## Renormalization-group study of the Ashkin-Teller-Potts model in two dimensions\*

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The critical behavior of the s-state Ashkin-Teller-Potts model on a square lattice is studied for s = 3, 4, and 5, using a variational renormalization-group transformation of the type introduced by Kadanoff. For the s = 3 and s = 4 models, the transformation correctly predicts a continuous phase transition. The calculated values of the critical exponents and the transition temperature are consistent with the results obtained from other approaches. For s = 5, however, the transformation fails to detect the first-order transition that is known to occur.

### I. INTRODUCTION

After a period of comparative neglect, there has recently been a renewed interest in the Ashkin-Teller-Potts (ATP) model.<sup>1,2</sup> The *s*-state ATP model is a generalization of the standard spin- $\frac{1}{2}$ Ising model in which each site of the lattice can lie in one of *s* distinct states. Nearest-neighbor sites interact with energy  $\epsilon_0$  if they are in the same state, and with a different energy  $\epsilon_1$  if they are in different states. There may also be external fields which favor a site being in one or another of the *s* states. Evidently, the spin- $\frac{1}{2}$  Ising model corresponds to s=2. In the  $s \rightarrow 1$  limit, this model describes the percolation problem.<sup>3-5</sup>

The question that has attracted the most attention is the order of the phase transition for the ferromagnetic ( $\epsilon_1 > \epsilon_0$ ) s-state ATP model. Landau mean-field theory<sup>5,6</sup> predicts a first-order transition in all dimensions for s > 2, essentially because the model permits a coupling trilinear in the magnetization variable. On the other hand, Baxter<sup>7</sup> has shown by an exact calculation that the s-state ATP model on a square lattice has a firstorder transition for s > 4, and a continuous transition for  $s \le 4$ . Series-expansion results<sup>8-10</sup> in two dimensions are consistent with a continuous transition for s = 3 and s = 4. There has been considerable numerical work<sup>10-13</sup> with series expansion for the three-state ATP model in three dimensions. These calculations indicate a continuous or nearly continuous phase transition.

Renormalization-group (RG) techniques have been used by many authors to study the continuum generalization<sup>14</sup> of the ATP model. Using an approximate RG recursion formula, Golner<sup>14</sup> has found the transition in the three-state model to be first order in both two and three dimensions.  $\epsilon$ -expansion calculations<sup>15-17</sup> near four dimensions indicate that all the fixed points are unstable with respect to the trilinear coupling. All indications are that this instability leads to a first-order transition for s > 2. Priest and Lubensky<sup>17</sup> have found a new fixed-point which is stable in  $6 - \epsilon'$  dimensions. For s = 1, this fixed-point can be identified as the one that describes the percolation problem. However, for s = 3 and s = 4, this fixed point can not be related to the continuous phase transition that is known to occur in two dimensions.

In recent years, many position-space RG schemes<sup>18-22</sup> have been developed and very successfully applied to the spin- $\frac{1}{2}$  Ising system. This paper describes the application of the variational RG scheme proposed by Kadanoff<sup>21,22</sup> to the sstate ATP model on a square lattice. The approximate RG recursion relations in this scheme are relatively easy to obtain and this scheme gives excellent results for the critical exponents for the spin- $\frac{1}{2}$  Ising model. The fact that the RG results for the continuum version of the ATP model contradict some of the known properties of the lattice model makes it a very interesting system to study in a position-space RG scheme.

In Sec. II, the application of Kadanoff's lowerbound RG transformation to the ATP model on a square lattice is described. The results for the three-, four-, and five-state models are discussed in Sec. III. The results for the  $s \rightarrow 1$  (percolation) limit have been reported in an earlier paper.<sup>23</sup>

# II. APPLICATION OF KADANOFF'S VARIATIONAL RG TRANSFORMATION TO THE ATP MODEL ON A SQUARE LATTICE

The *s*-state ATP model is defined by the Hamil-tonian

$$H^{(s)} = -J \sum_{\langle ij \rangle} (s \delta_{n_i n_j} - 1) - h \sum_i (s \delta_{n_i^1} - 1), \quad (1)$$

where for each site i, the ATP variable  $n_i$  as-

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sumes the values  $1, 2, \ldots, s$ , the sum  $\langle ij \rangle$  is over nearest-neighbor pairs, and  $\delta_{mn}$  is the Kronecker delta. The first term in the Hamiltonian represents the nearest-neighbor interaction. If two neighboring sites are in the same state, they interact with energy  $\epsilon_0 = -J(s-1)$ . If they are in different states, the interaction energy is  $\epsilon_1 = J$ . J > 0 corresponds to the ferromagnetic model. The second term in the Hamiltonian represents interaction with an external field in the "1" direction.

