Corner transfer matrix renormalization group analysis of the two-dimensional dodecahedron model

Hiroshi Ueda\textsuperscript{1,2}, Kouichi Okunishi\textsuperscript{3}, Seiji Yunoki\textsuperscript{1,4,5}, and Tomotoshi Nishino\textsuperscript{6}
\textsuperscript{1}Computational Materials Science Research Team, RIKEN Center for Computational Science (R-CCS), Kobe 650-0047, Japan
\textsuperscript{2}JST, PRESTO, Kawaguchi, 332-0012, Japan
\textsuperscript{3}Department of Physics, Niigata University, Niigata 950-2181, Japan
\textsuperscript{4}Computational Condensed Matter Physics Laboratory, RIKEN Cluster for Pioneering Research (CPR), Wako, 351-0198, Japan
\textsuperscript{5}Computational Quantum Matter Research Team, RIKEN Center for Emergent Matter Science (CEMS), Wako, 351-0198, Japan
\textsuperscript{6}Department of Physics, Graduate School of Science, Kobe University, Kobe 657-8501, Japan
(Dated: April 21, 2020)

We investigate the phase transition of the dodecahedron model on the square lattice. The model is a discrete analogue of the classical Heisenberg model, which has continuous $O(3)$ symmetry. In order to treat the large on-site degree of freedom $q = 20$, we develop a massively parallelized numerical algorithm for the corner transfer matrix renormalization group method, incorporating EigenExa, the high-performance parallelized eigensolver. The scaling analysis with respect to the cutoff dimension reveals that there is a second-order phase transition at $T_c = 0.4403(4)$ with the critical exponents $\nu = 2.88(5)$ and $\beta = 0.22(1)$. The central charge of the system is estimated as $c = 1.98(4)$.

I. INTRODUCTION

Clarification of the role of local symmetry in phase transition is important for the fundamental understanding of critical phenomena. Two-dimensional (2D) polyhedron models have been attracting theoretical interests, in particular in their variety of phase transitions. The models are discrete analogues of the classical Heisenberg model, which has continuous $O(3)$ symmetry. The polyhedron models are described by the pairwise ferromagnetic interaction $h_{s\sigma} = -\mathbf{v}^{(s)} \cdot \mathbf{v}^{(\sigma)}$ between neighboring sites, where $\mathbf{v}^{(s)}$ with $1 \leq s \leq q$ represents the unit-vector spin directing one of the $q$ vertices of the polyhedron. Figure 1 shows a pictorial representation of the dodecahedron model, where $q = 20$.

The regular polyhedron models on the square lattice have been intensively studied, and it has been revealed that each of them has a characteristic phase transition. The tetrahedron model ($q = 4$) can be mapped to four-state Potts model [1], and it exhibits second-order transition with logarithmic correction [2, 3]. The octahedron model ($q = 6$) exhibits a weak first-order phase transition [4, 5], whose latent heat is close to that of the five-state Potts model [6]. The cube model ($q = 8$) can be trivially mapped to three-set of Ising models, in the same manner as the square model corresponds to two sets [7]. Recent numerical studies on the icosahedron model ($q = 12$) clarified that the model exhibits a continuous phase transition [4, 8, 9], whose universality class may not be explained by the minimal unitary models in the conformal field theories (CFTs). Curiously, for the dodecahedron model ($q = 20$), the possibility of an intermediate phase was suggested by Monte Carlo simulations in Refs. [10] and [11], whereas a solo second-order transition was suggested by other Monte Carlo simulations in Ref. [8]. In this article, we investigate the dodecahedron model to resolve the unclear situation. This is a small step to answer the question how can these discrete symmetry model approximate the classical Heisenberg model, which has no order in finite temperature [12].

