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Abstract. We study thermal transitions of the generalized SU(N) Heisenberg models with four-body interactions on a square lattice and with six-body interactions on a honeycomb lattice. In both models for the N=3 and 4 cases, a singlet-dimer state is stabilized at a very low temperature, where a rotational symmetry of lattice is broken spontaneously. We discuss the universality class of thermal transition to the singlet dimer phases, performing quantum Monte Carlo calculations. From the finite-size scaling analysis, we find that the criticality for the square lattice case is well explained by the 2D weak Ising universality, while the 2D three-state Potts universality is observed in the honeycomb lattice case.

1. Introduction

In this decay, one of the most discussed topics is the possibility of deconfined critical phenomena (DCP) [1–3] in quantum spin systems. The phenomena are expected to be observed at a quantum phase transition (QPT) between the magnetic ordered phase such as Néel phase and the valence-bond-solid (VBS) phase in two dimension (2D). The remarkable feature is that it is continuous although the symmetry group in one phase is not the subset of another phase. The most famous models believed to show the DCP behavior are SU(N) JQ_m models on several 2D lattices [4]. Great numerical efforts have been devoted to clarify the critical properties of those models. However it has not been achieved yet satisfactory [4–11].

When we focus on the thermal properties of the SU(N) JQ_m models, the finite temperature transition to the VBS phase is expected because the VBS order can be characterized by the rotational symmetry breaking. For example, in the square lattice case, the VBS pattern is described by a columnar dimer configuration as shown figure 1 (b). This is the $\pi/2$-rotational symmetry breaking around the center of plaquette. Consequently the universality class is expected to be the same as the 2D classical models with Z_4 symmetry-breaking fields, such as the XY+Z_4 model[12] and the Ashkin-Teller model[13] and so on. Interestingly the criticality of the above classical models shows that the thermal exponent ν changes keeping relations among critical exponents with constant correlation exponent $\eta = 1/4 : \gamma/\nu = 7/4$ and $\beta/\nu = 1/8$. This

is known as the 2D weak Ising universality [14]. As for the SU(2) JQ_3 model on the square lattice case, the QMC calculations done in ref. [15] indicated that the criticality is well explained by the c=1 CFT and ν monotonically increases as the system approaches to the DCP point. When the Z_4 symmetry-breaking field becomes zero, it is expected that the Kosterliz-Thouless (KT) transition takes place and ν diverges in the classical model. Thus the authors in ref. [15] pointed out that the emergence of U(1) symmetry in the vicinity of the DCP point is associated with the KT physics at $T_c = T$ and $T \to 0$.

In contrast to the square lattice case, the situation is much different in the honeycomb lattice case. When the VBS order is columnar and accompanies the $\pi/3$-rotational symmetry breaking, the expected classical model is the XY model with the Z_3 symmetry-breaking field. Therefore the related classical model that can explain the universality is the 2D three-state Potts model [16]. The Z_3 field is always strongly relevant in 2D, and thus the critical exponents do not change depending on the coupling ratio as far as $T_c > 0$ and the symmetry of Hamiltonian is kept.

Based on the DCP scenario, the *quantum* criticality should not change depending on the lattice geometry. Indeed, in previous study [11], the same criticality is expected in both the square JQ_2 and honeycomb JQ_3 models at $T = 0$, while the possibility of the weak first order transition still remains especially in the SU(3) case. If the DCP point is the first order transition, the presence of the multi-critical point in the finite temperature region emerges. This indicates that the values of critical exponent ν should change when the system approaches to the multi-critical point or the discontinuous fixed point along the thermal transition line. From the above background, we focus on thermal phase transitions of SU(N) JQ_2 model on the square lattice and JQ_3 model on the honeycomb lattice in this paper.

2. Model and Method

The Hamiltonian for the SU(N) JQ_2 model on the square lattice and JQ_3 model on the honeycomb lattice can be simply expressed by introducing singlet projection operator P_{ij}. The singlet projection operator[11; 17] is defined in terms of the generators of the SU(N) algebra as $P_{ij} = -\frac{1}{N} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} S_i^{\alpha\beta} \bar{S}_j^{\beta\alpha}$, where $\bar{S}_j^{\beta\alpha}$ is conjugate operator of $S_i^{\alpha\beta}$. This singlet projection operator gives a simplified form for the Hamiltonian written as

$$\mathcal{H} = -J \sum_{(ij)} P_{ij} - Q_2 \sum_{(ij)(kl)} P_{ij} P_{kl}, \tag{1}$$

