Phase Transition of the four-dimensional Cross-Polytope Model

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Thermodynamic properties of the four-dimensional cross-polytope model, the 16-cell model, which is an example of higher dimensional generalizations of the octahedron model, are studied on the square lattice. By means of the corner transfer matrix renormalization group (CTMRG) method, presence of the first-order phase transition is confirmed. The latent heat is estimated to be \( L_4 = 0.3172 \), which is larger than that of the octahedron model \( L_3 = 0.0516 \). The result suggests that the latent heat increases with the internal dimension \( n \) when the higher-dimensional series of the cross-polytope models is considered.

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I. INTRODUCTION

There is a variety of spin models that contain vectors of unit length on regular lattices as site degrees of freedom. Typical examples are the \( n \)-vector models, which have the \( O(n) \) symmetry \[1\]. When the internal space dimension \( n \) is equal to or larger than 2, the \( O(n) \) symmetry is continuous. Thus the \( n \)-vector models do not exhibit any fixed order in finite temperature when \( n \geq 2 \) if the models are defined on one of the two-dimensional regular lattices, as it was proved by Mermin and Wagner \[2\]. The two-vector model is known as the classical XY model, which allows the presence of Berezinskii-Kosterlitz-Thouless (BKT) transition \[3\] on two-dimensional lattices. An ordered state can appear when discrete nature or perturbation is introduced to the \( O(n) \) symmetry. The two-dimensional ferromagnetic \( q \)-state clock models, which are the discrete analogues of the two-vector model, exhibit a fixed ordering when temperature is sufficiently low.

Discrete analogues of the three-vector model, which is the classical Heisenberg model, exhibit characteristic phase transitions on the two-dimensional lattices, and their thermodynamic properties depend on the type of the spin discretization. The polyhedron models are typical examples, where the site degrees of freedom are represented by the unit vectors pointing to all vertices of a regular polyhedron. For instance, the tetrahedron model, which can be mapped to the four-state Potts model, exhibits a second-order phase transition with logarithmic corrections \[3\]. The octahedron model, which has six states, exhibits a weak first-order phase transition \[7\]. The cubic model with eight states is equivalent to the four-state Potts model, which can be mapped onto the \( q \)-state Potts models \[6\], which exhibit the first-order phase transition for \( q \geq 5 \). The second family consists of hyper-cubic models, and they include the four-state clock model \( (n = 2) \), the cube model \( (n = 3) \), and the 8-cell model \( (n = 4) \). The site degrees of freedom are equal to \( 2^n \), and it is straightforward to show that those models are equivalent to a set of \( n \) independent Ising models. Thus, within this family, the phase transitions always remain of the second-order type. Finally, the third family consists of the cross-polytope models, which include the octahedron model \( (n = 3) \) and its higher-dimensional generalizations. In this article we mostly focus on the four-dimensional case \( (n = 4) \), which corresponds to the 16-cell model, and analyze its phase transition. The free energy, internal energy, and spontaneous magnetization are calculated by the CTMRG method. We observed the first-order phase transition, where the latent heat is obtained as \( L_4 = 0.3172 \). Additionally, we also re-examined the octahedron model, and re-estimated its latent heat to obtain \( L_3 = 0.0516 \). The calculated results suggest that \( L_n \) is an increasing function of the internal dimension \( n \).

The structure of this article is as follows. In the next section, we introduce the cross-polytope models. Numerical results by the CTMRG method are shown in Sec. III. Conclusions are summarized in Sec. IV. We also discuss the remaining studies for various discrete \( O(n) \) models.

II. CROSS-POLYTOPE MODELS

Let us now introduce the discrete analogues of the \( n \)-vector models that belong to the cross-polytope family.
Suppose that there is a vector of the unit length $S_i$ on each lattice point of the square lattice. The index $i$ specifies the location of the site on the square lattice. The vector can point to the vertices of the cross-polytope. For example, if $n = 3$, a vector $S_i$ of the octahedron model can be one of the six vectors
\[(\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1).\] (1)

If $n = 4$, the site vector $S_i$ of the 16-cell model can be any one of the eight vectors
\[(\pm 1, 0, 0, 0), (0, \pm 1, 0, 0), (0, 0, \pm 1, 0), (0, 0, 0, \pm 1).\] (2)

In general, $S_i$ is an $n$-dimensional vector where only one component is either 1 or $-1$, whereas all other components are 0. Thus, there are $2n$ site degrees of freedom in total.

In the following, we consider the model whose Hamiltonian is expressed as
\[H = -J \sum_{\langle i,j \rangle} S_i \cdot S_j,\] (3)

where $\langle i,j \rangle$ represents the neighboring pairs on the square lattice. The inner product $S_i \cdot S_j$ can result in 1, 0, or $-1$. For simplicity, we set the ferromagnetic coupling $J = 1$ throughout this article.