An efficient numerical method for the investigation of 2D statistical models is the corner transfer matrix renormalization group (CTMRG) method [13–15], which is a typical tensor network method based on the Baxter’s corner-transfer matrix (CTM) formalism [16–18]. Even for the polyhedron models with large on-site degrees of freedom, the CTMRG method enables us to collect precise numerical data with the use of a realistic computational resource. The computational cost in the method is roughly proportional to $O(m^3q^4)$ [19], where $m$ is the cutoff dimension. It should be noted that the computational cost required for the dodecahedron model ($q = 20$) is about 20 times larger than that of the icosahedron model ($q = 12$). We therefore develop a massively parallelized algorithm for the CTMRG method by means of the message-passing interface (MPI) [20], combined with

![FIG. 1. (Color online) Dodecahedron model on the square lattice. Each unit vector Dodecahedron model spin points one of the 20 vertices of the dodecahedron](image-url)
the numerical diagonalization package EigenExa [21, 22], which is also MPI parallelized.

In the previous study on the icosahedron model \((q = 12)\) [9], the calculations were performed up to \(m = 500\). Critical exponents associated with magnetization \(M\) and correlation length \(\xi\) are estimated by means of the finite \(m\)-scaling analysis [24–27]. The central charge \(c\) is also extracted from the finite-\(m\) scaling applied to the entanglement entropy \(S_E\). It was suggested that the model exhibits the second-order transition with a nontrivial central charge \(c = 1.90(2)\). Thus, a focus in the study of the dodecahedron model \((q = 20)\) is the nature of the phase transition. If it is second-order, what is the value of \(c\)? In this article we perform the finite \(m\)-scaling analysis for the dodecahedron model up to \(m = 800\).

This article is organized as follows. In the next section, we briefly explain the outline of the CTMRG method applied to polyhedron models. In Section III we explain a parallelization technique implemented to the CTMRG method, when it is combined with EigenExa. We benchmark the numerical program on the K computer, which was operated in RIKEN R-CCS, through the test application on the icosahedron model. In Section IV, we show temperature dependencies of the spontaneous magnetization and the entanglement entropy. We perform the finite-\(m\) scaling analysis in association with the effective correlation length induced by the finite cutoff effect. The conclusions are summarized in Section V, and role of dodecahedral symmetry is discussed.

II. CORNER TRANSFER MATRIX

FORMALISM

We represent the regular polyhedron model on the square lattice in terms of the 2D tensor network, which is written as the contraction among 4-leg ‘vertex’ tensors. Let us consider \(q\)-state vector spins \(v^{(s)}\), \(v^{(\sigma)}\), \(v^{(s')}\), and \(v^{(\sigma')}\) of unit length, which are located at each corner of a unit square on the lattice. The local energy associated with these vector spins is written as the sum of pairwise ferromagnetic interactions

\[ E_{\sigma\sigma'}^{s,s'} = h_{s\sigma} + h_{s\sigma'} + h_{s'\sigma'} + h_{s'\sigma}, \]

where \(h_{s\sigma}\) denotes \(-\mathbf{v}^{(s)} \cdot \mathbf{v}^{(\sigma)}\) as we introduced in the previous section. We have chosen interaction parameter as unity. The corresponding Boltzmann weight

\[ W_{s,s'}^{\sigma,\sigma'} = \exp \left[ - \frac{E_{s,s'}^{\sigma,\sigma'}}{k_B T} \right] \]

can be regarded as the local 4-leg vertex tensor [28], where \(k_B\) is the Boltzmann constant, and \(T\) is the thermodynamic temperature. Throughout this article we choose the temperature scale where \(k_B = 1\). It should be noted that the vertex tensors are defined on every other unit squares on the lattice. The product over all the vertex tensors contained in the system represents the Boltzmann weight for the entire system under a specific spin configuration. Taking the configuration sum for this weight, we obtain the partition function \(Z\).

In the CTM formalism [16–18], finite-size system with square geometry is considered. The partition function \(Z\) is then represented as

\[ Z \equiv \text{Tr} C^4, \]

where \(C\) denotes the CTM corresponding to each quadrant of the finite-size system. We have used the fact that \(C\) is real symmetric, since \(W_{s,s'}^{\sigma,\sigma'}\) defined in Eq. (2) is invariant under rotation and spacial inversions of indices. In this article, we assume the ferromagnetic boundary condition in order to choose one of the \(q\) types of the ordered state, where all the vector spins at the system boundary point the specified direction \(s = 1\).

