Deconfined criticality for the two-dimensional quantum

$S = 1$-spin model with the three-spin and biquadratic interactions

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Abstract. The criticality between the nematic and valence-bond-solid (VBS) phases was investigated for the two-dimensional quantum $S = 1$-spin model with the three-spin and biquadratic interactions by means of the numerical diagonalization method. It is expected that the criticality belongs to a novel universality class, the so-called deconfined criticality, accompanied with unconventional critical indices. In this paper, we incorporate the three-spin interaction, and adjust the (redundant) interaction parameter so as to optimize the finite-size behavior. Treating the finite-size cluster with $N \leq 20$ spins, we estimate the correlation-length critical exponent as $\nu = 0.88(3)$.

PACS. 75.10.Jm Quantized spin models – 05.30.-d Quantum statistical mechanics – 75.40.Mg Numerical simulation studies – 74.25.Ha Magnetic properties

1 Introduction

The phase transition between the Néel and valence-bond-solid (VBS) phases for the two-dimensional quantum spin system is attracting much attention recently [1-3, 4-5, 6-7, 8-9, 10-11, 12-13, 14-15]; see Ref. [17] for a review.

It is expected that the phase transition, the so-called deconfined criticality, belongs to a novel universality class, accompanied with unconventional critical indices. Originally, the idea was developed [12, 13] in the context of the gauge-field-theoretical description for the two-dimensional strongly-correlated-electron system. Meanwhile, it turned out that the underlying physics is common to a variety of systems in terms of the emergent gauge field [14, 15, 16, 17].

As a lattice realization of the deconfined criticality, the quantum $S = 1/2$-spin square-lattice antiferromagnet with the plaquette four-spin interaction, the so-called $J$-$Q$ model [15], has been investigated extensively; the
bipartite-lattice systems such as the square- and honeycomb lattice antiferromagnets do not conflict with the quantum Monte Carlo method, and large-scale-simulation results are available. However, it is still unclear whether the phase transition is critical or a weak first-order transition with a latent-heat release. The controversy may be reconciled by a recent renormalization-group analysis, which revealed an influence of a notorious marginal operator around the deconfined-critical fixed point; see Ref. as well. Because the character of the marginal operator depends on each lattice realization, it may be sensible to survey a variety of lattice realizations.

The $S = 1$-spin model is a clue to the realization of the deconfined criticality. A key ingredient is that the $S = 1$-spin model admits the biquadratic interaction, which stabilizes the VBS phase as the spatial anisotropy varies. The phase transition separating the VBS and nematic phases is expected to belong to the deconfined criticality. We consider a non-bipartite-lattice version (Fig. 1); the details and underlying ideas are explained afterward. In the preceding paper, the correlation-length critical exponent was estimated as $\nu = 0.92(10)$. In this paper, based on the preceding studies, we incorporate a rather novel interaction term intrinsic to the $S = 1$-spin model, namely, the three-spin-interaction term (in addition to the biquadratic one), and survey the extended parameter space so as to optimize the fine-size behavior.

