

# Deconfined criticality for the $S = 1$ spin model on the spatially anisotropic triangular lattice

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(Received 31 October 2010; revised manuscript received 18 December 2010; published 15 February 2011)

The quantum  $S = 1$  spin model on the spatially anisotropic triangular lattice is investigated numerically. The nematic and valence-bond-solid (VBS) phases are realized by adjusting the spatial anisotropy and the biquadratic interaction. The phase transition between the nematic and VBS phases is expected to be a continuous one with unconventional critical indices (deconfined criticality). The geometrical character (spatial anisotropy) is taken into account by imposing the screw-boundary condition (Novotny's method). Diagonalizing the finite-size cluster with  $N \leq 20$  spins, we observe a clear indication of continuous phase transition. The correlation-length critical exponent is estimated as  $\nu = 0.92(10)$ .

DOI: [10.1103/PhysRevB.83.054417](https://doi.org/10.1103/PhysRevB.83.054417)

PACS number(s): 75.10.Jm, 05.30.-d, 75.40.Mg, 74.25.Ha

## I. INTRODUCTION

According to the deconfined-criticality scenario,<sup>1-3</sup> in two dimensions, the phase transition separating the valence-bond-solid (VBS) and antiferromagnetic phases is continuous; naively,<sup>2</sup> such a transition should be discontinuous because the adjacent phases possess distinctive order parameters such as the VBS coverage pattern and the sublattice magnetization, respectively. A good deal of theoretical investigations<sup>4-11</sup> has been made to support this scenario. (On the contrary, in Refs. 12-19 it was claimed that the transition would be a weak first-order one.)

The magnetic frustration is a clue to the realization of the VBS phase. Actually, the square-lattice antiferromagnet with the next-nearest-neighbor interaction ( $J_1$ - $J_2$  model) exhibits the VBS phase around the fully frustrated ( $J_2/J_1 \approx 0.5$ ) regime.<sup>20</sup> The quantum Monte Carlo method is not applicable to this problem because of the negative-sign problem. So far, the  $J_1$ - $J_2$  model has been studied with the series-expansion<sup>20,21</sup> and numerical-diagonalization<sup>22</sup> methods.

Alternatively, one is able to realize the VBS phase through incorporating the biquadratic interaction;<sup>23,24</sup> correspondingly, one has to enlarge the magnitude of spin to  $S > 1/2$ . The biquadratic interaction (unlike the magnetic frustration) is tractable with the quantum Monte Carlo method. The deconfined criticality is realized by tuning the spatial anisotropy.<sup>25</sup> That is, as the interchain interaction increases, a transition from the VBS phase to either nematic or antiferromagnetic phase occurs.<sup>25</sup> Meanwhile, it turns out that the ring-exchange (plaquette-four-spin) interaction also induces the VBS phase even for  $S = 1/2$ . Extensive Monte Carlo simulations<sup>26,27</sup> support the deconfined-criticality scenario; the results are compared with ours in Sec. IV. The transition occurs for a considerably large ring exchange; the antiferromagnetic order would be far more robust than that of VBS. As mentioned above, the character of the singularity is controversial,<sup>12-19</sup> possibly, the log corrections<sup>28</sup> affect the scaling analysis. Even for the  $S = 1/2$  spatially anisotropic triangular antiferromagnet.<sup>29</sup> The ring exchange gives rise to the VBS phase.<sup>30,31</sup> This model is intractable with the quantum Monte Carlo method, and analytical considerations provide valuable information as to the deconfined criticality.<sup>32-34</sup>

In this paper, we investigate the  $S = 1$  spatially anisotropic-triangular-lattice model with the biquadratic interaction by

means of the numerical diagonalization method. To be specific, the Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle ij \rangle} [j \mathbf{S}_i \cdot \mathbf{S}_j + (\mathbf{S}_i \cdot \mathbf{S}_j)^2] - J' \sum_{\langle\langle ij \rangle\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2. \quad (1)$$

