

# Massively parallel Monte Carlo simulation of a possible topological phase transition in two-dimensional frustrated spin systems

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## Abstract

In two-dimensional frustrated Heisenberg spin systems, a topological defect, so called  $Z_2$ -vortex, often appears as an elemental excitation from magnetically ordered non-collinear ground states. In this paper, we investigate a possible topological phase transition driven by binding-unbinding of  $Z_2$ -vortices, the  $Z_2$ -vortex transition by means of massively parallel Monte Carlo simulations. In order to avoid the failure of global update Monte Carlo simulations in frustrated spin systems, we consider an effective model of the  $Z_2$  vortex transition, where  $SO(3)$  matrices ferromagnetically interact each other on the  $L \times L$  square lattice. We calculate an order parameter, the vorticity modulus, up to  $L = 16384$ . By extrapolating the data into the thermodynamic limit, we estimate the upper bound of the transition temperature as  $T/J \simeq 0.27$ . On the other hand, the spin correlation length at this temperature is estimated at least 20000 lattice spacings. Because the present system is limited  $L = 16384$ , we need further careful analysis to conclude the existence of the finite-temperature topological phase transition.

## 1 Introduction

Recently, frustrated magnets have attracted much interest [1–4]. Frustrated interactions often introduce two kinds of interesting features to spin systems. Firstly, in several frustrated systems, the classical ground states are macroscopically degenerated due to the competitions of interactions. These systems do not develop magnetic long-range order even at zero temperature. They have been considered to reveal possible quantum spin liquids as their ground state if we introduce strong quantum fluctuation typically appeared in the case of  $S = 1/2$ . Typical examples of such macroscopically degenerated ground state can be seen in the two dimensional kagomé lattice or in the three dimensional pyrochlore lattice.

Secondly, even if frustrated spin systems have magnetically ordered ground state, spins often cant from each other forming non-coplaner or non-collinear. A typical example showing non-collinear structure is the triangular lattice antiferromagnetic Heisenberg model. The ground state of the model is so called 120-degree structure where spins cant 120 degrees each other (see Fig. 1(a)). Such kind of canted structures often introduce novel phenomena to frustrated spin systems.

In two-dimensional frustrated Heisenberg spin systems with non-collinear ground state, a topologically stable point defect,  $Z_2$  vortex, often plays an important role in their ordering.

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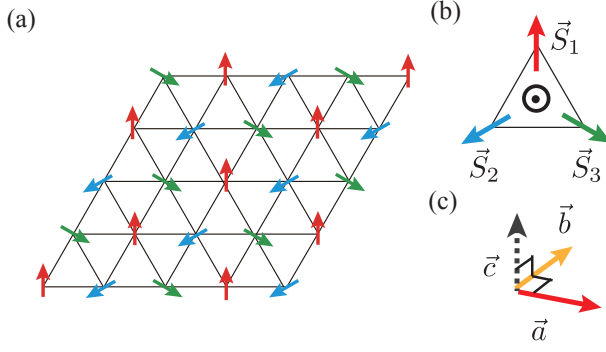


Figure 1: (a) Schematic view of 120-degree structure on the triangular lattice. (b) A local 120 degree structure together with the vector chirality  $\kappa \propto \vec{S}_1 \times \vec{S}_2$  perpendicular to the plane. (c) A local  $SO(3)$  vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$  defined from a local 120-degree structure.

A possible topological phase transition driven by binding-unbinding of the  $Z_2$  vortices was proposed by Kawamura and Miyashita about 30 years ago [5]. In this  $Z_2$ -vortex transition, the spin correlation length keeps finite. At the  $Z_2$ -vortex transition temperature  $T_v$ , only the vortex correlation length characterizing the typical separation of the free vortices diverges. This is a sharp contrast to the case of the Berezinskii – Kosterlitz – Thouless (BKT) transition in two dimensional  $XY$  spin systems, where the spin correlation length diverges together with the vortex correlation length below the transition temperature [6, 7].

