iDMRG for a system with an eight-site period. The blue parts highlight the difference between the parallel iDMRG for eight-site period structures and Hida’s iDMRG 10-site period structures in Fig. 3.

Fig. 6. Graphical representations of a unit of the uniform part for matrix product structures in Eq. (11) for $L = 6$. 

4. Benchmark Calculations

To test the numerical performance of our parallel iDMRG, we estimate the total energy, bond strength on nearest neighbor spins, spin-spin correlation functions, and correlation
lengths of the spin-1/2 Heisenberg model on a Kagome cylinder YC8 of infinite length. The Hamiltonian is given as $H = \sum_{\langle i,j \rangle} s_i \cdot s_j$, where the sum runs over nearest neighbor sites. The shape of the cylinder YC8 is shown in the inset of Fig. 7. The Hamiltonian of the cylinder can be represented by an MPO with $\ell = 12$ as in Eq. (7). The ground state of this model has been widely studied using the finite-size DMRG.\textsuperscript{22,24,25} We show that the parallel iDMRG can estimate consistent physical quantities using only $m$ up to 2800. In this paper, we do not introduce block diagonalizations with respect to typical quantum numbers, for example, the total spin and its $z$ component. Of course, our parallel iDMRG is compatible with the use of Abelian and non-Abelian symmetries.\textsuperscript{26–28}

### 4.1 Parallel performance

We first checked the parallel performance of our iDMRG as shown in Fig. 7. The time for calculation was fitted by a linear function $t = ax + b$, where $x = (qr)^{-1}$, and $a$ and $b$ are the reciprocal of the parallel cores, and the parallel and serially processed parts of our calculations, respectively. Parallel efficiency $\rho$ is defined by $a/(a+b)$, and we obtained $p = 99.6\%$ in the calculations. This means that the parallelization worked well up to several hundred cores in this system.

![Fig. 7. (Color online) Parallel performance of our iDMRG while maintaining $m = 1000$ states. Computations were performed by using 32-core Fujitsu SPARC64 XIfx 1.973 GHz nodes. Each pair of numbers $(q, r)$ located nearby each plot, respectively, indicates the number of nodes and threads per node in the hybrid MPI/OpenMP parallel calculations. Calculation time $t$ is defined by the average time of parallel iDMRGs per iteration, where the number of iterations $n$ is up to 1200. In the inset, the paths of the matrix product of our MPO and MPS are denoted by bold red lines on the YC8, where blue broken lines separate the MPO into periods of the MPO.](image)

Note: The figure shows a graph with a linear fit to the data, indicating that the parallel performance was stable up to several hundred cores. The inset of the figure shows the matrix product of our MPO and MPS, with a blue broken line separating the MPO into periods.

### 4.2 Effect of wavefunction prediction

The wavefunction prediction methods in Step 3 of the parallel iDMRG are used to accelerate iteration methods for eigenvalue problems. The degree of acceleration for solving problems using prediction can be discussed using a fidelity error

$$
\epsilon_i^{(n)} = 1 - \frac{||\Psi_i^{(n)}|\Psi_i^{(n)}||}{||\Psi_i^{(n)}||}. \tag{12}
$$

As the Schmidt rank of $\Psi_i^{(n)}$ is up to $m$, the fidelity error $\epsilon_i^{(n)}$ must be not less than the best fidelity error $\epsilon_i^{(n)}$, given by

$$
\epsilon_i^{(n)} = 1 - \frac{\Phi_i^{(n)}|\Phi_i^{(n)}||}{||\Phi_i^{(n)}||} = 1 - \sqrt{\sum_{j=1}^{m} (\lambda_j^{(n)})^2}, \tag{13}
$$

where $\Phi_i^{(n)}$ is an approximated eigenvector defined by $\Phi_i^{(n)} = \sum_{m=1}^{n} \psi_{i,m}^{(n)} \phi_{i,m}^{(n)}$. This behavior can be confirmed in Fig. 8. Due to the prediction, the numerical error in eigenvalue $\epsilon_i^{(n)}$ with respect to the Lanczos iterations becomes less than $10^{-13}$ at around 40 iterations, a third of that without the prediction in $n \geq 72$ [Fig. 8 (a)]. In this region, as $\epsilon_i^{(n)}$ is comparable with $\epsilon_i^{(n)}$, as shown in Fig. 8 (b), we can find that the wavefunction prediction gives a nearly best-approximated eigenvector.