for the square lattice case and

$$\mathcal{H} = -J \sum_{(ij)} P_{ij} - Q_3 \sum_{(ij)(kl)(mn)} P_{ij} P_{kl} P_{mn}, \tag{2}$$

for the honeycomb lattice case, where (ij) is the nearest-neighbor sites. The summation for the Q_m terms runs over all pairs without breaking the rotational symmetry of lattice as illustrated in figure 1. Since the present lattices are bipartite, the fundamental (conjugate) representation is adapted for SU(N) spins on A(B) sites. By tuning the two coupling parameters J and Q_m, the ground state of the above Hamiltonians changes from the VBS state to the Néel state. Thus it is convenient to introduce the coupling ratio defined as

$$\lambda = J/(J + Q_m). \tag{3}$$

The values of the QPT points between the Néel state and the VBS state were already evaluated in ref. [11], and summarized as $(N, \lambda_c) = (3, 0.665)$ and $(N, \lambda_c) = (4, 0.918)$ for the square lattice case, and $(N, \lambda_c) = (3, 0.797)$ and $(N, \lambda_c) = (4, 0.985)$ for the honeycomb lattice case.
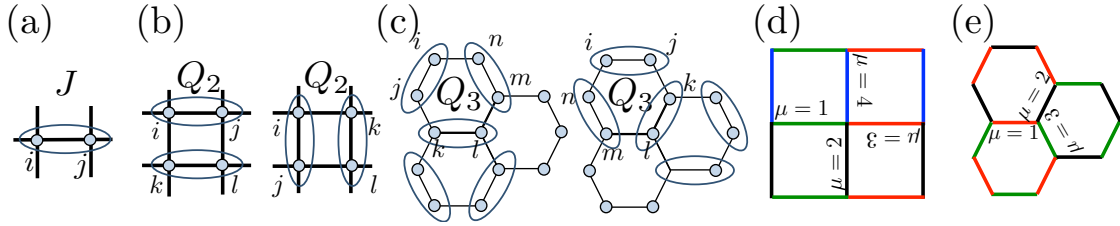
Figure 1. Singlet projection operator on a bond (a). Bold ellipsoids denote projection operator P_{ij} and color-singlet dimer state. Projection operator for Q_2 term (b) and Q_3 term (c). (d) and (e) are coordination indexes μ.

For the Hamiltonian (1) and (2), we carried out the QMC calculations up to $L=192$ for the square lattice case and $L=96$ for the honeycomb lattice case, changing the coupling ratio λ with the fixed energy scale, $J+Q_m=1$. The computations were executed by using the massively parallelized Loop algorithm code [18] provided in ALPS project [19]. To discuss the thermal transition to the VBS phase, we defined the complex-VBS magnetization defined as $\Psi_r \equiv \sum_{\mu=1}^{z} \exp[\frac{2\pi i}{z}\mu]\hat{P}_{r,r_\mu}$, where $\hat{P}_{r,r_\mu}$ is the diagonal component of projection operator, z is the coordination number of a lattice, and r_μ represents the neighboring site of r along the μ direction, respectively.

3. Results and discussion

In the QMC calculations, we evaluated the VBS order parameter $\Psi = L^{-2}\sum_r \Psi_r$. From the obtained Ψ_r, we further calculated the VBS correlation function given by $C(r) \equiv \langle \Psi_r \Psi_0 \rangle$, the static structure factor $S(Q) = L^{-2}\sum_r \exp[-iQr]\Psi_r$, the Binder ratio $B_R \equiv \langle \Psi^4 \rangle/\langle \Psi^2 \rangle^2$, and the correlation length, $\xi \equiv \frac{1}{|\Delta Q|}\sqrt{\frac{S(0)}{S(|\Delta Q|)}-1}$, where ΔQ denotes the smallest distance from the Γ point, namely $(0, 2\pi/L_y)$ or $(2\pi/L_x, 0)$.