The nature of the possible  $Z_2$ -vortex transition has been investigated typically on the triangular-lattice Heisenberg antiferromagnet [5, 8–10]. Recent Monte Carlo (MC) simulation up to  $L = 1536$  suggested the occurrence of  $Z_2$ -vortex transition at a finite temperature  $T_v/J \simeq 0.285$  with a finite spin-correlation length  $\xi \simeq 2000$  [8]. However, the existence of topological phase transition has not been fully resolved because the estimated spin correlation length at  $T_v$  is larger than the maximum system size  $L = 1536$ . In order to clarify the true nature of the  $Z_2$ -vortex transition, we need larger systems beyond the spin-

correlation length at the transition temperature.

However the increase of the system sizes is not so easy because the cluster update MC techniques such as Swendsen-Wang and Wolff algorithms [11, 12] do not work efficiently in the case of frustrated spin systems. By using local update, typically we suffered from *critical slowing down* which means the relaxation time behaves as

$$\tau \propto L^z, \quad (1)$$

where  $z$  is usually  $z \geq 2$ . Thus, if we increase the systems size by twice as  $L' = 2L$ , we at least need four times long MC steps than that of  $L$  in order to obtain sufficient statistics. In addition, we also need to cover the increase of computational cost per unit MC step which is usually proportional to  $L^2$  in the case of two-dimensional systems.

In order to overcome these difficulties, we consider the following strategy. First, we change the model from original frustrated triangular lattice model to a low temperature effective model where we consider  $SO(3)$  rotational matrices as elemental degree of freedoms. As we see in the followings, in this effective model the  $SO(3)$  matrices interact each other ferromagnetically and there is no explicit frustration. Thus we can introduce a cluster algorithm which seems to work well at least for smaller system [13, 14]. Second, in order to cover the increase of computational costs, we introduce MPI parallelization of a cluster MC algorithm based on the real space division. Note that in contrast to the local update MC, we need a global communication to determine the cluster structure in the case of global update.

By combining these two techniques, we perform massively parallel MC simulations for the system sizes up to  $L = 16384$ , which is ten times larger than the previous numerical simulations. It turns out that if we assume the existence of phase transition, the transition temperature  $T_v$  is estimated to be actually finite

by using finite size scaling. On the other hand, the spin correlation length at the estimated  $T_v$  is larger than the maximum system size  $L = 16384$ . Thus we need further studies to confirm the existence of  $Z_2$  vortex transition without doubt.

The rest of the paper is organized as follows. In Sec. 2 we introduce an effective model of the  $Z_2$ -vortex transition. Then we describe numerical methods to investigate the model in Sec. 3. The main results are provided in Sec. 4. Finally, we give concluding remarks and future issues in Sec. 5.

## 2 Model

In order to investigate the possible  $Z_2$ -vortex transition, we consider an effective model which describes low temperature properties of several frustrated Heisenberg systems, *e.g.* the triangular lattice antiferromagnet Heisenberg model [14,15]. The Hamiltonian of the triangular lattice antiferromagnetic Heisenberg model is given by

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \quad (2)$$

where  $\vec{S} = (S_x, S_y, S_z)$  is a three-component unit-vector,  $J > 0$ , and  $\sum_{\langle i,j \rangle}$  means the sum over the nearest-neighbor pairs on the triangular lattice.

The ground state of the model is the 120-degree structure. Note that a “direction” of a 120-degree structure on a triangle can be characterized by a  $SO(3)$  matrix. For example, we construct three orthogonal unit vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$  as

$$\begin{aligned} \vec{a} &= \vec{S}_1 \\ \vec{c} &\propto \vec{S}_1 \times \vec{S}_2 \\ \vec{b} &= \vec{c} \times \vec{a}, \end{aligned} \quad (3)$$

(see Fig. 1(b,c)). Thus, a low-temperature effective model of the triangle lattice Heisenberg

model is given by

$$\mathcal{H}_{\text{eff}} = - \sum_{\langle i,j \rangle_t} \left( p_1 \vec{a}_i \cdot \vec{a}_j + p_1 \vec{b}_i \cdot \vec{b}_j + p_3 \vec{c}_i \cdot \vec{c}_j \right), \quad (4)$$

where a set of vectors  $(\vec{a}_i, \vec{b}_i, \vec{c}_i)$  is located at a upper triangle of the original triangular lattice and  $\sum_{\langle i,j \rangle_t}$  is the sum over the nearest-neighbors on the coarse grained triangular lattice formed by upper triangles. Note that interaction coefficients  $p_1$  and  $p_3$  are non-negative (ferromagnetic), and  $p_3$  is generally different from  $p_1$  because  $\vec{c}$  is perpendicular to the original 120-degree structure, while  $\vec{a}$  and  $\vec{b}$  are on the plane formed by the 120-degree structure. In a previous study done by Kawamura and Kikuchi, they used a model with  $p_3 = 0$  [15]. Because the the model only has ferromagnetic interactions, the underlying lattice structure might be irrelevant to the nature of the ordering. Thus, hereafter we consider the model on the square lattice for the simplicity.