In the CTMRG method [13–15], we recursively update \(C\) and the half row-to-row or half column-to-column transfer matrices \(P\) toward their bulk fixed point. Thus the fixed boundary condition can be imposed just fixing the boundary spins in the initial transfer matrices. In order to prevent the exponential blow-up of the matrix dimension, these matrices are successively compressed by means of the truncated orthogonal transformations, which are obtained from the diagonalization of \(C\). In this renormalization group (RG) process, the number of ‘kept’ eigenvalues \(m\) plays the role of the cutoff dimension [29, 30].

After a sufficient number of iterations in the CTMRG calculation, we obtain the fixed point matrices \(C\) and \(P\), which are dependent on both \(T\) and \(m\). It is convenient to create the normalized density matrix

\[ \tilde{\rho} \equiv \frac{\hat{C}^4}{\text{Tr} C^4} \]

for the evaluation of one point functions. Spontaneous magnetization in the thermodynamic limit can be approximately obtained as

\[ M(T, m) = \text{Tr} \left[ \mathbf{v}^{(1)} \cdot \mathbf{v}^{(s)} \tilde{\rho} \right], \]

where \(\mathbf{v}^{(s)}\) is the vector spin located at the center of the system. The entanglement entropy

\[ S_E(T, m) = -\text{Tr} \tilde{\rho} \ln \tilde{\rho} \]

is essential for the determination of the central charge \(c\). In addition to these one point functions, we can calculate the effective correlation length \(\xi_c(T, m)\) by diagonalizing the renormalized row-to-row transfer matrices reconstructed from \(\tilde{P}\). These physical functions are dependent on \(m\), and therefore we have to take the extrapolation \(m \to \infty\) by any means, which we consider in section IV.

III. PARALLEL COMPUTATION

By the end of this section, we explain the massively parallelized numerical algorithm, which is implemented
to the CTMRG method. The incorporation of the parallelized diagonalization routine ‘EigenExa’ [21] is essential in this computational programming. To the readers who do not care about numerics, we recommend to skip this part and proceed to the next section.

Under the use of MPI [20], we distribute all the elements of large-scale matrices to n processes along “the 1 × 1 2D block-cyclic distribution” shown in Fig. 2, where n is the number of processes in MPI. We can then employ the PDGEMM routine contained in “the Basic Linear Algebra Communication Subprograms” (BLACS) package [31] for the matrix-matrix multiplication, and can also employ EigenExa package for the diagonalization of CTMs. Both of these linear numerical procedures support the block-cyclic distribution.

To achieve a high performance in matrix-matrix multiplications, we often encounter the situation where reordering of tensor indices is necessary. Suppose that we have a 4-leg tensor $A_{pqrs}$, and that we have to store the elements to another one $B_{prqs} := A_{pqrs}$, where := denotes substitution from the right to the left. This reordering can be quickly done even under the block-cycle distribution, as it is abbreviated in the numerical pseudocode Algorithm 1. For the legs p, q, r, and s, respectively, we denote their leg dimension by a, b, c, and d. In the algorithm, the 4-leg tensor $A_{pqrs}$ is represented as a matrix $A_{ij}$ with the use of combined indices $i := p + a(q - 1)$ and $j := r + c(s - 1)$. Such an ‘addressing’ is often used in the tensor-network frameworks. Note that the symbol MPIAlltoallv in line 2 denotes the address management — to arrange which tensor elements should be stored in which array address under which process — in MPI. This management enables the substitution of tensor elements in consistent with the block-cyclic distribution. In addition to the substitution $B_{prqs} := A_{pqrs}$, another type of reordering $B_{prq} := A_{prqs}$, between 3-leg tensors is often necessary. This process is represented by the pseudocode Algorithm 2.