An RG transformation takes a Hamiltonian  $H_{\vec{k}}(\sigma)$ where  $\sigma$  represents the initial set of spin variables and  $\vec{K}$  represents a set of coupling constants, to a new Hamiltonian  $H_{\vec{K}'}(\mu)$  involving a new set of coupling constants  $\vec{K}'$  and a smaller number of variables  $\mu$ . For the *s*-state ATP model on a square lattice, we consider a Hamiltonian of the form

$$H_{\vec{k}}(\sigma) = -k_B T \sum_{\text{squares}} h_{\vec{k}}(\sigma_1, \sigma_2, \sigma_3, \sigma_4) , \qquad (2)$$

where  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$ , and  $\sigma_4$  represent, in cyclic order, the four ATP variables at the corners of the square. The variational RG transformation used in this paper has the form

$$h_{\vec{k}'}(\mu_{1}, \mu_{2}, \mu_{3}, \mu_{4}) = \ln \operatorname{Tr}_{\sigma_{1} \cdots \sigma_{4}} \exp \left\{ x \left[ s \left( \delta_{\mu_{1}\sigma_{1}} + \delta_{\mu_{2}\sigma_{2}} + \delta_{\mu_{3}\sigma_{3}} + \delta_{\mu_{4}\sigma_{4}} \right) - 4 \right] + 4h_{\vec{k}} \left( \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4} \right) - f \left( \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4} \right) \right\},$$

$$f \left( \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4} \right) = \ln \operatorname{Tr}_{\mu} \exp \left\{ x \left[ s \left( \delta_{\mu\sigma_{1}} + \delta_{\mu\sigma_{2}} + \delta_{\mu\sigma_{3}} + \delta_{\mu\sigma_{4}} \right) - 4 \right] \right\}.$$
(3)

Here, x is a variational parameter. This transformation, which yields a lower-bound to the exact free energy, is a straightforward generalization of the lower-bound transformation used by Kadanoff in his treatment of the spin- $\frac{1}{2}$  Ising model. For s=2, Kadanoff's spin- $\frac{1}{2}$  Ising transformation is recovered. At each renormalization step, the number of variables is reduced by a factor of 4. [For the details of how the transformation (3) is constructed, see Ref. 23.]

 $h_{\vec{k}}(\sigma_1, \ldots, \sigma_4)$  is written in the form

$$h_{\vec{\mathbf{K}}}(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = \sum_{i} K_i s_i(\sigma_1, \sigma_2, \sigma_3, \sigma_4), \qquad (4)$$

where, within each square, the set  $\{s_i\}$  includes all the possible interactions which are consistent with the point-group symmetries of the square. These interactions are listed in Appendix A. All these interactions have been made traceless with respect to each of the variables involved. When there is no symmetry-breaking external field, only the first seven interactions  $s_0, s_1, \ldots, s_6$  (the so-called "even-spin" interactions) have to be considered. If an external field is introduced in the "1" direction, the remaining ten interactions  $s_7, \ldots, s_{16}$  (the "odd-spin" interactions) have to be taken into account.