Here, the quantum  $S = 1$  spins  $\{\mathbf{S}_i\}$  are placed at each triangular-lattice point  $i$ ; see Fig. 1(a). The summation  $\sum_{\langle ij \rangle}$  ( $\sum_{\langle\langle ij \rangle\rangle}$ ) runs over all possible nearest-neighbor (skew-diagonal) pairs. The parameter  $J$  ( $J'$ ) denotes the corresponding coupling constant. Hereafter, we consider  $J'$  as the unit of energy ( $J' = 1$ ). Along the  $J$  bond, both quadratic and biquadratic interactions exist, and the parameter  $j$  controls a strength of the former component. The  $J'$ -bond interaction is purely biquadratic. The interaction  $J$  interpolates the one-dimensional ( $J = 0$ ) and square-lattice ( $J' \rightarrow \infty$ ) structures. Correspondingly, the VBS and spin-nematic phases appear, as the interaction  $J$  varies; see a schematic phase diagram, Fig. 2. To take into account such a geometrical character, we implement the screw-boundary condition [Fig. 1(b)] through resorting to Novotny's method (Sec. II).

The rest of this paper is organized as follows. In Sec. II, we explain the simulation scheme. We also make an overview on the biquadratic-interaction spin models relevant to ours. In Sec. III, we demonstrate that the present model exhibits a clear indication of deconfined criticality at a moderate value of  $J$ . We also analyze the criticality with the finite-size-scaling theory. In Sec. IV, we present the summary and discussions.

## II. SCREW-BOUNDARY CONDITION: NOVOTNY'S METHOD

In this section, we present the simulation scheme (Novotny's method<sup>35,36</sup>). A brief overview on the biquadratic-interaction spin models follows.

Before commencing an explanation of the technical details, we present a basic idea of Novotny's method. We implement the screw-boundary condition for a finite cluster with  $N$  spins; see Fig. 1(b). Basically, the spins  $\{\mathbf{S}_i\}$  ( $i \leq N$ ) constitute a one-dimensional ( $d = 1$ ) structure, and the dimensionality is lifted to  $d = 2$  by the bridges over the long-range pairs. The present system (1) has a spatial anisotropy governed by  $J$ . We take into account such a geometrical character through imposing the screw-boundary condition. According to Novotny, the

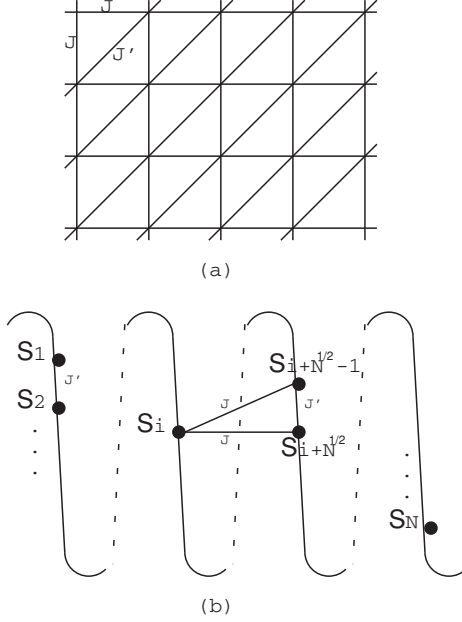


FIG. 1. (a) We consider a spatially anisotropic triangular lattice; the Hamiltonian is given by Eq. (1). The interaction  $J$  interpolate the one- and two-dimensional lattice structures in the limiting cases  $J = 0$  and  $J \rightarrow \infty$ , respectively. (b) To take into account such a geometrical character, we implement the screw-boundary condition. As shown in the drawing, a basic structure of the cluster is an alignment of spins  $\{S_i\}$  ( $i \leq N$ ). Thereby, the dimensionality is lifted to  $d = 2$  by the bridges over the  $(\sqrt{N})$ th neighbor pairs through the  $J$  bonds. Technical details are explicated in Sec. II.

long-range interactions are introduced systematically by the use of the translation operator  $P$ ; see Eq. (3), for instance. The operator  $P$  satisfies the formula

$$P|S_1, S_2, \dots, S_N\rangle = |S_N, S_1, \dots, S_{N-1}\rangle. \quad (2)$$

Here, the base  $\{|S_i\rangle\}$  diagonalizes each of  $\{S_i^z\}$ ; namely, the relation  $S_k^z|S_i\rangle = S_k|S_i\rangle$  holds.