Here, the symbol $S_i$ denotes the quantum $S = 1$-spin operator placed at each square-lattice point $i$ (Fig. 1). The summations, $\sum_{(ij)}$, $\sum_{\langle\langle ij\rangle\rangle}$, and $\sum_{\langle ijk\rangle}$, run over all possible rectangular (nearest-neighbor) edges $(ij)$, skew-diagonal pairs $(\langle ij\rangle)$, and skew-diagonal adjacent three sites $[ijk]$, respectively. Correspondingly, the coupling constants, $J$, $J'$, and $J''$, denote the nearest-neighbor-, skew-diagonal- and skew-diagonal-adjacent-three-spin-interaction parameters. Hereafter, the coupling constant $J'$ is considered as the unit of energy ($J' = 1$). The underlying physics behind each interaction parameter is as follows. For sufficiently large nearest-neighbor interaction $J(> 0)$, the system reduces to a two-dimensional model, and the nematic phase emerges; here, the quadratic component of the Heisenberg interaction is set to $j = 0.5$ throughout this study. On the contrary, the coupling constants $J'(= 1)$ and $J''(> 0)$ strengthen the spatial anisotropy, promoting the formation of singlet dimers along the skew-diagonal bonds; a schematic phase diagram is presented in Fig. 2. In this paper, we incorporate the latter interaction term and adjust this (redundant) interaction parameter $J''$ as well as the three-spin-interaction component $j_3$ so as to optimize the finite-size-scaling behavior.
It has to be mentioned that in the pioneering study \cite{24}, the bipartite-lattice version (without the diagonal interaction) of Eq. (1) was investigated by means of the quantum Monte Carlo method; for the bipartite lattice, the spatial anisotropy $J'$ inevitably violates the symmetry between the horizontal and vertical directions, and the asymmetry might alter the nature of the transition \cite{15}. Our non-bipartite-lattice version (1) retains the symmetry (between the horizontal and vertical directions), as would be apparent from Fig. 1. In order to cope with the non-bipartite-type lattice, we employ the exact diagonalization method with the aid of Novotny’s method (screw-boundary condition) \cite{31}, which enables us to treat a variety of system sizes $N = 10, 12, \ldots$ in a systematic manner; note that the number of spins constituting a rectangular cluster is restricted within $N = 4, 9, \ldots$.

The rest of this paper is organized as follows. In Sec. 2 we present the simulation results. The technical details as to the screw-boundary condition are presented as well. In Sec. 3 we address the summary and discussions, providing a brief overview on the past studies of the correlation-length critical exponent $\nu$.

## 2 Numerical results

In this section, we present the simulation results. To begin with, we explain the simulation scheme to implement the screw-boundary condition, namely, Novotny’s method \cite{31}, briefly. Owing to this scheme, we are able to treat an arbitrary number of spins, $N = 10, 12, \ldots$, constituting a two-dimensional cluster. The linear dimension $L$ of the cluster is given by $L = \sqrt{N}$, because the $N$ spins form a rectangular cluster.

The Hamiltonian (1) has been investigated extensively in some limiting cases. In order to elucidate the phase diagram, Fig. 2 we recollect a number of related studies \cite{27,28,29,30}; we also address a brief account of the parameter range surveyed in our preliminary study. In the limit $J \to \infty$, the model reduces to the two-dimensional Heisenberg model with the biquadratic interaction. According to Ref. \cite{28}, around $j = 0.5$, the nematic phase is realized. With $J = 0$ and $J'' = 0$, the one-dimensional biquadratic-interaction Heisenberg model is realized, and the VBS phase emerges \cite{27}. Similarly, with $J = 0$ and $J' = 0$, the VBS phase is realized for sufficiently large $j_3 > 0.111$ \cite{29}. Hence, the interaction parameter $J$ interpolates smoothly these limiting cases, and the phase diagram, Fig. 2 follows. In the preliminary stage of the research, we dwelt on the subspace $J'' = 0$, which was studied in Ref. \cite{29}. Turning on the interaction $J''$ gradually, we arrive at the optimal regime $J'' \approx 0.08$, as indicated in Fig 5. At least for a moderate range of $J'' < 0.2$, a fundamental feature of the phase diagram, Fig. 2 is kept maintained; namely, no signature such as an appearance of a certain intermediate phase could be detected.

### 2.1 Simulation method: Screw-boundary condition

In this section, we explain Novotny’s method \cite{31} to implement the screw-boundary condition. The screw-boundary condition enables us to treat a variety of system sizes $N = 10, 12, \ldots$; note that naively, the system size is re-
stricted within quadratic numbers $N = 4, 9, \ldots$ for a rectangular cluster.

In this paper, we follow the simulation scheme reported in Ref. [26], where the $J''$ term of the Hamiltonian (1) was not taken into account. The missing term is incorporated by the addition of the following term to Eq. (5) of Ref. [26]:

$$ J'' \sum_{i=1}^{N} \{ \mathbf{S}_i \cdot \mathbf{S}_{i+1} + j_3 [\mathbf{S}_i \cdot (\mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2}) + h.c.] \}. \tag{2} $$

(The index $i$ runs over a one-dimensional alignment $i = 1, 2, \ldots, N$ in a way intrinsic to the screw-boundary condition.) Thereby, we diagonalize the Hamiltonian matrix given by Eq. (5) of Ref. [26] with the term (2), employing the Lanczos algorithm for a finite-size cluster with $N \leq 20$ spins. Rather technically, the diagonalization was performed within the zero-momentum subspace, at which the magnetic- (triplet-) excitation gap $\Delta E$ opens.