From the temperature dependence, we found that B_R and ξ for each system sizes show a good cross at a critical point. Assuming the scaling forms, $\xi/L \sim g_\xi[L^{1/\nu}(T-T_c)]$ and $B_R \sim g_{B_R}[L^{1/\nu}(T-T_c)]$, we evaluated the critical temperature T_c and thermal exponent ν. Figure 2 show the results for $(N, \lambda) = (3, 0.10)$ and $(4, 0.20)$. In the finite-size scaling (FSS) analysis, we evaluated the two variables T_c and ν simultaneously by the Bayesian-scaling-analysis scheme [20]. The obtained values are $(T_c, \nu) = (0.2550(6), 1.30(4))$ for $(N, \lambda) = (3, 0.10)$ and $(T_c, \nu) = (0.2542(7), 1.08(3))$ for $(N, \lambda) = (4, 0.20)$. Therefore we find that ν apparently depends on the coupling ratio λ and SU(N) spins.

Next, we evaluate γ/ν from the static structure factor with the obtained critical temperatures. In the present case, a single peak structure at the Γ point is expected for $S(Q)$. Figure 3(a) and (c) present the system size dependence of $S(Q=\Gamma)$ in the vicinity of critical temperatures. We find that $S(Q)$ well scales as $S(Q) \sim L^{\gamma/\nu}$ at T_c and $\gamma/\nu = 7/4$ is satisfied independently of SU(N) spins. In fact, as shown in figure 3 (b) and (d), temperature dependence of $S(Q)L^{-\gamma/\nu}$ shows a good cross when we assume $\gamma/\nu = 7/4$. The crossing temperature, namely T_c, is the same value within the error bar that is estimated from the FSS analysis for the Binder ratio and correlation length. The value of γ/ν also indicates that the critical exponent for the correlation function satisfies $\eta = 1/4$ if the hyper scaling relation is assumed. As not shown here, we found that γ/ν is constant independently of λ. [17]

The obtained results strongly suggest that the thermal transition for the SU(N) JQ_2 model on the square lattice is explained by that of the 2D XY+Z_4 model, because the critical exponents satisfy the condition in the 2D Ising weak universality class[14]; ν changes depending on the
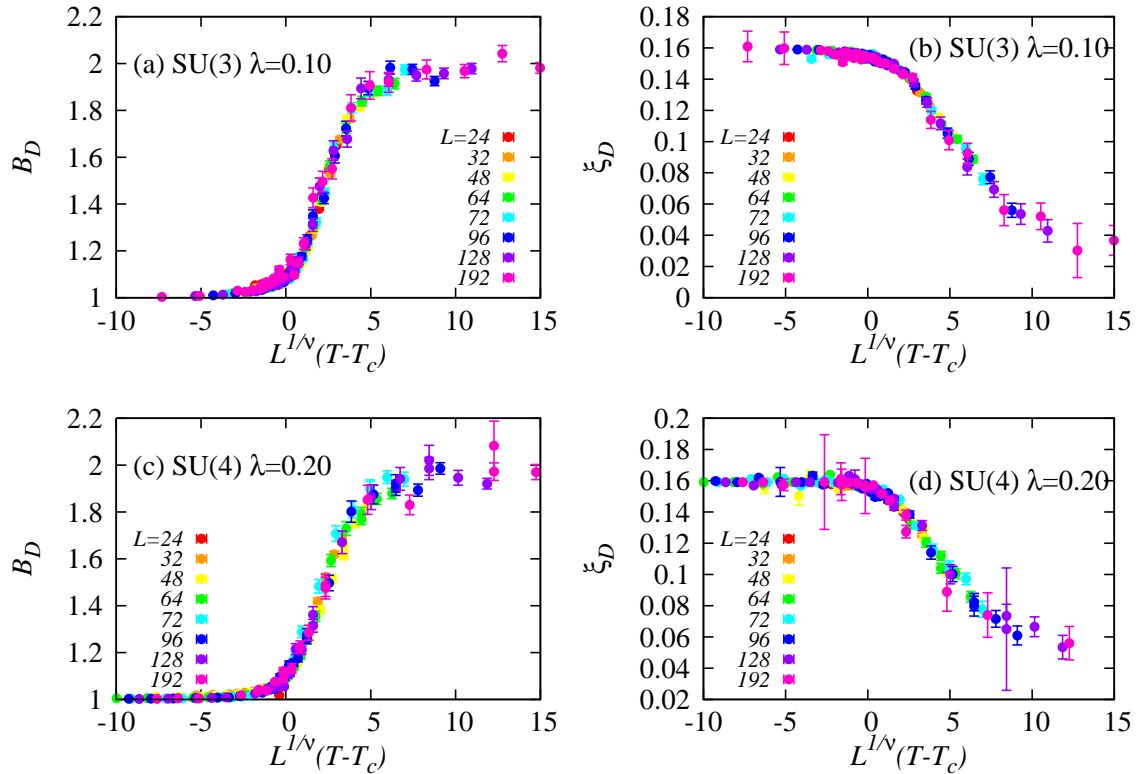
Figure 2. Finite-size scaling analysis for the Binder ratio and correlation length. (a) and (b) ((c) and (d)) are the results for the SU(3) (SU(4)) spin case.