![Fig. 8. (Color online) (a) The number of iterations for the Lanczos method with/without wavefunction prediction (+/×) versus the number of iterations for the parallel iDMRG. (b) Fidelity errors $\epsilon_i^{(n)}$ in Eq. (12), $\epsilon_i^{(n)}$ in Eq. (13) and truncation error $\epsilon_i^{(n)}$ in Eq. (14) are denoted by black lines, block circles, and red lines with a circle, respectively.](image)

### 4.3 Ground state energy in the bulk limit under a fixed $m$

Taking the double limit, namely, the number of iterations of calculations $n \to \infty$ and the number of maintained states $m \to \infty$ of iDMRG, we can address the true physical quantity of the cylinder in the thermodynamic limit. In this and the next subsection, we show how to take the double limit properly when estimating the ground state energy per site of the cylinder.

We first focus on the convergence of energy per site with respect to $n$ under a fixed $m$. As shown in Step 6 of Section 3, we used the subtraction method\textsuperscript{13} for convergence acceleration to obtain energy per site in the limit $n \to \infty$. If this treatment is suited to accelerating convergence, $\epsilon_i^{(n)}$ can rapidly converge to the energy per site of $\lim_{n \to \infty} \epsilon_i^{(n)}/(2n+2)$. As shown in Fig. 9, energies per site had an almost linear dependence with respect to $1/L$ as depicted by the broken black line. We found that the energy per site $\lim_{n \to \infty} \epsilon_i^{(n)}/(2n+2)$ agreed with the convergent values of subtracted energies $\epsilon_i^{(n)} = -0.43796022(2)$ up to $n \geq 1200$, where the error was owing to a common
cancellation of significant digits due to subtraction analysis. Using this subtraction method, we thus avoided a careful extrapolation of the energy per site with respect to the length of the cylinder.

![Fig. 9](image-url) (Color online) The energies per site of finite systems $\varepsilon_i^{(n)}/(2n + 2)$ and the subtracted energies $\varepsilon_i^{(m)}$ of the Kagome cylinder YC8 as a function of the reciprocal of cylinder length $1/L = (2n + 2)/L$ with $m = 1000$.

4.4 Definition of truncation error in the parallel iDMRG

Following the above, to obtain the energy of the true ground state, we extrapolate $\varepsilon_i^{(n)}$ to the limit $m \to \infty$. In the parallel iDMRG, we define truncation error $\varepsilon = \max[|\varepsilon_i^{(n)}|]$ as

$$e_i^{(n)} = 1 - \sum_{\beta=1}^{m} (x_i^{(\beta)})^2 = (2 - e_i^{(n)})e_i^{(n)}, \quad (14)$$

and extrapolate $\varepsilon_i^{(n)}$ to the limit $\varepsilon \to 0$ because this truncation error is reduced by increasing $m$, and must be zero in the limit $m \to \infty$. The reasons for using $i = 1$ and the maximum of $|\varepsilon_i^{(n)}|$ are as follows:

i) The leftmost site of the cluster, represented by the renormalized Hamiltonian $H_i^{(n)}$, is fixed at the $t$-th site irrespective of $n$ as shown in Fig. 5, and the series of $\{H_i^{(n)}\}$ have a chance of achieving the same boundary condition as the original Hamiltonian in Eq. (7).

ii) Reflecting the $t$-site period structure of the system, the value $e_i^{(n)}$ has the periodicity with respect to $n$ shown in Fig. 8. We assume that the largest truncation error mainly determines the quality of the MPS.

If the value of $\varepsilon$ is appropriate, we find that the expectation values fit well with the quadratic form of $\varepsilon$. The extrapolated value agrees with the reported values where the error is the standard deviation of the fit. The extra $p$-site unit cells as in Eq. (11). Therefore, the correlation functions $\langle (S_{i+2n} \cdot S_{j+2n}) \rangle_{i,j}$ are equivalent to one another in our MPS, where the number of sites for the cylinder YC8 is shown in Fig. 11 (a). Moreover, if the numerical calculations are executed exactly, the four correlation functions $\{\langle S_{i+3k} \cdot S_{r+3k} \rangle \mid 0 \leq k \leq 3, s_{i+3k} = s_{i+3k} \}$ if mod$I + 3k - 1, 12 [ = \text{mod}(j - 1, 12) + 1]$ identically reflect translational symmetry along the direction of the circumference of the cylinder. However, in our parallel iDMRG, these identities do not hold because of the finite-$m$ effect. Figure 11 (b) shows the differences between bond strengths and the average value.