By introducing a  $3 \times 3$  matrix  $R_i$  as  $R_i = (\vec{a}_i, \vec{b}_i, \vec{c}_i)$ , the Hamiltonian is transformed into the form as

$$\mathcal{H}_{\text{eff}} = - \sum_{\langle i,j \rangle} \text{Tr} R_i^t P R_j, \quad (5)$$

where  $P$  is a diagonal matrix  $P = \text{diag}(p_1, p_1, p_3)$ . From this notation, we can see that the Hamiltonian is unchanged under the transformation

$$R'_i = U R_i V, \quad (6)$$

where  $U$  is a  $SO(3)$  rotational matrix and  $V$  is a  $O(2)$  rotational matrix which mixes  $\vec{a}$  and  $\vec{b}$ . Thus, the effective model often called as  $SO(3) \times O(2)$  model. At the special parameter  $p_3 = p_1$  the model becomes  $SO(3) \times SO(3)$  symmetric, *i.e.*, the Hamiltonian is unchanged under the transformation (6) with both of  $U$  and  $V$  are  $SO(3)$  matrices.

Because the effective model has  $Z_2$ -vortices as topological defects independent on the value of  $p_3$ , here we concentrate to the case  $p_3 = p_1$ .

In this special case, the  $SO(3) \times SO(3)$  model can be mapped onto so called  $RP^3$  model [14]. In the  $RP^3$  model *four-component* unit vectors  $\vec{S}_i = (S_{i,0}, S_{i,1}, S_{i,2}, S_{i,3})$ , interact through the ferromagnetic biquadratic interaction as

$$\mathcal{H}_{RP^3} = -\tilde{J} \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j)^2. \quad (7)$$

The effective spin  $\vec{S}$  is related to the matrix  $R$  through the relation

$$R_{kl} = 2 \left( S_k S_l - \frac{1}{4} \delta_{k,l} \right) + 2 \sum_{m=1}^3 \epsilon_{klm} S_0 S_m + 2 \left( S_0^2 - \frac{1}{4} \right) \delta_{kl}. \quad (8)$$

A general  $RP^{n-1}$  model defined as  $n$ -component spin system interacting through the biquadratic term has been investigated, *e.g.*, as a model for liquid crystals [13, 16–18]. In the case of  $n = 2$ , the model is equivalent to the XY model and it exhibits the BKT transition on two-dimensional lattices. For  $n \geq 3$ , the two dimensional  $RP^{n-1}$  models have  $Z_2$ -vortex excitations and they could exhibit the  $Z_2$ -vortex transition, although no clear evidence of the transition has been reported. In the limit of  $n \rightarrow \infty$ , the model is soluble: the model exhibits a finite temperature first-order phase transition [17].

### 3 Method

In order to investigate the  $RP^3$  model on the  $L \times L$  square lattice, we perform MC simulations. Because the Hamiltonian contains no frustrated interactions, conventional cluster algorithms are likely to work efficiently. Actually, Kunz and Zumbach have proposed a Wolff-Swendsen-Wang type cluster algorithm for general  $RP^{n-1}$  models [13] and Caffarel *et al.*, have extended it to  $SO(3) \times O(2)$  model [14]. In their algorithm, first we generate a random (unit) vector  $\vec{e}$  in  $O(n)$  space, and then we calculate the projection of  $\vec{S}_i$  onto the  $\vec{e}$  as

$\sigma_i = \vec{S}_i \cdot \vec{e}$ . Finally, we perform the Swendsen-Wang cluster algorithm [11] by constructing clusters defined through effective Ising variables  $\sigma_i$ .