Novotny's method was adapted to the quantum  $S = 1$  XY model in  $d = 2$  dimensions.<sup>36</sup> Our simulation scheme is based on this formalism. In the following, we present the modifications explicitly for the sake of self-consistency. The XY interaction  $H_{XY}$ , Eq. (4) of Ref. 36, has to be replaced with the Heisenberg interaction

$$H_{XXX}(v) = \sum_{i=1}^N (P^v S_i^x P^{-v} S_i^x + P^v S_i^y P^{-v} S_i^y + P^v S_i^z P^{-v} S_i^z). \quad (3)$$

Additionally, we introduce the biquadratic interaction

$$H_4(v) = -\frac{1}{2}H_{XXX}(v) + \frac{1}{2} \sum_{i=1}^N \sum_{\alpha=1}^5 P^v Q_i^\alpha P^{-v} Q_i^\alpha. \quad (4)$$

The definition of  $\{Q_i^\alpha\}$  and an algebra are presented in the Appendix. Based on these expressions, we replace Eq. (3) of Ref. 36 with

$$\mathcal{H} = -J[jH_{XXX}(\sqrt{N}) + jH_{XXX}(\sqrt{N}-1) + H_4(\sqrt{N}) + H_4(\sqrt{N}-1)] - J'H_4(1). \quad (5)$$

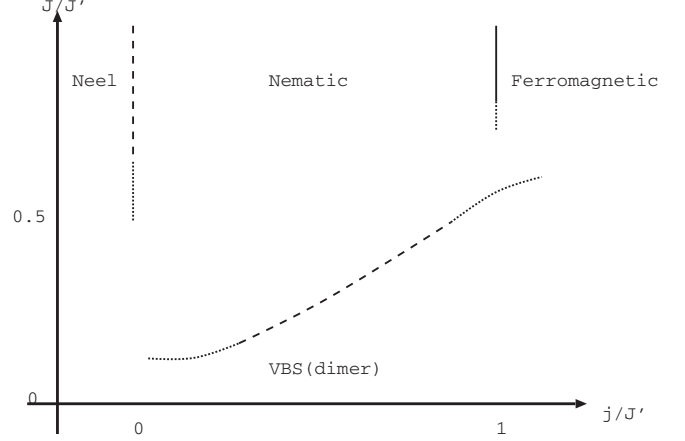


FIG. 2. A schematic phase diagram for the  $S = 1$  spatially anisotropic-triangular-lattice model, Eq. (1), is presented. The limiting cases  $J \rightarrow 0$  and  $J \rightarrow \infty$  were studied in Refs. 37 and 38, respectively. The solid (dashed) lines stand for the phase boundaries of discontinuous (continuous) character. The dotted lines are ambiguous. We investigate the phase boundary separating the nematic and VBS phases.

We diagonalize this matrix for  $N \leq 20$  spins in Sec. III. The above formulas complete the formal basis of our simulation scheme. However, to evaluate the above Hamiltonian-matrix elements efficiently, one may refer to a number of techniques addressed in Refs. 35 and 36.

Last, we overview the biquadratic-interaction spin models. As mentioned in the Introduction, the present model reduces to the one-dimensional and square-lattice models in the limiting cases  $J = 0$  and  $J \rightarrow \infty$ , respectively. Each of these limiting cases has been studied extensively. Here, we devote ourselves to the nearest-neighbor interaction of the generic form  $\cos \theta \mathbf{S}_i \cdot \mathbf{S}_j + \sin \theta (\mathbf{S}_i \cdot \mathbf{S}_j)^2$ , parameterized by  $\theta$ . The regime  $\pi < \theta < 2\pi$  is relevant to the present research. As for  $d = 1$  (Ref. 37), the dimer phase appears in  $5\pi/4 < \theta < 7\pi/4$ . Namely, around  $\theta \approx 3\pi/2$ , the stability of the dimer (VBS) phase would be maximal. For  $d = 2$  (Ref. 38), the ferromagnetic, nematic, and antiferromagnetic phases appear in  $\theta < 5\pi/4$ ,  $5\pi/4 < \theta < 3\pi/2$ , and  $3\pi/2 < \theta$ , respectively. The phase diagram in Fig. 2 is based on these preceding studies.