parameters but η and the others scaled by ν, for example β/ν and γ/ν, take constant values. (This is related with the fact that the Z_4 symmetry-breaking field becomes marginal just on the critical temperature.) When we discuss whether the universality is same or not, it is important clue to check the form of scaling function each other. In figure 4, we show the Binder ratio as a function of inverse correlation. The scaling form of the Binder ratio is expressed by $B_R(L/\xi) = g_{B_R}[L/\xi]$. The Binder ratio is analytical function and takes a characteristic value depending only on the universality class at the critical point [21]. Therefore if the value at the critical point is same each other, the scaling function $g[x]$ should be same. Unfortunately, the value of binder ratio at the critical point changes depending on the coupling ratio λ. Thus it is difficult to estimate the corresponding magnitude of Z_4 fields in the classical models from the coupling ratio in the quantum SU(N) JQ_2 model directly. However, we can check the trend when λ or Z_4 field changes and then, can give a discussion, whether the universality class for both models is same or not and the possibility of the first order transition. (In the first-order transition case, it is expected that the Binder ratio itself shows a dip structure [21].)

In figure 4, we show $B_R(L/\xi)$ for the SU(N) JQ_2 model and the 2D XY+Z_4 model. Note that the data set for the 2D XY+Z_4 model is obtained from the Monte Carlo calculations for $\mathcal{H} = J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) - h_4 \sum_i \theta_i$. Any dip structure is not confirmed in the results for the SU(N) JQ_2 model. We also find the quite small system-size dependence of $B_R(L/\xi)$ and a relatively weak dependence for λ and $\alpha = h_4/(J + h_4)$. The important point is that the same trend of $B_R(L/\xi)$ is confirmed in both quantum and classical models; the behavior of $B_R(L/\xi)$ closes to that of the 2D Ising model case, when $\lambda \to 0$ and $\alpha \to 1$. This is reasonable because
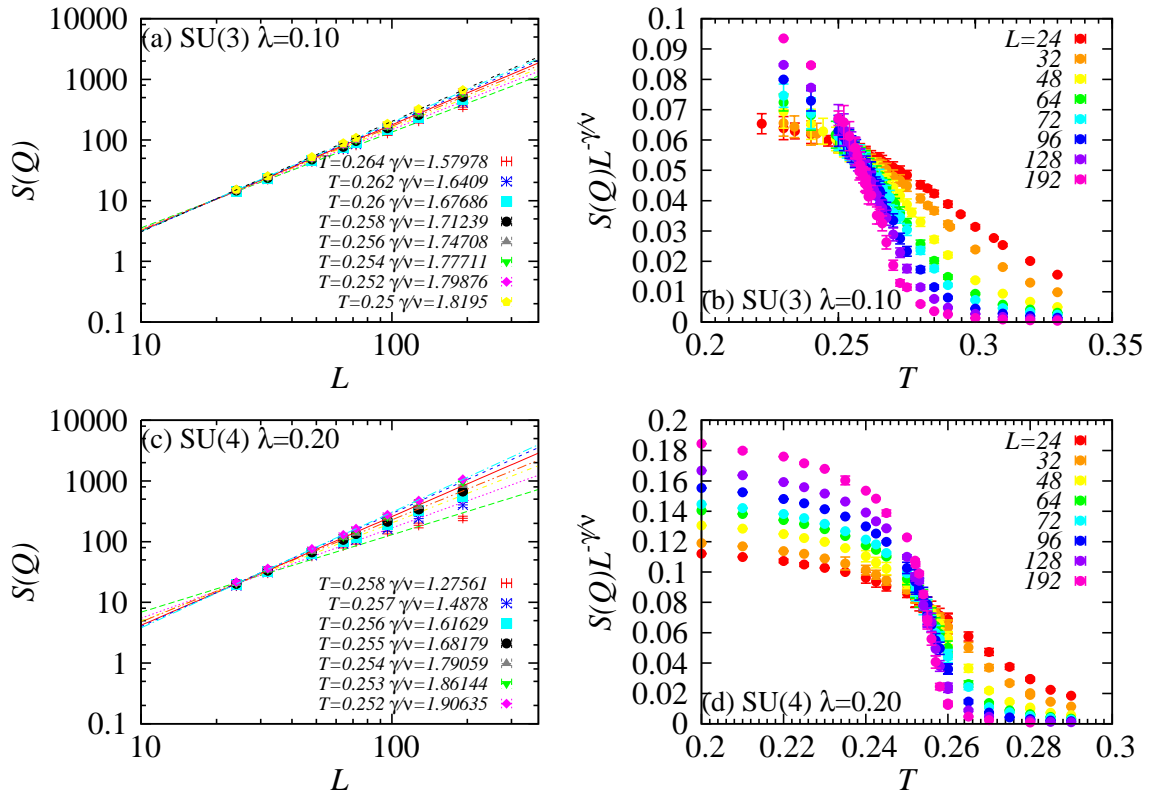
Figure 3. Size dependence of $S(Q = \Gamma)$ in the vicinity of critical temperatures and temperature dependence of $S(Q)$.