### 2.2 Finite-size scaling of $\Delta E$: Critical point

In this section, based on the simulation method explained in Sec. 2.1, we evaluate the excitation gap $\Delta E$. Thereby, we estimate the location of the critical point via the scaling analysis of $\Delta E$.

In Fig. 3, we plot the scaled energy gap $L \Delta E$ for various $J'' / J'$ and $N = 10, 12, \ldots, 20$ ($L = \sqrt{N}$); here, the interaction parameters are set to $J'' / J' = 0.08$ and $j_3 = 0.45$. According to the finite-size-scaling theory, the intersection point of $L \Delta E$ indicates a location of the critical point $J_c \approx 0.3$, because the scaled energy gap should be scale-invariant (dimensionless) at the critical point.

In Fig. 4 we plot the approximate critical point $J_c(L_1, L_2)$ for $[2/(L_1 + L_2)]^2$ with $10 \leq N_1 < N_2 \leq 20$ ($L_{1,2} = \sqrt{N_{1,2}}$); the interaction parameters are the same as those of Fig. 3. Here, the approximate critical point $J_c(L_1, L_2)$ is defined by the formula

$$ L_1 \Delta E(L_1)|_{j=J_c(L_1, L_2)} = L_2 \Delta E(L_2)|_{j=J_c(L_1, L_2)}. \tag{3} $$

for a pair of system sizes $(L_1, L_2)$. The least-squares fit to the data in Fig. 4 yields $J_c = 0.2998(45)$ in the thermodynamic limit $L \to \infty$. This extrapolated value does not affect the subsequent analysis (Sec. 2.3), and we do not go into the discussion of the extrapolation error; actually, the approximate critical point $J_c(L_1, L_2)$ (rather than the extrapolated $J_c$) is fed into the formula, Eq. (4).

Last, we address a number of remarks. First, in Fig. 4 the finite-size behavior seems to be oscillatory; actually, the data exhibit successive bumps for quadratic values of $N(= L^2) \approx 9, 16, \ldots$. Such an oscillatory deviation is an artifact of the screw-boundary condition. Second, the set of the coupling constants $J'' = 0.08$ and $j_3 = 0.45$ were determined so as to optimize the finite-size behavior of Fig. 4 (as well as Fig. 5 mentioned afterward). Actually, as for $J'' \neq 0.08$ and $j_3 \neq 0.45$, the finite-size behavior of $J_c(L_1, L_2)$ suffers from steep finite-size drift and enhanced bumps. Last, in the scaling analysis, Fig. 3 we postulated the dynamical critical exponent $z = 1$. Here, we followed the conclusion $z = 1$ obtained in the pioneering studies [4, 5].
2.3 Correlation-length critical exponent $\nu$

In this section, we estimate the correlation-length critical exponent $\nu$. Based on the approximate critical point $J_c(L_1, L_2)$, we are able to calculate the approximate correlation-length critical exponent

$$\nu(L_1, L_2) = \frac{\ln(L_1/L_2)}{\ln[\partial_J[L_1\Delta E(L_1)]/\partial_J[L_2\Delta E(L_2)]]}_{J=J_c(L_1, L_2)},$$

for a pair of system sizes $(L_1, L_2)$. In Fig. 5, as the symbol +, we plot $\nu(L_1, L_2)$ for $[2/(L_1 + L_2)]^2$ with $10 \leq N_1 < N_2 \leq 20$ ($L_{1,2} = \sqrt{N_{1,2}}$); here, the interaction parameters are the same as those of Fig. 3. The data exhibit an oscillatory deviation (bump at $N \approx 16$), which is an artifact of the screw-boundary condition [31]. The least-squares fit to the data in Fig. 5 yields $\nu = 0.88(10)$ in the thermodynamic limit.