Generally speaking, the number of processes n and the dimensions of tensor legs can vary during numerical calculations, therefore in principle the allocation managements should be performed dynamically. In the case of the CTMRG calculation, however, the maximum dimensions of all the matrices are always $qn$. Thus, we can make lists for the address management in advance to reduce communication complexity in MPI.

Combining the Algorithm 1, 2, and EigenExa, we can construct the CTMRG algorithm that is MPI parallelized. In Algorithm 3, we present the resulting pseudocode for a lattice model that is invariant under 90° rotation. The main loop contains four MPIAlltoall communications with the cost $O(m^2q^2)$, five matrix-matrix multiplications labeled by PDGEMM with the cost $O(m^3q^2 + m^2q^4)$, and the EigenExa with the cost $O(m^3q^4)$. Thus, in this algorithm, EigenExa could be the numerical bottle neck. Note that Algorithm 3 is executable on any standard computer if MPI is implemented, and if EigenExa is replaced by a matrix diagonalization package such as PDSYEV in ScalAPACK [32].

We check the performance of the Algorithm 3 by means of a benchmark computation applied to the icosahedron model ($q = 12$) at the critical temperature [9]. Figure 3(a) shows the elapsed time t for single iteration in the CTMRG method with respect to n, the number of nodes used, up to n = 16,380 (∼ 130 × 126). All the calculations were performed on the K computer (CPU:...
Algorithm 3 Main part of the CTMRG calculation for a vertex model with the fixed boundary condition

Require:
Input: positive integer $L, q,$ and $m$; real $T$ and $\epsilon$

2. $\sum_{q=0}^{m} q^{2}$.
3. $\sum_{q=0}^{m} q^{2}$.
4. $\sum_{q=0}^{m} q^{2}$.
5. $\sum_{q=0}^{m} q^{2}$.

Ensure:
Output: real $S_{E}$

1: function SYMMETRIC-CTMRG($L, q, m, T, \epsilon$)
2: $k := 1$; $S := 0$ \> initialization
3: $P = \{p_{\alpha \beta}\}$; $P_{\alpha \beta} := \begin{cases} 1 & \alpha = \beta = 1 \\ 0 & \text{otherwise} \end{cases}$ \> initialization.
4: $\Omega = \{\omega_{\beta}\}$; $\omega_{\beta} := \begin{cases} 1 & \beta = 1 \\ 0 & \text{otherwise} \end{cases}$ \> initialization.
5: $U = \{u_{\beta\beta}\}$ := 0 \> initialization.
6: $W = \{w_{ij}\}$; $w_{i+q(s-1), j+q(s'-1)} := W_{s'\beta, s'}$ \> local Boltzmann weight in Eq. (2)
7: while $k \leq L$ \& $c \geq \epsilon$ do \> CTMRG iteration
8: $P' := \{\omega_{\beta}P_{\alpha \beta}\}$ \> Using PDGEMM
9: $C := \text{Sub-CTMRG}(P, P', W)$ \> Sub-CTMRG
10: $(\{u_{\gamma\gamma}\}, \{w_{ij}\}) := \text{EigenExa}(\{c_{\gamma\gamma}\})$
11: with $1 \leq \gamma \leq \min(q^{2}, mq)$ \> diagonalization
12: $U' := P^{\text{-INDEX}}(\{u_{\beta\beta}\}, m, q, m)$ \> Using PDGEMM
13: $X := \text{Sub-CTMRG}(P, U', W)$ \> Sub-CTMRG
14: $P := P/\max_{\alpha \beta}P_{\alpha \beta}$ \> normalization
15: $\Omega := \Omega/\sqrt{\sum_{\beta} \omega_{\beta}^2}$ \> normalization
16: $S_{E} := -\sum_{\beta} \omega_{\beta} \ln \omega_{\beta}^2$ \> equivalent to Eq. (6)
17: $c := |1 - S_{E}/S|$
18: $S := S_{E}$
19: $k := k + 1$
20: end while
21: return $S_{E}$
22: end function