$$\Delta_i^m = \max_k \{\langle S_{i+3k} \cdot S_{r+3k} \rangle - \langle S_i \cdot S_r \rangle_{av}\}, \quad (15)$$

$$\Delta_i^m = \min_k \{\langle S_{i+3k} \cdot S_{r+3k} \rangle - \langle S_i \cdot S_r \rangle_{av}\}, \quad (16)$$

where $\langle S_i \cdot S_r \rangle_{av}$ is the arithmetic average of $\{\langle S_{i+3k} \cdot S_{r+3k} \rangle\}$. The difference $\Delta_i^m$ approaches zero in the limit $\varepsilon \to 0$, and we can confirm the extrapolated values $\lim_{m \to -\Delta_i^m}$ by ensuring that the quadratic fits for data for $\varepsilon < 6 \times 10^{-5}$ are less than $1.0 \times 10^{-5}$. This behavior is consistent with the fact that translational symmetry along the circumference must be recovered to the limit $m \to \infty$. Thus, we can focus on $\langle S_i \cdot S_r \rangle_{av}$ if we discuss the values to the limit $\varepsilon \to 0$.

As there are two types of translational symmetry, we estimate only a set of bond strengths $B = \{\langle S_i \cdot S_r \rangle_{av} \mid \beta, \beta', \beta'' \} = (1, 2), (2, 3), (3, 4), (2, 4), (3, 13)$ and (3, 14) to discuss the bond strength of nearest neighbor spins on the cylinder YC8. Figure 11 (c) shows $\langle S_i \cdot S_r \rangle_{av}$ in $B$ versus $\varepsilon$. The values extrapolated to the limit $\varepsilon \to 0$ can be grouped into two values $-0.2158(1)$ and $-0.2208(1)$. The configuration of the strength of nearest neighbor spins corresponding to this result are shown in 11(a). A similar configuration result was reported in a Kagome cylinder XC8.$^{23}$

4.5 Bond strength of nearest neighbor spins

To better understand the convergence behavior of the parallel iDMRG, we discuss the bond strength of the nearest neighbor spins as a typical local observable. The parallel iDMRG can predict and assume a spatially uniform MPS with 12-site unit cells as in Eq. (11). Therefore, the correlation functions $\{\langle S_{i+12n} \cdot S_{r+12n} \rangle_{i,j} \}$ are equivalent to one another in our MPS, where the number of sites for the cylinder YC8 is shown in Fig. 11 (a). Moreover, if the numerical calculations are executed exactly, the four correlation functions $\{\langle S_{i+3k} \cdot S_{r+3k} \rangle \mid 0 \leq k \leq 3, s_{i+3k} = s_{i+3k} \}$ if mod$I + 3k - 1, 12 [ = \text{mod}(j - 1, 12) + 1]$ identically reflect translational symmetry along the direction of the circumference of the cylinder. However, in our parallel iDMRG, these identities do not hold because of the finite-$m$ effect. Figure 11 (b) shows the differences between bond strengths and the average value.

$$\Delta_i^m = \max_k \{\langle S_{i+3k} \cdot S_{r+3k} \rangle - \langle S_i \cdot S_r \rangle_{av}\}, \quad (15)$$

$$\Delta_i^m = \min_k \{\langle S_{i+3k} \cdot S_{r+3k} \rangle - \langle S_i \cdot S_r \rangle_{av}\}, \quad (16)$$

where $\langle S_i \cdot S_r \rangle_{av}$ is the arithmetic average of $\{\langle S_{i+3k} \cdot S_{r+3k} \rangle\}$. The difference $\Delta_i^m$ approaches zero in the limit $\varepsilon \to 0$, and we can confirm the extrapolated values $\lim_{m \to -\Delta_i^m}$ by ensuring that the quadratic fits for data for $\varepsilon < 6 \times 10^{-5}$ are less than $1.0 \times 10^{-5}$. This behavior is consistent with the fact that translational symmetry along the circumference must be recovered to the limit $m \to \infty$. Thus, we can focus on $\langle S_i \cdot S_r \rangle_{av}$ if we discuss the values to the limit $\varepsilon \to 0$.