### III. NUMERICAL RESULTS

In this section, we present the simulation results. We employed the simulation scheme developed in Sec. II. We devote ourselves to the analysis of the transition between the nematic and VBS phases (deconfined criticality); see Fig. 2. We treat a variety of system sizes  $N = 10, 12, \dots, 20$  ( $N$  is the number of spins within a cluster). The linear dimension  $L$  of the cluster is given by

$$L = \sqrt{N}. \quad (6)$$

#### A. Critical point $J_c$

In this section, we investigate a location of the phase boundary separating the VBS and nematic phases.

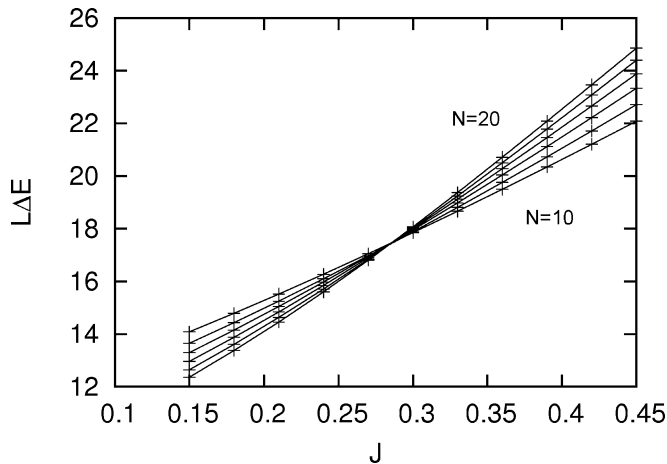


FIG. 3. The scaled energy gap  $L\Delta E$  is plotted for various  $J$  and  $N = 10, 12, \dots, 20$ . The quadratic-interaction strength  $j$  is fixed to  $j = 0.5$ . ( $J'$  is the unit of energy.) We observe a clear indication of the deconfined criticality around  $J \approx 0.28$ .

In Fig. 3, we plot the scaled energy gap  $L\Delta E$  for various  $J$  and  $N = 10, 12, \dots, 20$ . The quadratic-interaction strength  $j$  is fixed to  $j = 0.5$ . The symbol  $\Delta E$  denotes the first excitation gap. According to the finite-size scaling, the scaled energy gap  $L\Delta E$  should be scale-invariant at the critical point. In fact, we observe an intersection point at  $J_c \approx 0.28$ , which indicates an onset of the  $J$ -driven phase transition. As mentioned in the Introduction, the nature of this singularity is under current interest. The present result indicates that the singularity is a continuous one; the critical phenomena (below the upper critical dimension) should be described by the finite-size scaling.

In Fig. 4, we plot the approximate transition 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 parameters are the same as those of Fig. 3. Here, the approximate transition point denotes a scale-invariant point with respect to a pair of system sizes  $(L_1, L_2)$ . Namely, the following relation holds:

$$L_1 \Delta E(L_1)|_{J=J_c(L_1, L_2)} = L_2 \Delta E(L_2)|_{J=J_c(L_1, L_2)}. \quad (7)$$

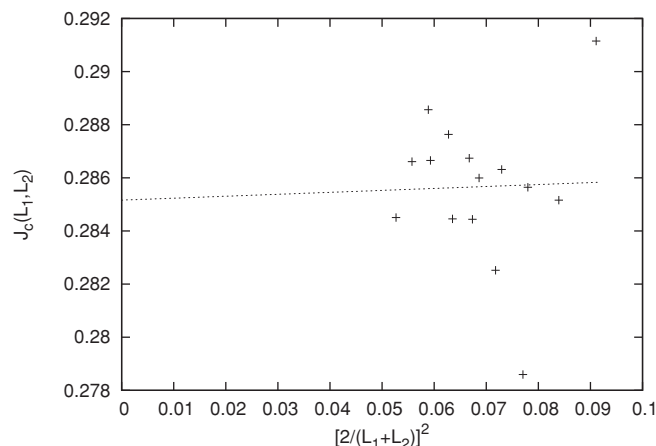


FIG. 4. The approximate critical point  $J_c(L_1, L_2)$  (7) is plotted for  $[2/(L_1 + L_2)]^2$  with  $10 \leq N_1 < N_2 \leq 20$ . The parameters are the same as those of Fig. 3. The least-squares fit to these data yields  $J_c = 0.285(5)$  in the thermodynamic limit.