Indeed, the Wolff-Swendsen-Wang algorithm for the  $RP^{n-1}$  and the  $SO(3) \times O(2)$  models have worked efficiently at least for smaller system sizes [13, 14]. On the other hand, for systems of  $L = O(1000)$ , we found that the relaxation of  $Z_2$ -vortex degree of freedoms feel a kind of critical slowing down and the total relaxation time scaled as  $\tau \propto L^z$ , where  $z \simeq 2$ . Thus, for the present model the cluster algorithm works not surprisingly well, although it can largely reduce the relaxation time from that of the local updates.

In order to investigate much larger sizes than the previous simulations, we also implemented MPI parallelization of the Wolff-Swendsen-Wang algorithm. We split the two-dimensional square lattice into  $M \times M$  cells, and a MPI process is assigned to each cell (see Fig. 2). In total, we have  $M^2$  MPI processes. A MPI process store the information of spins in its cell. Different from the local update methods, we need global communication to perform the cluster algorithm. For this purpose, we implemented a simple hierarchical communication, known as the butterfly type communication.

In Fig. 3, we show benchmark results of our code performed at the K computer and the previous ISSP super computer, Kashiwa. We performed the benchmark up to 16384 MPI processes (2048 nodes) at the K computer and up to 1024 MPI processes (128 nodes) with the flat MPI parallelization. Although the parallelization efficiency is lower than the ideal scaling for large nodes, we can get sufficient speed-up by using MPI parallelization. Based on benchmark calculations, we performed the product calculations *e.g.* of the largest size  $L = 16384$  on 512 node of the K computer.

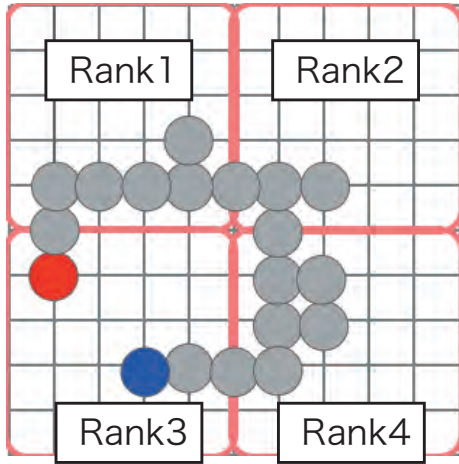


Figure 2: Schematic view of assignment of MPI processes on the square lattice together with a cluster determined by *e.g.* Wolff-Swendsen-Wang algorithm. Because two sites on a cell could be connected through the all other cells, we need information of the whole system to detect the cluster structure.

## 4 Results

By using parallel Wolff-Swendsen-Wang algorithm, we performed MC simulation of the  $RP^3$  model on the square lattice up to  $L = 16384$ . The calculations have been performed in the K computer and the system B in ISSP University of Tokyo.

In Fig. 4, we show the vortex density  $n_v$  for various system sizes. We define vortices on every elemental plaquet of the square lattice, and  $n_v$  is defined as the ratio between the number of vortices and the volume  $L^2$ . The vortex density does not show strong size dependence and it rapidly varies around  $T/\tilde{J} \simeq 0.28$ . In the low temperature phase, the vortices appear only as pairs and the vortex density is expected to be described by the thermal activation of such pairs. The inset of Fig. ?? shows the semi-log plot of  $n_v$  as a function of  $\tilde{J}/T$ . For  $T \gtrsim 0.28\tilde{J}$ , we see clear deviation from the low-temperature behavior  $n_v \propto e^{-\mu/T}$ , indicating at least something happens in the vortex sector around  $T/\tilde{J} \simeq 0.28$ . However, note