Similar analyses were carried out independently for various values of $J''$ with $j_3 = 0.45$ fixed. As a consequence, the approximate critical point is plotted in Fig. 5 for $(\times) J'' = 0$, $(\ast) 0.04$, and $(\Box) 0.12$. The least-squares fit to these data yields $\nu = 0.8642(87)$, $0.8823(93)$, and $0.883(12)$, respectively, in the thermodynamic limit. Notably enough, the interaction parameter $J''$ governs the convergence of $\nu(L_1, L_2)$ to the thermodynamic limit. Particularly, in the optimal regime $0.04 \leq J'' \leq 0.12$, the extrapolation to the thermodynamic limit can be taken reliably, allowing us to appreciate the critical exponent $\nu \approx 0.88$ rather systematically. For exceedingly large $J'' > 0.12$, there emerge a notable finite-size drift (to the counter direction) as well as enhanced oscillatory deviations (steep bumps around $N \approx 16$) as to $\nu(L_1, L_2)$ and even $J_c(L_1, L_2)$, preventing us from extrapolating $\nu$ unambiguously. Surveying various $J''$ as well as $j_3$, we observed that the uncertainty of the extrapolation is bounded by $\Delta \nu = 0.03$. As a result, we estimate the correlation-length critical exponent as

$$\nu = 0.88(3).$$

The result is consistent with the estimate $\nu = 0.92(10)$ reported in Ref. [26], where the three-spin interaction was not taken into account.

In Fig. 5, we assumed implicitly that the dominant scaling correction should obey the power law $1/L^2$. However, as mentioned in Introduction, there might be a logarithmic correction [22,23], which is not negligible for large system sizes. We cannot exclude a possibility that such a correction gives rise to an ambiguity as to the estimate [4]. Here, aiming to provide a crosscheck, we carry out an alternative analysis of criticality as presented in the next section.

2.4 Scaling plot for $\Delta E$

In this section, we present the scaling plot for $\Delta E$ as a cross-check of the analyses in Sec. 2.2 and 2.3.

In Fig. 6, we present the scaling plot, $(J - J_c)L^{1/\nu} - L\Delta E$ for the same interaction parameters as those of Fig. 3. Here, the scaling parameters are set to $J_c = 0.2998$ (Sec. 2.2) and $\nu = 0.88$ (Sec. 2.3). The scaled data appear to fall into a scaling curve satisfactorily for an appreciable range of $J$, confirming the validity of the analyses in Sec. 2.2 and 2.3. As mentioned in Introduction, corrections-to-scaling
behavior \cite{22,23} may depend on each lattice realization. In this respect, we stress that the present $S = 1$-spin model is less affected by severe scaling corrections.

This is a good position to address a remark on the validity of the deconfined-criticality scenario. As mentioned in Introduction, it is still unclear whether the (Néel-VBS) phase transition is continuous or not. The scaling analysis in Fig. 6 suggests that the (spatial-anisotropy-driven nematic-VBS) phase transition would be continuous. A notable point is that the estimate $\nu = 0.88(3)$ \cite{25} takes a rather enhanced value; actually, it appears to be larger than, for instance, that of the Heisenberg universality class, $\nu = 0.7112(5)$ \cite{32}. Because of the following reason, such a feature might exclude a possibility of the discontinuous phase transition. As a matter of fact, the discontinuous phase transition does exhibit a pseudo-critical behavior (for finite system sizes) with an enhanced effective specific-heat critical exponent $\alpha = 2 - 3\nu$, one arrives at a suppressed $\nu = 0.4$, which is inaccordant with ours. Such a tendency is reasonable, because the discontinuous transition is accompanied with a latent-heat release, enhancing the specific-heat critical exponent $\alpha$ to a considerable extent. A comparison with other existing estimates for $\nu$ is presented in the next section.