The least-squares fit to the data of Fig. 4 yields an estimate  $J_c = 0.285(5)$  in the thermodynamic limit  $L \rightarrow \infty$ . To appreciate possible extrapolation errors, we made an alternative extrapolation with the  $1/L^3$ -abscissa scale. Thereby, we obtain  $J_c = 0.285(3)$ . The extrapolation errors appear to be negligible. (As a matter of fact, we surveyed a wide range of  $j$ , and found that the parameter  $j = 0.5$  yields an optimal finite-size behavior.) Hence, we obtain an estimate  $J_c = 0.285(5)$ .

Making similar analyses for various values of  $j$ , we arrived at a phase diagram, Fig. 2. The phase boundary around  $j \approx 0$  and 1 is ambiguous because of finite-size errors. Possibly, around  $j \approx 1$ , the magnetic structure (antiferromagnetic order) conflicts with the screw-boundary condition, resulting in an enhancement of finite-size errors. On the one hand, in  $j < 0$ , the character of the transition changes to a discontinuous one, and the finite-size-scaling method becomes invalid. Hence, the finite-size behavior improves around the midst ( $j \approx 0.5$ ) of  $0 < j < 1$ .

Last, we address a number of remarks. First, in the scaling analysis, Fig. 3, we assumed the dynamical critical exponent  $z = 1$ , following the conclusion of the Monte Carlo simulations.<sup>26,27</sup> Second, we argue a possible systematic error for the data  $J_c(L_1, L_2)$  in Fig. 4. As a matter of fact, for large system sizes, the data  $J_c(L_1, L_2)$  exhibit an enhancement, suggesting that the extrapolated value of  $J_c$  should be larger than 0.285(5). However, in the subsequent analyses, the extrapolated value of  $J_c$  is no longer used, and systematic deviations are less influential. Nevertheless, as to the singularity of  $J_c$ , it has to be mentioned that the present data cannot exclude a possibility of weak-first-order transition, for which the scaling approach becomes invalidated.

## B. Correlation-length critical exponent $\nu$

In this section, we analyze the criticality found in Sec. III A. In Fig. 5, we plot the approximate critical exponent

$$\nu(L_1, L_2) = \frac{\ln(L_1/L_2)}{\ln\{\partial_J[L_1 \Delta E(L_1)]/\partial_J[L_2 \Delta E(L_2)]\}|_{J=J_c(L_1, L_2)}}, \quad (8)$$

for  $2/(L_1 + L_2)$  with  $10 \leq N_1 < N_2 \leq 20$ . The parameters are the same as those of Fig. 3. The least-squares fit to these data yields  $\nu = 0.97(2)$  in the thermodynamic limit. This estimate may be affected by systematic errors. (The statistical error would be an underestimate.) To appreciate an error margin, we made an alternative extrapolation with the  $1/L^2$ -abscissa scale. Thereby, we obtain  $\nu = 0.86(1)$ . The discrepancy indicates an amount of systematic errors. As a result, we arrive at an estimate

$$\nu = 0.92(10), \quad (9)$$

which covers the above results obtained via independent extrapolations.

This is a good position to address a remark on the scaling behaviors of Figs. 3 through 5. As mentioned in the Introduction, notorious log corrections were observed for the  $S = 1/2$  square-lattice antiferromagnet with the ring exchange. Our data, on the contrary, appear to exhibit moderate corrections to scaling, particularly, in Figs. 3 and 4. For the former antiferromagnet, the VBS phase emerges for a considerably

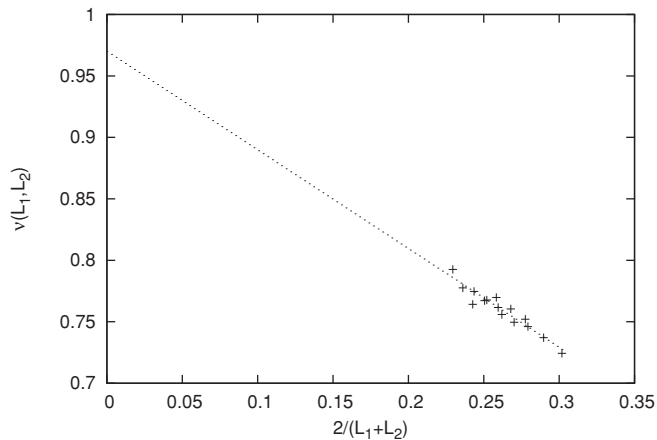


FIG. 5. The approximate critical exponent  $\nu(L_1, L_2)$  (8) is plotted for  $2/(L_1 + L_2)$  with  $10 \leq N_1 < N_2 \leq 20$ . The parameters are the same as those of Fig. 3. The least-squares fit to these data yields  $\nu = 0.97(2)$  in the thermodynamic limit. A possible systematic error is considered in the text.