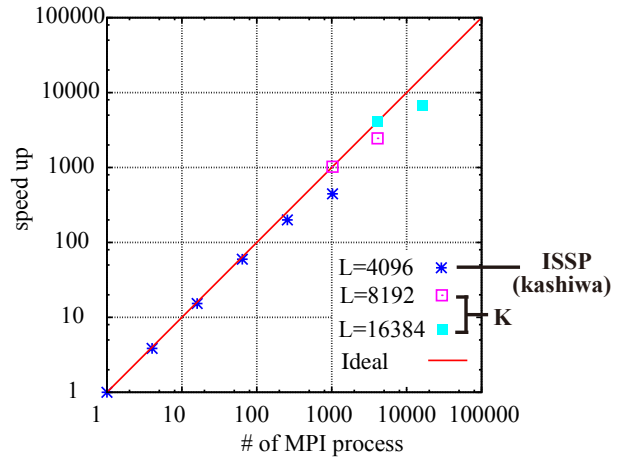


Figure 3: Benchmark results of MPI parallelized cluster MC method for  $RP^3$  model. The speed up is the inverse of elapsed time normalized at 1, 1024, and 4096 MPI processes for  $L = 4096, 8192,$  and  $16384$ , respectively. In this benchmark calculation, we include not only the MC updates but also calculation of observable. The calculations performed at the K computer and ISSP super computer (Kashiwa) with flat MPI parallelization.

that  $n_v$  contains information from both of free and paired vortices, while  $Z_2$ -vortex transition is governed by a binding-unbinding of free vortices. At the phase transition, the density of the free vortices becomes zero, while  $n_v$  keeps finite due to the contribution from paired vortices. Thus, we need a proper order parameter for  $Z_2$ -vortex transition rather than  $n_v$ .

In order to further clarify the existence of  $Z_2$ -vortex transition, here we investigate the so called *vorticity modulus* as an order parameter of the topological phase transition [10, 15]. The vorticity modulus is conceptually defined through the free energy difference between the cases with and without a free vortex [15]. The free energy difference  $V$  is expected to show logarithmic size dependence for sufficiently large  $L$  as

$$V = C + v \log L, \quad (9)$$

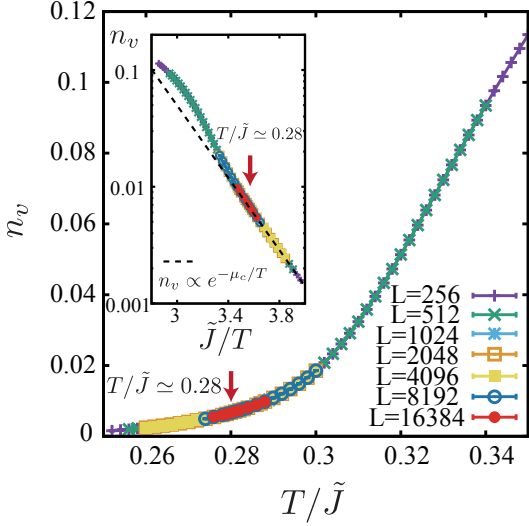


Figure 4: Temperature dependence of the vortex density. Red arrows indicate the position of  $T/\tilde{J} = 0.28$ , where the vortex density rapidly varies. The inset shows the vortex density in the semi-log plot as a function of  $1/T$ .

and the coefficient  $v$  before  $\log L$  is the vorticity modulus. In the thermodynamic limit, the vorticity modulus is equal to zero ( $v = 0$ ) for  $T > T_v$  and it is finite ( $v > 0$ ) for  $T < T_v$ . Thus we can determine the transition temperature  $T_v$  through size and temperature dependence of the vorticity modulus.

In actual calculation, we assume a simple vortex structure and calculate the free energy difference at size  $L$ ,  $V(L)$ , through the fluctuation in the equilibrium configurations under the periodic boundary condition; it is similar to the conventional calculation of the helicity modulus [10]. Then, we extract the vorticity modulus  $v$  by using  $V(L)$ s of two system sizes  $L_1$  and  $L_2$  as

$$v(L_1, L_2) \equiv \frac{V(L_1) - V(L_2)}{\log L_1/L_2}. \quad (10)$$

In Fig. 5, we plot thus obtained vorticity moduli for various sizes, where we set  $L_2 = L_1/2$ . As we expect, for sufficiently high temperature  $v \simeq 0$ , and for  $T \lesssim 0.28\tilde{J}$ ,  $v > 0$ . We also see that as decreasing the temperature,  $v$  becomes negative slightly higher tem-

perature before  $v > 0$ . It might be a finite size effect comes from *e.g.* the size dependence of  $C$  term in Eq. (9). However, owing to this negative part, we can easily define a characteristic temperature  $T_v(L)$  as the temperature where  $v$  change the sign, which is expected to converge to the true transition temperature  $T_v$  in the thermodynamic limit.