the Q term flavors the columnar dimer configuration along the x or y -axis. In the classical case, the similar behavior is also observed when $\alpha \to 1$, where the system can be expressed by the double Ising model exactly. The above result is consistent with the result for the SU(2) JQ_3 model case reported in ref. [15]. Consequently we conclude that the universality class of the SU(N) JQ_2 model possesses the same feature of the classical $XY + Z_4$ model and this is independent of SU(N) spins.

In the honeycomb lattice case, the expected columnar VBS pattern is characterized by the $\pi/3$-rotational symmetry breaking, with reflecting the honeycomb-lattice background. This implies that the related classical model showing the same universality class is the 2D $XY+Z_3$ model. The most different point from the square lattice case is that Z_3 symmetry-breaking field is always relevant. This may warrant that the critical exponents should be independent of the coupling ratio λ. Therefore we assume the critical exponents for the 2D 3-state Potts universality class, namely $\nu = 5/6$ and $\gamma/\nu = 26/15$. Adopting the fixed values for the critical exponents, we perform the FSS analysis for the correlation length and static structure factor. The results are shown in figure 5. From the FSS results, we obtain the critical temperatures $T_c = 0.083(1)$ for the SU(3) case and $T_c = 0.205(1)$ for the SU(4) case, and find that the universality class is independent of the SU(N) spin and coupling ratio λ. Interestingly the critical exponents for the SU(3) spin case are well explained by those of the 3-state Potts universality even in the vicinity of the QPT point.

In the previous study[11], the possibility of the weak first-order transition at $T = 0$ was discussed. Our present results for ν do not change in the vicinity of the QPT point. This
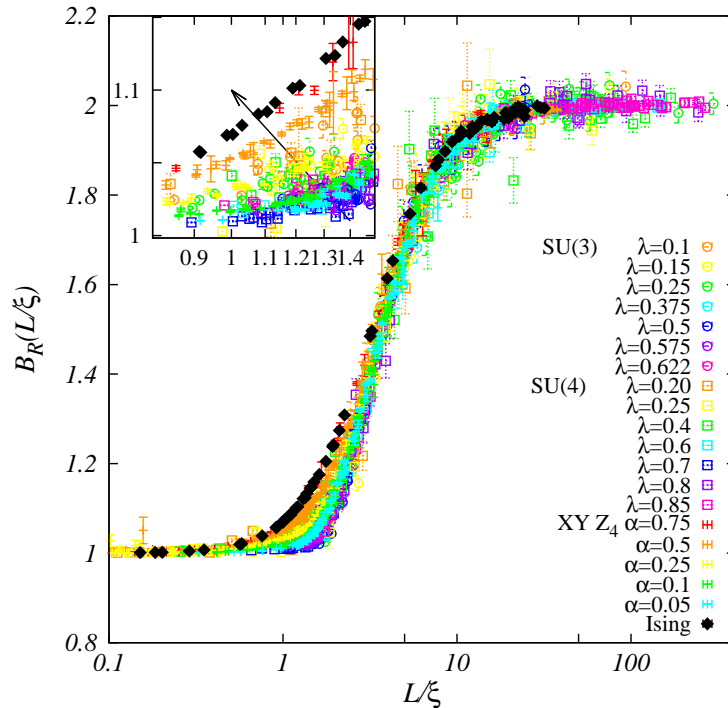
Figure 4. The Binder ratio as a function of L/ξ. Colored symbols are results for the SU(N) JQ_2 models and classical XY+Z_4 model. Open colored circles (squares) are the results for SU(3) (SU(4)) spin case. Plus symbols are the results for the classical case. Black diamonds are the results for the two dimensional Ising model. All data in figure include several different system-size results.