large ring exchange, indicating that the antiferromagnetic phase is robust. On the one hand, our model exhibits a stable VBS state owing to the spatial anisotropy (one-dimensionality in the  $J = 0$  limit), and the nematic phase turns into the VBS phase at a moderate coupling strength,  $J_c \approx 0.3$ . We suspect that these peculiarities of the present (rather artificially designed) model bring about improved scaling behaviors.

Last, we make a consideration of the abscissa scale of Fig. 5 (4). The critical exponent (point) has a leading correction of  $O(L^{-\omega})$  [ $O(L^{-\omega-1/\nu})$ ]; here, the symbol  $\omega$  denotes the index for corrections to scaling. At present, the index  $\omega$  for the deconfined criticality is unclear. As a reference, one may refer to that of the  $d = 3$  Heisenberg universality class,  $\omega = 0.773$  (Ref. 39). Making use of this value, we set the abscissa scale to that depicted in Fig. 5 (4).

#### IV. SUMMARY AND DISCUSSIONS

The  $S = 1$  spin model on the spatially anisotropic triangular lattice, Eq. (1), was investigated numerically. As the spatial

anisotropy  $J$  changes, the VBS and nematic phases appear (Fig. 2). Hence, this rather artificial model provides a candidate for the analysis of the deconfined criticality, which is arousing much attention recently. We employed Novotny's method (screw boundary condition) to take into account such a geometrical character (spatial anisotropy).

As a result, we observe a clear indication of the  $J$ -driven criticality through the finite-size-scaling analysis (Fig. 3). This result supports the deconfined-criticality scenario. Thereby, we estimate the correlation-length critical exponent as  $\nu = 0.92(10)$ .

As a reference, we overview related studies. For the square-lattice antiferromagnet with the ring exchange, the estimates,  $\nu = 0.78(3)$  (Ref. 26) and  $\nu = 0.68(4)$  (Ref. 27), were reported. As for the spatially anisotropic-triangular antiferromagnet with the ring exchange, the exponent  $\nu = 0.80(15)$  was obtained<sup>30</sup>. These results are to be compared with the index,  $\nu = 0.7112(5)$  (Ref. 40), for the  $d = 3$  Heisenberg universality class. Our result indicates a tendency toward an enhancement for the correlation-length critical exponent, as compared to that for the  $d = 3$  Heisenberg universality class. Taking the advantage of the numerical diagonalization method, we are able to extend the interactions so as to eliminate finite-size errors. A frustrated interaction along the  $J'$ -bond direction may stabilize (extend the regime of) the VBS phase substantially. This problem will be addressed in future study.

#### APPENDIX: A REDUCTION FORMULA FOR THE BIQUADRATIC INTERACTION

The biquadratic interaction  $(\mathbf{S}_i \cdot \mathbf{S}_j)^2$  reduces to a seemingly quadratic form

$$(\mathbf{S}_i \cdot \mathbf{S}_j)^2 = -\mathbf{S}_i \cdot \mathbf{S}_j / 2 + \sum_{\alpha=1}^5 Q_i^\alpha Q_j^\alpha / 2 + 4/3. \quad (\text{A1})$$

Here, the operators  $\{Q_i^\alpha\}$  are given by the relations,  $Q_i^1 = (S_i^x)^2 - (S_i^y)^2$ ,  $Q_i^2 = [2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2] / \sqrt{3}$ ,  $Q_i^3 = S_i^x S_i^y + S_i^y S_i^x$ ,  $Q_i^4 = S_i^y S_i^z + S_i^z S_i^y$ , and  $Q_i^5 = S_i^x S_i^z + S_i^z S_i^x$ . This reduction formula is a key ingredient in Sec. II.

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