The transformation (3) has the property that, if  $h_{\vec{k}}(\sigma_1, \ldots, \sigma_4)$  is completely symmetric in the four  $\sigma$  variables, then  $h_{\vec{k}'}(\mu_1, \ldots, \mu_4)$  is also symmetric in the four  $\mu$  variables. Difficulties arising from extra relevant variables<sup>22</sup> are encountered if this transformation is used outside this invariant subspace of Hamiltonians. To avoid such difficulties, we confine our attention to that 12-dimensional subspace of the full 17-dimensional coupling-constant space in which  $K_1 = K_2$ ,  $K_5 = K_6$ ,  $K_8 = K_9$ ,  $K_{1\ 1} = K_{12}$ , and  $K_{15} = K_{16}$ . This corresponds to considering the Hamiltonian

$$H_{\vec{K}}(\sigma) = -k_B T \sum_{\text{squares}} \sum_{i} K_i S_i(\sigma_1, \sigma_2, \sigma_3, \sigma_4), \quad (5)$$

where  $S_0 = s_0$ ,  $S_1 = s_1 + s_2$ ,  $S_2 = s_3$ ,  $S_3 = s_4$ ,  $S_4 = s_5 + s_6$ ,  $S_5 = s_7$ ,  $S_6 = s_8 + s_9$ ,  $S_7 = s_{10}$ ,  $S_8 = s_{11} + s_{12}$ ,  $S_9 = s_{13}$ ,  $S_{10} = s_{14}$ , and  $S_{11} = s_{15} + s_{16}$ . Starting from the Hamiltonian defined in Eq. (1), one can enter this symmetric subspace by performing an exact decimation transformation<sup>19</sup> in which every other ATP variable on the lattice is summed over.

The transformation (3) can be written as a transformation on the coupling constants of the form  $\vec{K}' = R_x(\vec{K})$ . Both the fixed-point structure of this transformation and the location of a fixed point in the coupling-constant space depend on the value of the variational parameter x. The value of x appropriate for a given fixed point  $x^*$  is taken to be the value which maximizes the lower bound to the free energy for the fixed-point Hamiltonian.

#### III. RESULTS

For the three-state model, not all the 12 interactions  $S_0, S_1, \ldots, S_{11}$  are linearly independent. We find that the following relations are satisfied for all possible configurations of the four ATP variables on the square

$$2S_3 = S_4, \quad S_7 = S_8, \quad 4S_9 = 4S_{10} + S_{11}. \tag{6}$$

So, one has to consider recursion relations for the following nine coupling constants:  $K_0$ ,  $K_1$ ,  $K_2$ ,  $K_3 + 2K_4$ ,  $K_5$ ,  $K_6$ ,  $K_7 + K_8$ ,  $K_9 + 4K_{11}$ , and  $K_{10} - 4K_{11}$ . These recursion relations exhibit several fixed points. However, for only one of these is there an  $x^*(=0.562)$  that maximizes the lower bound to the free energy of the fixed-point Hamiltonian. This fixed-point, which for  $x = x^*$ , is located at  $K_1 = 0.09080$ ,  $K_2 = 0.02413$ ,  $K_3 + 2K_4 = -0.00386$ ,  $K_5 = K_6 = K_7 + K_8 = K_9 + 4K_{11} = K_{10} - 4K_{11} = 0$ , has the characteristics of a second-order fixed point (only one relevant eigenoperator with even-spin symmetry). This is in agreement with the Baxter result that the three-state ATP model on a square lattice undergoes a second-order phase transition in the absence of any external symmetry-breaking field.

We have used the standard procedure<sup>24,25</sup> to calculate the critical exponents from the optimal lower-bound recursion relations  $\vec{K}' = R_{x*}(\vec{K})$ . The exponents  $\nu$  and  $\delta$  are obtained by using the relations

$$\nu = \ln 2 / \ln \lambda_e, \qquad (7)$$
  
$$\delta = \ln \lambda_0 / (\ln 4 - \ln \lambda_0),$$

where  $\lambda_e$  is the eigenvalue for the relevant eigenoperator with even-spin symmetry and  $\lambda_0$  is the eigenvalue for the most relevant eigenoperator with odd-spin symmetry (there are two relevant eigenoperators with odd-spin symmetry). The values of the other static exponents  $\alpha$ ,  $\beta$ , and  $\gamma$ are then obtained by using the scaling relations  $d\nu = 2 - \alpha$ ,  $\alpha + \beta(\delta + 1) = 2$ , and  $\alpha + 2\beta + \gamma = 2$ . The results are listed and compared with series expansion results in Table I. The agreement is found to be quite good. Berker and Wortis<sup>26</sup> have used a position-space renormalization-group

TABLE I. Numerical results for the critical exponents for the three-state ATP model.