As there are two types of translational symmetry, we estimate only a set of bond strengths $B = \{\langle S_i \cdot S_r \rangle_{av} \mid \beta, \beta', \beta'' \} = (1, 2), (2, 3), (3, 4), (2, 4), (3, 13)$ and (3, 14) to discuss the bond strength of nearest neighbor spins on the cylinder YC8. Figure 11 (c) shows $\langle S_i \cdot S_r \rangle_{av}$ in $B$ versus $\varepsilon$. The values extrapolated to the limit $\varepsilon \to 0$ can be grouped into two values $-0.2158(1)$ and $-0.2208(1)$. The configuration of the strength of nearest neighbor spins corresponding to this result are shown in 11(a). A similar configuration result was reported in a Kagome cylinder XC8.$^{23}$

4.6 Spin-spin correlations and correlation length

As the final demonstration, we estimated the spin-spin correlation function $\langle S_i \cdot S_r \rangle$ along the cylinder YC8 and determined its correlation length. We set $i' = 2$, and swept $i = 2, 14, 35, 47...$ along the axis of the cylinder [see Fig. 11(a)]. The absolute values of the correlation function decayed exponentially with respect to distance $|r_i - r_i'|$ between sites $i$ and 2, as shown in Fig. 12. We fit the data for $|r_i - r_i'| > 5$ with an exponential function $\propto e^{-|r_i - r_i'|/\xi}$ and obtained the correlation length $\xi = 1.25(7)$, where the error was the standard deviation of the fit. The length of the spin-spin correlation with finite length $L$ up to 12 had already been evaluated by the non-Abelian DMRG.$^{25}$ We confirmed that the correlation length $L \to \infty$ obtained by our parallel iDMRG agreed with...
quantum systems and a variant of McCulloch’s wavefunction order of sites for the MPS of iDMRG. (b) The difference between Eqs. (15) and (16) depends on the truncation error, where the triangles and inverted triangles represent $\Delta_{12}$ and $\Delta_{23}$, respectively. (c) The average values of bond strength $\langle s_i \cdot s_i' \rangle_{\text{av}}$, where the broken lines are quadratic-fitted curves for data of $\varepsilon < 6 \times 10^{-5}$ in each pair of $(i,i')$.

the value extrapolated from the data for $L = 10$ and 12 with a linear fit.

5. Conclusions

In this study, we investigated a parallel iDMRG method applied to 1D quantum systems with a large unit cell. This parallel iDMRG is based on Hida’s iDMRG \(^{17}\) for 1D random quantum systems and a variant of McCulloch’s wavefunction prediction. \(^{15}\) The numerical efficiency of our parallel iDMRG was demonstrated for the spin-1/2 Heisenberg model on the Kagome cylinder YC8. Using truncation errors proposed in this work, we succeeded in obtaining correct observables, including the ground state energy per site, bond strength on nearest neighbor spins, and spin-spin correlation functions and their correlation lengths with the number of renormalized states $m$ up to 2800, approximately a third (sixth) of the number of renormalized states in Ref. 22 (Ref. 24). The wavefunction prediction sped up the Lanczos methods in the our parallel iDMRG by approximately three times. This effectively reduced the numerical cost of the iDMRG.

Several remarks are in order. First, Hida’s iDMRG is intimately related to the real-space parallel DMRG. \(^{23}\) Figure 13 shows the entire picture of the real-space parallel DMRG, starting from Hida’s iDMRG, where the diagrams, including overbraces and arrows, have the same meaning as shown in Fig. 3 and Fig. 5. The region shaded in green is identical to Hida’s iDMRG. In the procedures shown in Figure 13, the initial MPS is no longer needed to start parallel DMRG calculations.

Second, the physical background of wavefunction prediction in the iDMRG is understood well from the viewpoint of 2D classical vertex models. By applying the quantum-classical correspondence discussed in Ref. 16, we can easily find that our parallel iDMRG algorithm is also applicable to analyses of 2D classical vertex models with arbitrary periodic structures along only the horizontal (vertical) direction.

Third, our parallel iDMRG is compatible with other parallel algorithms, such as those used to parallelize over different terms in the Hamiltonian \(^{30}\) and the block diagonalization of a matrix with respect to the quantum number. \(^{31,32}\)

We expect that our parallel iDMRG and its extensions can be used in a variety of other quantum systems.

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Fig. 13. (Color online) Schematic procedure of real-space parallel DMRG, starting from the Hida’s iDMRG for random systems.\textsuperscript{17}

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