supports the absence of conventional first order transition, because the apparent decrease of ν toward the trivial value $1/d = 1/2$ is not observed. Although we can not discuss the order of the QPT point directly from the thermal transitions, the clarification of phase boundary in the finite temperature region is important because the quantum criticality is expectable to appear in the boundary curvature. The further discussions for the parameter λ dependence of critical exponents and phase boundaries are challenging tasks and we will discuss the details in the other paper [17].

4. Summary
We have investigated the thermal transitions of JQ_2 models on the square lattice and JQ_3 models on the honeycomb lattice for SU(3) and SU(4) spins. We have found that the criticality can be explained by the 2D weak Ising universality class in both SU(3) and SU(4) in the square lattice case. This is the same result for the SU(2) JQ_3 model, as Jin and Sandvik discussed [15]. In the honeycomb lattice case, reflecting that Z_3 field is strongly relevant, thermal exponent ν always takes the value of the 2D three-state Potts one.
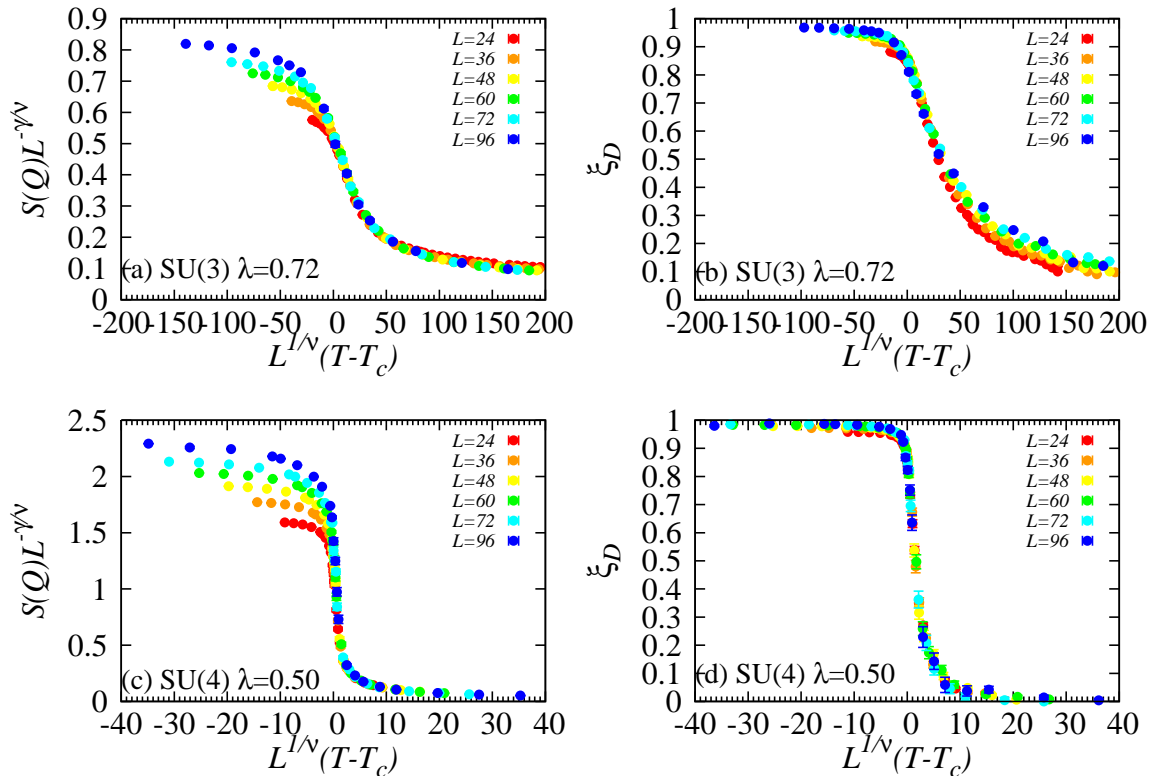
Figure 5. Finite-size scaling analysis for the static structure factor and correlation length. (a) and (b) ((c) and (d)) are the results for the SU(3) (SU(4)) spin case.

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