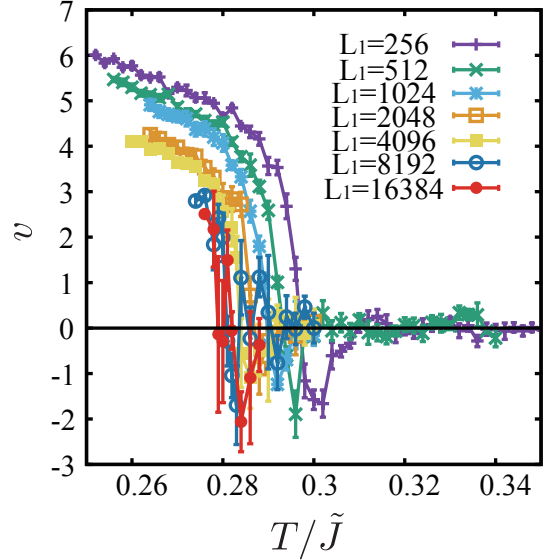


Figure 5: Vorticity modulus obtained by MC simulations for  $128 \leq L \leq 16384$ . The vorticity modulus is calculated through Eq. (10) by setting  $L_2 = L_1/2$ .

In Fig. 6, we plot the characteristic temperature  $T_v(L)$  as a function of the system size, where we set  $L = (L_1 + L_2)/2$ . Because the correlation length for vortices  $\xi_v$ , which could be defined as characteristic separation length of the free vortices, diverges exponentially at  $T_v$  as

$$\xi_v \propto \exp \left[ \frac{A}{(T - T_v)^\alpha} \right] \quad (T > T_v), \quad (11)$$

we expect that  $T_v(L)$  converges to  $T_v$  by logarithmic form as

$$T_v(L) = T_v + a [\log(L/L_0)]^{-\frac{1}{\alpha}} \quad (12)$$

[8]. In the previous MC simulation of the triangular lattice antiferromagnetic Heisenberg

model,  $\alpha$  was estimated as  $\alpha = 0.42 \pm 0.15$  [8]. The estimated  $\alpha$  is not so different from  $\alpha = 0.5$ , which is the case of BKT transition. Note that even if there is no  $Z_2$  vortex transition, Eqs. (11) and (12) are applicable by setting  $T_v = 0$  and  $\alpha = 1$  [19].

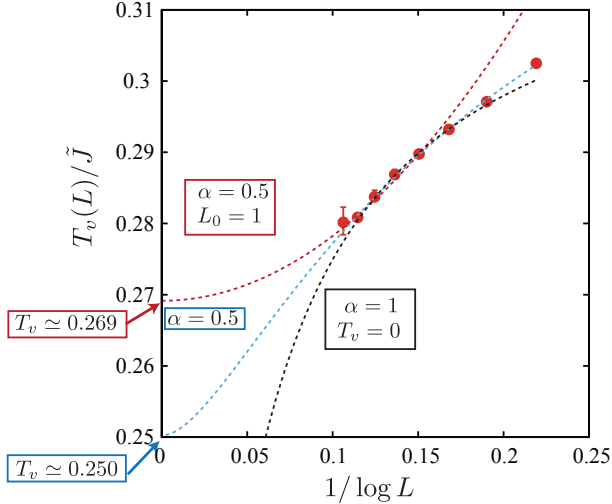


Figure 6: Extrapolation of characteristic temperature  $T_v(L)$  to the thermodynamics limit. Based on Eq. (12), we extrapolated the data by assuming three kind of situations: (red) ( $\alpha = 0.5, L_0 = 1$ ), (blue) ( $\alpha = 0.5$ ), and (black) ( $\alpha = 1, T_v = 0$ ).

Based on Eq. (12), we extrapolate  $T_v(L)$  to the thermodynamic limit by assuming  $\alpha = 0.5$  or  $\alpha = 0$ , which correspond to assuming finite temperature  $Z_2$ -vortex transition or no  $Z_2$ -vortex transition, respectively. In the former case, we also try two extrapolations by fixing  $L_0 = 1$  or freely change  $L_0$  because  $L_0 = 1$  was used in the analysis of the triangular lattice antiferromagnetic Heisenberg model [8]. The fitting curves are also plotted in Fig. 6. The two curves assuming  $\alpha = 0.5$  give  $T_v/\tilde{J} \simeq 0.269$  and  $T_v/\tilde{J} \simeq 0.250$  for fixed  $L_0 = 1$  and free  $L_0$  cases, respectively. There extrapolation indicate that if we assume the existence of the  $Z_2$  vortex transition, indeed we obtain finite transition temperature. However, note that the fitting curve obtained by assuming  $\alpha = 1.0$  and  $T_v = 0.0$  seems to be not bad except for the

largest size data. Unfortunately, the statistical error of the largest size is rather large and it is difficult to exclude the possibility of no phase transition from the present data set.