3 Summary and discussions

The deconfined criticality between the nematic and VBS phases for the two-dimensional $S = 1$-spin model with both three-spin and biquadratic interactions was investigated with the numerical diagonalization method for a finite-size cluster with $N \leq 20$ spins; so far, the case without the three-spin interaction has been investigated extensively \cite{24,26}. The extended interaction-parameter space enables us to search for a regime of suppressed finite-size corrections. Actually, the interaction parameter $J''$ governs the convergence to the thermodynamic limit, as shown in Fig. 5. In fact, for $0.04 \leq J'' \leq 0.12$, the extrapolation can be taken reliably. As a result, we estimate the correlation-length critical exponent as $\nu = 0.88(3)$; the result agrees with the preceding estimate $\nu = 0.92(10)$ \cite{26}.

As a comparison, we recollect related studies of the deconfined criticality, placing an emphasis on the critical exponent $\nu$. First, as mentioned in Introduction, the $J$-$Q$ model has been investigated extensively. Pioneering studies reported $\nu = 0.78(3) \cite{4}$ and $0.68(4)$ \cite{5}. Possibly, there emerges the logarithmic corrections to scaling in the vicinity of the deconfined criticality \cite{22,23}, preventing us from identifying the character of the phase transition definitely. A recent simulation result for the honeycomb-lattice model indicated a rather suppressed value of $\nu = 0.54(5) \cite{16}$. Second, a unique approach to the deconfined criticality was made by the extension of the internal symmetry to SU($N$) with the continuously variable $N$ \cite{34}. There was reported a clear evidence of the phase transition of a continuous character with the enhanced critical exponent $\nu = 0.75$-1. Third, the “fermionic” criticality \cite{18,19} indicates $\nu = 0.80(3)$ \cite{20} and $\approx 0.88$ \cite{21}. Last, we overview simulation results for the classical coun-
For the dimer model, the critical exponent was estimated as $\nu = 0.73(5)$, $0.5$, $0.5-0.53$, and $0.5-0.6$. The hedgehog-suppressed O(3) model indicates an enhanced exponent $\nu = 1.0(2)$. These conclusions have not been settled yet. Nonetheless, our result indicates a tendency toward an enhancement of $\nu$ such as the fermionic criticality.

The present simulation result supports the deconfined-criticality scenario at least for the (spatial-anisotropy-driven) nematic-VBS phase transition; see the discussion in Sec. as well. In Ref. [40], a novel two-dimensional quantum-spin model with the three-spin-interaction was introduced. The model may be a good clue to the realization of the deconfined criticality without the spatial anisotropy. However, its rich phase diagram has not been fully clarified. A progress toward this direction is remained for the future study.

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Fig. 3. The scaled energy gap $L\Delta E$ is plotted for various $J/J'$ and the system sizes of (+) $N=L^2 = 10$, ($\times$) 12, ($\ast$) 14, ($\square$) 16, ($\blacksquare$) 18, and ($\circ$) 20; here, the interaction parameters were set to $J''/J' = 0.08$ and $j_3 = 0.45$. The intersection point of the curves, $J_c \approx 0.3$, indicates the location of the critical point.

Fig. 4. The approximate critical point $J_c(L_1,L_2)$ is plotted for $2/(L_1 + L_2)^2$ ($10 \leq N_1 < N_2 \leq 20$) with the interaction parameters, (+) $(J'', j_3) = (0.08, 0.45)$, ($\times$) $(0, 0.45)$, ($\ast$) $(0.04, 0.45)$, and ($\square$) $(0.12, 0.45)$. The least-squares fit to these data yields $\nu = 0.889(10), 0.8642(87), 0.8823(93)$ and 0.883(12), respectively, in the thermodynamic limit. Clearly, in an optimal regime $0.04 \leq J'' \leq 0.12$, the extrapolation can be taken reliably; see text for details. An oscillatory finite-size deviation (bump around $N \approx 16$) is an artifact of the screw-boundary condition [31].

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Fig. 6. The scaling plot, $(J - J_c)L^{1/\nu} - L\Delta E$, is shown for (+) $N=L^2 = 10$, ($\times$) 12, ($\ast$) 14, ($\square$) 16, ($\blacksquare$) 18, and ($\circ$) 20; the interaction parameters are the same as those of Fig. 3. Here, the scaling parameters are set to $J_c = 0.2998$ and $\nu = 0.88$. The data collapse into a scaling curve satisfactorily, providing a cross-check for the analyses in Sec. 2.2 and 2.3.
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