23: function Sub-CTMRG($P, P', W$)
24: $X_{1} := P^{\text{INDEX}}P'$ \> Using PDGEMM
25: $X_{2} := P^{\text{-INDEX}}(X_{1}, m, q, m, q)$ \> Using PDGEMM
26: $X_{3} := X_{2}W$ \> using the $1 \times 1$ 2D block-cyclic distribution. Matrices $P'$, $U'$, $X_{1}$, $X_{2}$, and $X_{3}$ are working arrays. The 2D arrays $C$ and $X$ can share the common physical memory in this algorithm.
27: $X_{1} := P^{\text{-INDEX}}(X_{3}, m, q, m, q)$ \> using the $1 \times 1$ 2D block-cyclic distribution. Matrices $P'$, $U'$, $X_{2}$, and $X_{3}$ are working arrays. The 2D arrays $C$ and $X$ can share the common physical memory in this algorithm.
28: return $X_{1}$
29: end function

We examine a scaling hypothesis given by

$$t = N^3 n^{-1} F(nN^{-K}) \quad (7)$$

in order to capture the relation among $t$, $N$, and $n$. The scaling function $F(y)$ has the asymptotic forms $F(y) \sim y^{3/K}$ for $y \gg 1$, namely $t \sim n^{-1+3/K}$, and $F(y) \sim const.$ for $y \rightarrow 0$. Under the ideal MPI parallelization, the exponent $K$ could be three, but it is empirically less than that in practical computations. For the estimation of $K$, we invoke the benchmark data in EigenExa with $N = 1 \times 10^{4}$, $5 \times 10^{4}$, and $1.3 \times 10^{5}$, which are available on the web page of EigenExa [22]. Performing the polynomial fitting to the scaling form in Eq. (7), we obtain $K = 1.66$. Assuming that the data shown in Fig. 3(a) shares the same exponent, we show the scaling plot for all the bench-mark data in Fig. 3(b). The plotted points almost collapse on a certain scaling curve, and the result supports the fact that the diagonalization of CTMs by EigenExa is certainly the numerical bottleneck.

FIG. 3. (Color online) (a) Elapsed time (sec.) per single iteration in the parallelized CTMRG algorithm performed by means of K computer, when the method is applied to the icosahedron model. [9]. The horizontal axis denotes the number of nodes $N$. The maximum matrix dimension $N = mq$ is shown by numbers beside the legends. (b) Scaling plot for computational times required for EigenExa and for the time shown in Fig. 3(a).

If the maximum matrix dimension $N = mq$ is much larger than $n$, the elapsed time decreases with respect to $n$, implying that the parallelization properly works. For $n \gg N/10$, however, the parallelization efficiency saturates, where the MPI communication time among the nodes becomes non-negligible.
IV. SCALING ANALYSIS

We performed the CTMRG calculation for the dodecahedron model, assuming the ferromagnetic boundary conditions. We choose the cutoff dimensions $m = 500$, 600, 700, and 800 [23] for all the numerical data analyses shown in this section. Figure 4 shows the temperature dependence of the spontaneous magnetization $M(T, m)$. The overall behavior of the magnetization, which exhibits a shoulder-like structure in the region $0.45 \leq T \leq 0.5$, is very similar to $M(T, m)$ observed in the icosahedron model [9].