Thermodynamic properties of the system are obtained through the partition function formally written as
\[Z = \text{Tr} \, e^{-\beta H},\] (4)

which is the function of $\beta = 1/k_B T$, where $T$ is the temperature and $k_B$ represents the Boltzmann constant. For simplicity, we set $k_B = 1$ in the following. We have expressed the configuration sum for all the vectors on the lattice using the trace notation. For the convenience in the numerical calculations, we express the system as the interaction round a face (IRF) model, where each IRF weight is represented by the Boltzmann factor
\[W(S_i, S_j, S_k, S_\ell) = \exp \left[ \frac{\beta J}{2} (S_i \cdot S_j + S_j \cdot S_k + S_k \cdot S_\ell + S_\ell \cdot S_i) \right],\] (5)

where the vectors $S_i, S_j, S_k, S_\ell$ are located on the corners of a square-shaped unit cell.

A variety of the thermodynamic functions can be obtained from the free energy
\[F = -k_B T \ln Z.\] (6)

Alternatively, one-point functions can be directly calculated from the thermal average with respect to the Boltzmann factor $e^{-\beta H}$. An example is the spontaneous magnetization per site
\[M(T) = \langle S_i \rangle = \frac{1}{Z} \text{Tr} \left[ S_i \cdot \sigma \, e^{-\beta H} \right],\] (7)

which is independent on the location $i$ in the thermodynamic limit, and is finite in the low-temperature ordered state. The unit vector $\sigma$ represents the direction of the ordering. Another example is the bond energy
\[U(T) = -J \langle S_i \cdot S_j \rangle = -\frac{J}{Z} \text{Tr} \left[ S_i \cdot S_j \, e^{-\beta H} \right],\] (8)

where $S_i$ and $S_j$ are the nearest neighbors.

If the first-order phase transition is present in the discrete $n$-vector model of the polytope type, the latent heat
\[L_n = \lim_{T \to T_n^+} U(T) - \lim_{T \to T_n^-} U(T)\] (9)
is finite, where $T_n^+$ and $T_n^-$, respectively, denote the limits to the transition temperature $T_n$ from high- and low-temperature side.

### III. NUMERICAL RESULTS

We consider a set of finite-size systems with the square geometry, and denote the size of each system by the linear dimension $N$. Let us express the corresponding partition function by $Z(N)$. We calculate $Z(N)$ iteratively by means of the CTMRG method, starting from $Z(3)$ and increasing the system size $N$ by 2 in each numerical iteration step. It is possible to choose boundary conditions for the square systems, by setting the appropriate conditions for the initial tensors. Under the fixed boundary condition, all the boundary vectors are kept aligned in an identical direction. Under the free boundary condition, the boundary vectors can point to arbitrary directions.

It should be noted that the numerically calculated value for $Z(N)$ is slightly dependent on the number of the renormalized block-spin state $m$ in the CTMRG method. We denote the approximated value by $Z(N,m)$. We keep $m = 300$ states at most, the condition of which enables us to estimate the latent heat $L_n$ quantitatively in the large-$m$ limit. Let us introduce the calculated free energy per site
\[f_n(N,m) = -\frac{1}{N^2} k_B T \ln Z(N,m).\] (10)

In the cases $n = 3$ and 4 that we examine in the following, the convergence of $f_n(N,m)$ with respect to $N$ to the limit $f_n(\infty,m)$ is fast enough regardless of the temperature $T$. Such a rapid convergence suggests that the system is always off-critical.

We first show the calculated result for the case $n = 4$, the 16-cell model. Figure 1 shows the spontaneous magnetization $M(T)$ in Eq. (7) in the thermodynamic limit $N \to \infty$, calculated under the condition $m = 100$. There is a discontinuity at the temperature $T_n = 0.80620$. (We put ‘*’ mark for the calculated cross-over temperature, which can be dependent on $m$.) The behavior suggests the presence of the first-order phase transition. In order to get complementary information, we observe the
Fig. 1: Spontaneous magnetization $M$ of the 16-cell model ($n = 4$) with respect to $T$ in the limit $N \to \infty$ when $m = 100$. There is a discontinuity at $T^*_4 = 0.80620$. The inset shows the free energy per site under the fixed boundary conditions $f_4^{[\text{FBC}]}$ and the open ones $f_4^{[\text{OBC}]}$.

The effect of boundary conditions on the free energy per site $f_4(\infty, m)$. The inset of Fig. 1 shows $f_4^{[\text{FBC}]}(\infty, m)$ under the fixed boundary conditions and $f_4^{[\text{OBC}]}(\infty, m)$ under the open ones. As it is shown, there is a crossover at $T^*_4 = 0.80620$ between the ordered state at low temperatures and the disordered one at high temperatures.