In addition, as we can see from the “spin” correlation length<sup>1</sup> plotted in Fig. 7, even at the higher estimation of the transition temperature,  $T_v/\tilde{J} = 0.269$ , the correlation length seems to be longer than the largest system size of the present simulation,  $L = 16384$ . It means that although we investigated the model ten times larger than the previous simulations, the situation remains unclear for persons skeptical about the  $Z_2$ -vortex transition because we cannot ruled out the possibility of “fictitious order” due to smaller systems sizes than the spin correlation length. Thus, we probably need much larger scale calculations to conclude the existence of the  $Z_2$ -vortex transition without doubt. From the present data, we only conclude that the upper bound of the  $Z_2$ -vortex transition is  $T_v/\tilde{J} = 0.27$ .

## 5 Conclusion

In this paper, we investigated the possible topological phase transition, the  $Z_2$ -vortex transition, in two-dimensional frustrated Heisenberg spin systems. The most characteristic feature of the  $Z_2$ -vortex transition is that the spin correlation length at the phase transition keeps finite and only the topological nature, existence of free vortices, changes at the phase transition. In order to clarify the existence of transition and to distinguish with a cross over by numerical simulations, we need to calculate larger systems than the spin correlation length at the transition temperature. We attacked this challenging problem by investigating the  $RP^3$  model on the square lattice as an effective model for the  $Z_2$ -vortex transition.

<sup>1</sup>Here we define correlation length through the ferromagnetic correlation of  $\vec{S}_i$  in  $RP^3$  model, or equivalently through the ferromagnetic correlation of  $\vec{a}$ ,  $\vec{b}$ , or  $\vec{c}$  in  $SO(3) \times SO(3)$  model.

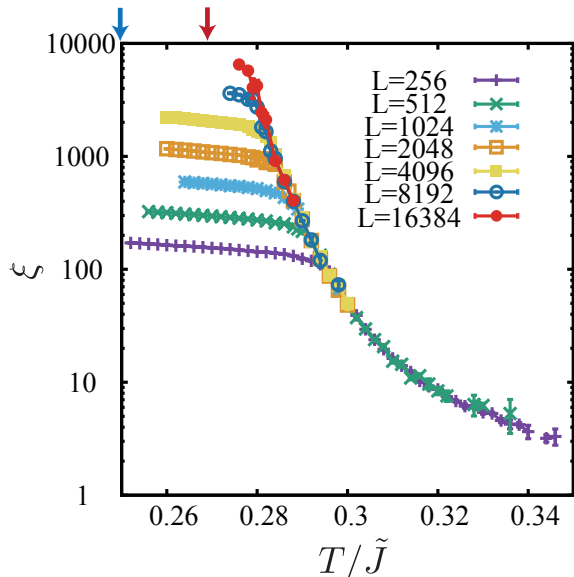


Figure 7: "Spin" correlation length of  $RP^3$  model for various system sizes. red and blue arrows indicate the position of estimated  $T_v$ s,  $T_v/\tilde{J} \simeq 0.269$  and  $T_v/\tilde{J} \simeq 0.250$ , respectively.

By using massively parallel cluster MC simulation, we successfully equilibrated the system up to  $L = 16384$ . We extrapolated the characteristic temperature to the thermodynamic limit by assuming the scaling of the  $Z_2$ -vortex transition, and obtained an upper limit of the transition temperature  $T_v/\tilde{J} \simeq 0.27$ . However, when we extrapolated the data by assuming no phase transition, it also gave us satisfactory fittings. In addition, the spin correlation length at  $T_v$  seems to be clearly beyond the maximum size  $L = 16384$ . These analysis indicates that although we have performed ten times larger size than the previous MC simulation, it is still difficult to show the existence of  $Z_2$ -vortex transition without doubt.

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