We perform the finite-$m$ scaling analysis [24–27], in order to check whether the transition is second-order or not. At the fixed point — the large system size limit — of the CTMRG method, the presence of finite cutoff dimension $m$ modifies the intrinsic correlation length $\xi(T)$ to an effective one $\xi_e(T, m)$. At the critical temperature $T = T_c$, the behavior $\xi_e(T_c, m) \sim m^\kappa$ is expected, where $\kappa$ is a particular exponent [24–26]. Meanwhile, the intrinsic correlation length $\xi(T)$ away from the critical point obeys $\xi(T) \sim |T - T_c|^\nu$, where $\nu$ is the exponent characterizing the divergence of the correlation length. Taking account of these relations, we can assume the finite-$m$ scaling form

$$\xi_e(T, m) \sim m^\kappa f \left( (T - T_c)m^{\kappa/\nu} \right), \quad (8)$$

where the scaling function behaves as $f(y) \sim |y|^{-\nu}$ for $y \gg 1$ and $f(y) \sim \text{const.}$ for $y \to 0$. We can also assume the finite-$m$ scaling form

$$M(T, m) \sim m^{\kappa\beta/\nu} g \left( (T - T_c)m^{\kappa/\nu} \right) \quad (9)$$

for the spontaneous magnetization, where $\beta$ denotes the critical exponent for the magnetization, and $g$ is a scaling function. It should be noted that Eqs. (8) and (9) are basically equivalent to the conventional finite-size scalings if we substitute the system size $\ell$ to $\xi_e(T_c, m) \sim m^\kappa$. For the bipartite entanglement entropy, the finite-size scaling form $S_{E}(T_c, \ell) \sim \frac{1}{\ell} \log \ell + \text{const.}$ suggests that the effective scaling dimension for $e^{S_E(T_c, m)}$ can be expressed as $c/6$ [33, 34]. Thus, we can assume the finite-$m$ scaling form

$$e^{S_E(T_c, m)} \sim m^{c\kappa/6} h \left( (T - T_c)m^{\kappa/\nu} \right) \quad (10)$$

for the entanglement entropy, where the scaling function behaves as $h(y) \sim |y|^{-\nu}$ for $y \gg 1$ and $h(y) \sim \text{const.}$ for $y \to 0$.

We perform the Bayesian scaling analysis proposed in Ref. [35] for the estimation of scaling parameters in Eqs. (8), (9), and (10). We empirically find that the analysis on $\xi_e(T, m)$ is more stable than that for $M(T, m)$ and $e^{S_E(T_c, m)}$. From the calculated $\xi_e(T_c, m)$ in the temperature range $0.35 \leq T \leq 0.56$, the values $T_c \approx 0.4403(4)$, $\nu \approx 2.88(5)$, and $\kappa \approx 0.844(4)$ are extracted. Figure 5(a) shows the corresponding scaling plots for $\xi_e(T, m)$, where the data well collapse to a scaling function, which exhibit an intermediate plateau, as it was observed in the icosahedron model [9].

Using the obtained $T_c$, $\nu$, and $\kappa$, we can further estimate $\beta = 0.22(1)$ by means of the Bayesian analysis applied to $M(T, m)$ and $e^{S_E(T_c, m)}$. From the calculated $\xi_e(T_c, m)$ in the temperature range $0.35 \leq T \leq 0.56$, the values $T_c \approx 0.4403(4)$, $\nu \approx 2.88(5)$, and $\kappa \approx 0.844(4)$ are extracted. Figure 5(a) shows the corresponding scaling plots for $\xi_e(T, m)$, where the data well collapse to a scaling function, which exhibit an intermediate plateau, as it was observed in the icosahedron model [9].

It should be noted that for a 2D classical system at criticality, the central charge $c$ and $\kappa$ can be related with each other through the nontrivial relation

$$c \kappa/6 = \frac{1}{1 + \sqrt{12/c}}^{-1}, \quad (11)$$

which was originally derived from the matrix-product-state description of 1D critical quantum systems [27]. The relation is satisfied within the error bars when the above estimations $c = 1.98$ and $\kappa = 0.844$ are substituted. The fact provides a complementary check to the present finite-$m$ scaling analysis performed to the numerically calculated results. Since the estimated values of the exponents in the dodecahedron model are different from those in the icosahedron model, phase transitions of these two models belong to different universality classes.