Precisely speaking, the crossover temperature $T^*_4$ slightly depends on $m$, even around $m = 100$. Figure 2 shows the $m$-dependence of $T^*_4$, which is almost converged around $m = 200$. Fitting the plotted data with the function $T^*_4 + c e^{a/m}$ within the range $100 \leq m \leq 300$, we estimate the phase-transition temperature $T^*_4 = 0.806183$. The inset of Fig. 2 shows the difference of the internal energy per site between the ordered and the disordered states at the crossover temperature $T^*_4$. Even when $m = 300$, there is a non-negligible $m$-dependence, and, therefore, we perform the extrapolation with the use of the fitting function $L^*_4 + c e^{a/m}$ within the range $160 \leq m \leq 300$. As a result, we estimate the latent heat $L^*_4 = 0.3172$.

For comparison, let us focus on the thermodynamic property of the octahedron model ($n = 3$). In our previous study, we obtained the transition temperature $T^*_3 = 0.908413$ from the CTMRG calculation under $m = 300$ only, where we estimated the latent heat to be $L^*_3 = 0.073$. In the study the $m$-dependence in $T^*_3$ was not carefully examined. We thus perform re-estimation of $T^*_3$ and $L^*_3$. In the same manner as we have analyzed the 16-cell model, we calculate $f_3^{[\text{FBC}]}(\infty, m)$ and $f_3^{[\text{OBC}]}(\infty, m)$ in order to determine their crossover temperature $T^*_3$. In Fig. 3, we plot $T^*_3$ with respect to $1/m$. Fitting the plotted data to the function $T^*_3 + c e^{a/m}$ within the range $80 \leq m \leq 300$, we obtain $T^*_3 = 0.908358$, which is slightly lower than the value we had previously reported [8]. The inset of Fig. 3 shows the jump in the internal energy per site with respect to $1/m$. In this case, the exponential convergence is not observed. We, therefore, carried out a linear fit to the plotted data within the range $80 \leq m \leq 300$. The estimated latent heat, $L^*_3 = 0.0516$, is smaller than the value we had reported earlier [8]. It is worth to mention that the estimated $L^*_3 = 0.0516$ is of the same order as the latent heat measured in the 5-state Potts model $L \approx 0.0265$ [6, 15].

We have recognized that $L^*_4$ is larger than $L^*_3$. In order to roughly capture the $n$-dependence in the latent heat $L_n$, we also calculate the cases with the higher internal dimensions ($n \geq 5$). Figure 4 shows the internal energy $U(T)$ for those cases from $n = 1$ to $n = 10$. For the cases $n = 5, 6,$ and $10$, respectively, the value of $m$ is chosen to be $m = 120, 50,$ and $50$. Discontinuous nature in $U(T)$ is evident for $n \geq 3$. The observed discontinuity $L^*_n$ at each cross-over temperature $T^*_n$ is summarized in Tab. 4. Although careful extrapolation with respect to $m$ is not performed here, the increasing nature of the jump
n of the site vectors were focused on the two cases in which the internal dimensions cross-polytope models on the square lattice. We have found that the latent heat is a monotonously increasing function of $n$.

TABLE I: The list of the cross-over temperature and the jump in the calculated internal energy for higher $n$. The value of $m$ used in the CTMRG calculation is also shown.

| $n$ | $m$ | $T^*_n$ | $L^*_n$ |
|-----|-----|---------|---------|
| 5   | 120 | 0.74388(2) | 0.568(7) |
| 6   | 50  | 0.70049(40) | 0.757(12) |
| 10  | 50  | 0.60326(5)  | 1.159(2)  |

$L^*_n$ with respect to the internal dimension $n$ is apparent. It can be conjectured that the latent heat $L_n$ is a monotonously increasing function of $n$.

IV. CONCLUSIONS

We have studied the thermodynamic properties of the cross-polytope models on the square lattice. We have focused on the two cases in which the internal dimensions of the site vectors were $n = 3$ and $n = 4$. The free energy and the internal energy were calculated by means of the CTMRG method. The presence of the first-order phase transition is confirmed for both models from the temperature dependence of these functions. For the 16-cell model ($n = 4$), we evaluated the latent heat $L_4 = 0.3172$, which is larger than that for the octahedron model $L_3 = 0.0516$. The increasing tendency in the latent heat with respect to $n$ is similar to the latent heat of the $q$-state Potts models, which is increasing with $q$ when $q \geq 5$.

It is worth mentioning that the octahedron model ($n = 3$) is similar to the 5-state Potts model, in the point that there are 4 type of single spin flip, which increases the energy by $4J$ on the square lattice, from the completely ordered ferromagnetic ground state. This is the reason why both the octahedron and the 5-state Potts models reveal the small latent heat. Similar correspondence can be considered between the 16-cell model ($n = 4$) and 7-state Potts model.

In four dimensions, there are exceptional polytope models, which are 24-, 120-, and 600-cell models. There is an interest in the clarification of the nature of their phase transitions. It should be noted that these models have rich sub-group structure in their site-vector symmetry. Since these models contain huge amount of the site degrees of freedom, algorithmic improvements of the CTMRG method is necessary in order to carry out their numerical investigation.

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