Exponent	Value obtained from		
	This work	Series expansion	
α	0.326	$0.05 \pm 0.10^{a}$	
β	0.107	$0.103 \pm 0.010$ <sup>b</sup>	
		$0.105 \pm 0.005$ <sup>c</sup>	
γ	1.460	$1.5 \pm 0.1^{b}$	
		$1.45 \pm 0.15$ °	
		$1.42 \pm 0.05^{d}$	
ν	0.837		
δ	14.644	$15.2 \pm 0.5$ °	
		$15.0 \pm 0.5^{e}$	

<sup>a</sup>See Ref. 8. Later calculations (Refs. 9 and 10) indicate that these authors underestimated the value of  $\alpha$ .

<sup>d</sup>See Ref. 10.

<sup>e</sup>See Ref. 13.

TABLE II. Numerical results for the critical exponents for the four-state ATP model.

Exponent	Value obtained from		
	This work	Series expansion	
α	0.488	$0.64 \pm 0.05^{a}$	
β	0.091	$0.089 \pm 0.03^{a}$	
γ	1.330	$1.20 \pm 0.05^{b}$	
ν	0.756		
δ	15.527	$15.8 \pm 0.8$ <sup>c</sup>	
See Ref. 30.	<sup>b</sup> See Ref. 1	0. <sup>c</sup> See Ref.	

transformation of the Niemeyer-van Leeuwen<sup>18</sup> type to study the Blume-Emery-Griffiths model on a square lattice and have calculated the critical exponents for the three-state ATP model to which the Blume-Emery-Griffiths model reduces for specific values of the interaction constants. Their results ( $\alpha = 0.192$ ,  $\beta = 0.117$ ,  $\gamma = 1.574$ ) are in reasonable agreement with those presented here. Burkhardt, Knops, and den Nijs<sup>27</sup> have independently obtained almost identical results by using a transformation similar to the one used here.

The transition temperature is determined by finding the value of  $J/k_BT$  for which the fixed point can be reached by first applying the decimation transformation to the Hamiltonian defined in Eq. (1) (with h=0) and then repeatedly applying the lower-bound transformation. Numerically, we find that  $J/k_BT_c = 0.346$ , in good agreement with the exact result,  $J/k_BT_c = 0.335$ , ..., obtained by locating the fixed point of the dual transformation<sup>2,28</sup> which is known to exist for the *s*-state ATP model on a square lattice.

For s = 4, we find that  $3S_9 = 3S_{10} + S_{11}$  for all possible configurations on the square. So, we consider recursion relations for the 11 coupling constants,  $K_0$ ,  $K_1$ ,  $K_2$ ,  $K_3$ ,  $K_4$ ,  $K_5$ ,  $K_6$ ,  $K_7$ ,  $K_8$ ,  $K_9 + 3K_{11}$ , and  $K_{10} - 3K_{11}$ . The fixed-point structure is found to be qualitatively similar to that for the three-state model. The second-order fixed point is the only one at which the lower bound to the free energy can be maximized. This is in agreement with the Baxter result of a continuous transition for the four-state ATP model on a square lattice. For  $x = x^* = 0.444$ , the fixed-point is located at  $K_1 = 0.06465$ ,  $K_2 = 0.01887$ ,  $K_3 = -0.00450$ ,  $K_4 = 0.00123$ ,  $K_5 = K_6 = K_7 = K_8 = (K_9 + 3K_{11}) = (K_{10} - 3K_{11}) = 0$ .

The numerical results for the critical exponents are listed and compared with series results in Table II. The calculated value of  $J/k_BT_C$  (= 0.283) is quite close to the exact value,  $J/k_BT_C$ = 0.2748, ....

Baxter has shown that the s-state ATP model on a square lattice exhibits a first-order phase

<sup>&</sup>lt;sup>b</sup>See Ref. 8.