V. SUMMARY AND DISCUSSION

We have investigated the phase transition and critical properties of the dodecahedron model on the square lattice, where the vector spin has twenty degrees of freedom ($q = 20$). In order to deal with the large on-site degree of freedom, we developed the massively parallelized CTMRG algorithm cooperating with the
FIG. 5. (Color online) Scaling plots for (a) effective correlation length \( \xi_e(T, m) \), (b) magnetization \( M(T, m) \), and (c) the exponential of the entanglement entropy \( e^{S_E(T, m)} \).

EigenExa [21, 22]. Spontaneous magnetization \( M(T, m) \), effective correlation length \( \xi_e(T, m) \), and entanglement entropy \( S_E(T, m) \) are calculated for the cutoff dimensions \( m = 500, 600, 700, \) and \( 800 \). The finite-\( m \) scaling analyses [9, 24–27] around the transition temperature revealed that the model undergoes a solo second-order phase transition at \( T_c = 0.4403(4) \), which is consistent with the Monte Carlo simulations in Ref. [8]. We also estimated the scaling exponents \( \nu = 2.88(5) \), \( \beta = 0.22(1) \), and the central charge \( c = 1.98(4) \).

Let us summarize the critical temperatures and central charges for the series of regular polyhedron models in Fig. 6. The transition temperature monotonically decreases with respect to the number of on-site degree of freedom \( q \). The behavior in \( T_c \) is consistent with the fact that it converges to zero in the large-\( q \) limit, which is the classical Heisenberg model [12]. Note that the octahedron model \((q = 8)\) is known to exhibit a weak first-order phase transition. Meanwhile, the central charge monotonically increases with \( q \). The exact value \( c = 1 \) is known for the tetrahedron model \((q = 4)\), which corresponds to four-state Potts model. Also for the cubic model \((q = 6)\), which is nothing but three set of Ising models, the value \( c = 3/2 \) is known.

So far, we have no theoretical explanation for the central charges \( c = 1.90(2) \) and \( c = 1.98(4) \), respectively, for the icosahedron model and dodecahedron model. How can we explain the universality classes of the phase transitions, and can interpret the intermediate shoulder structures in the scaling functions? In these two models, there are several ways of introducing anisotropy to the vector spins, according to the subgroup structure of the polyhedral symmetry [36]. A preliminary numerical calculation suggest that introduction of XY anisotropy to these models induce KT transitions. A more promising deformation is the introduction of the cubic anisotropy. If the phase transition splits into two different ones subject to different subgroup symmetries, the value of central charge in each transition would explain the value of \( c \) obtained in this study. Complementary, an effective field theoretical treatment within the regular polyhedron symmetry is also a non-trivial future problem.

If we consider polyhedron models in general, in addition to the regular ones, semi-regular (or truncated) polyhedron model would be important candidates for the future study of attacking the large-\( q \) limit. The pioneering work by Krčmár, et al shows that truncated tetrahedron model exhibit two phase transitions [5]. If we introduce the truncation scheme to the current study, we have to treat the truncated icosahedron, which has 60 on-site degrees of freedom. In a couple of years realistic computation will be possible for this system. At present, rhombic icosahedron model \((q = 24)\) can be the next target of the
analysis in near future.

ACKNOWLEDGMENT

H.U. thanks Y. Hirota and T. Imamura for helpful comments on the EigenExa and S. Morita for discussions of the MPI parallelization. The work was partially supported by KAKENHI No. 26400387, 17H02926, 17H02931, and 17K14359, and by JST PRESTO No. JP-MJPR1911, and by MEXT as “Challenging Research on Post-K computer” (Challenge of Basic Science: Exploring the Extremes through Multi-Physics Multi-Scale Simulations). This research used computational resources of the K computer provided by the RIKEN R-CCS through the HPCI System Research project (Project ID:hp160262) and of the HOKUSAI-Great Wave supercomputing system at RIKEN.

[1] F.Y. Wu, Rev. Mod. Phys. 54, 235 (1982).
[2] M. Nauenberg and D.J. Scalapino, Phys. Rev. Lett. 44, 837 (1980).
[3] J.L. Cardy, N. Nauenberg, and D.J. Scalapino, Phys. Rev B 22, 2560 (1980).
[4] A. Patrasciou and E. Seiler, Phys. Rev. D 64, 065006 (2001).
[5] R. Krňmar, A. Gendiar, and T. Nishino, Phys. Rev. E 94, 022134 (2016).
[6] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 67, 1492 (1998).
[7] D.D. Betts, Can. J. Phys. 42, 1564 (1964).
[8] T. Surungan and Y. Okabe, in Proceedings of 3rd JOGJA International Conference on Physics (2012); arXiv:1709.03720.
[9] H. Ueda, K. Okunishi, R. Krňmar, A. Gendiar, S. Yunoki and T. Nishino, Phys. Rev. E 96, 062112 (2017).
[10] A. Patrasciou, J.-L. Richard, and E. Seiler, Phys. Lett. B 241, 229 (1990).
[11] A. Patrasciou, J.-L. Richard, and E. Seiler, Phys. Lett. B 254, 173 (1991).
[12] N.D. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966).
[13] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 65, 891 (1996).
[14] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 66, 3040 (1997).
[15] R. Orus and G. Vidal, Phys. Rev. B 80, 094403 (2009).
[16] R.J. Baxter, J. Math. Phys. 9, 650 (1968).
[17] R.J. Baxter, J. Math. Phys. 19, 461 (1978).
[18] R.J. Baxter, Exactly Solved Models in Statistical Mechanics (Academic Press, London, 1982).
[19] In general, a larger cutoff dimension $m$ is also required for a CTMRG calculation with a large $q$ model.
[20] Message Passing Interface Forum. MPI: A Message-Passing Interface Standard. International Journal of Supercomputer Applications and High Performance Computing, 8(3-4), (1994); MPI Forum, http://www.mpi-forum.org/.
[21] T. Sakurai, Y. Futamuro, A. Imakura, and T. Imamura, Scalable Eigen-Analysis Engine for Large-Scale Eigenvalue Problems In: Sato, M. (ed.) Advanced Software Technologies for Post-Peta Scale Computing, pp. 37-57 (Springer, Singapore, 2019).
[22] EigenExa, https://www.r-ccs.riken.jp/labs/lpmctrt/en/projects/eigenexa.
[23] We requested computational time around a day with 24×24 nodes on the K computer, where each node has a process.
[24] T. Nishino, K. Okunishi, and M. Kikuchi, Phys. Lett. A 213, 69 (1996).
[25] M. Andersson, M. Boman, and S. Östlund, Phys. Rev. B 59, 10493 (1999).
[26] L. Tagliacozzo, T.R. de Oliveira, S. Iblisdir, and J.I. Latorre, Phys. Rev. B 78, 024410 (2008).
[27] F. Pollmann, S. Mukerjee, A.M. Turner, and J.E. Moore, Phys. Rev. Lett. 102, 255701 (2009).
[28] The term ‘vertex’ used here corresponds to a square on the diagonal square lattice, not to a vertex of the polyhedron.
[29] S.R. White, Phys. Rev. Lett. 69, 2863 (1992).
[30] S.R. White, Phys. Rev. B 48, 10345 (1993).
[31] J. Dongarra and R.C. Whaley, A user’s guide to the BLACS v1.1, Computer Science Dept. Technical Report CS-95-281, (University of Tennessee, Knoxville, 1995). (Also LAPACK Working Note #94).
[32] L.S. Blackford, J. Choi, A. Cleary, E. D’Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, R.C. Whaley, ScalA-PACK Users’ Guide (Society for Industrial and Applied Mathematics, Philadelphia, 1997).
[33] G. Vidal, J.I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[34] P. Calabrese and J. Cardy, J. Stat. Mech., P06002 (2004).
[35] K. Harada, Phys. Rev. E 84, 056704 (2011).
[36] L.L. Foster, Mathematics Magazine, 63, 106 (1990).