<sup>&</sup>lt;sup>c</sup>See Ref. 9.

transition for s > 4. According to Nienhuis and Nauenberg,<sup>29</sup> the occurrence of a first-order transition is indicated by the presence of a "discontinuity" fixed point, characterized by a relevant eigenoperator with eigenvalue  $l^d$  (l is the change of scale of length under the RG transformation) corresponding to each order parameter that changes discontinuously at the transition. So, for s = 5, one would expect to find a fixed point with  $\lambda_{e} = \lambda_{0}$ =4, corresponding to the discontinuities in the derivatives of the free energy with respect to the temperature and the external field variables respectively. The calculations, however, do not show such a fixed point. For s = 5, all the 12 interactions are linearly independent. The lower bound to the free energy can be maximized at only one fixed point, which for  $x = x^* = 0.370$ , is located at  $K_1 = 0.04995$ ,  $K_2 = 0.01410$ ,  $K_3 = -0.00224$ ,  $K_4$ = 0.00042,  $K_5 = K_6 = \cdots = K_{11} = 0$ . This fixed point corresponds to  $J/k_BT_C = 0.241$  (exact value: 0.2349,...) and has one relevant even-spin eigenoperator with eigenvalue 2.643 and two relevant odd-spin eigenoperators with eigenvalues 3.698 and 1.336. The fact that both  $\lambda_e$  and  $\lambda_0$  increase with s indicates a trend towards a first-order transition for large s. However, the calculated values of  $\lambda_e$  and  $\lambda_0$  for s = 5 are quite different from the expected values,  $\lambda_e = \lambda_0 = 4$ . The reason for this discrepancy is not clear. The most probable explanation is that the single-parameter variational transformation (3) fails to give a sufficiently good fit to the free energy for s = 5. (Application of Midgal's approximate recursion relations to the ATP model in two dimensions<sup>31</sup> yields second-order exponents for all s. Series calculations<sup>9,10</sup> for the s = 5 model in two dimensions also fail to show a first-order transition. These results indicate that a very good approximation is necessary in order to detect the true nature of the transition.) The excellent agreement between the results obtained by using this transformation and the results obtained from other approaches for the s = 1,<sup>23</sup> s = 2,<sup>22</sup> and s = 3 (see Table I) models indicates that the transformation works very well for small values of s. However, it can be seen from Table II that the agreement is not so good for s = 4. Thus, it seems that the fit to the free energy deteriorates as s is increased. A better approximation can, in principle, be obtained by using a transformation that involves more variational parameters. In particular, the three-spin interaction  $S_2$ , which gives rise to a term trilinear in the magnetization variable in the mean-field free energy, is expected to become more and more important as s is increased. This seems to indicate that, for a sufficiently good approximation for the free energy for large s, one should include in the

transformation a new term that corresponds to the three-spin interaction. Unfortunately, such a term in the transformation cannot be handled within the framework of the present scheme.

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#### APPENDIX A: INTERACTIONS WITHIN A SQUARE

For the *s*-state ATP model with an external field in the "1" direction, the following 17 interactions have to be considered.

#### Even-spin interactions

$$\begin{split} s_{0} &= 1 , \quad s_{1} = \sum_{P} \left( s \, \delta_{\sigma_{1} \sigma_{2}} - 1 \right) , \quad s_{2} = \frac{1}{2} \sum_{P} \left( s \, \delta_{\sigma_{1} \sigma_{3}} - 1 \right) , \\ s_{3} &= \sum_{P} \left[ s^{2} \delta_{\sigma_{1} \sigma_{2} \sigma_{3}} - s \left( \delta_{\sigma_{1} \sigma_{2}} + \delta_{\sigma_{2} \sigma_{3}} + \delta_{\sigma_{3} \sigma_{1}} \right) + 2 \right] , \\ s_{4} &= \sum_{P} \left[ \frac{1}{4} s^{3} \delta_{\sigma_{1} \sigma_{2} \sigma_{3} \sigma_{4}} - s^{2} \left( \delta_{\sigma_{1} \sigma_{2} \sigma_{3}} \right) + s \left( \delta_{\sigma_{1} \sigma_{2}} + \frac{1}{2} \delta_{\sigma_{1} \sigma_{3}} \right) - \frac{3}{4} \right] , \\ s_{5} &= \sum_{P} \left( \frac{1}{2} s^{2} \delta_{\sigma_{1} \sigma_{2}} \delta_{\sigma_{3} \sigma_{4}} - s \, \delta_{\sigma_{1} \sigma_{2}} + \frac{1}{2} \right) , \\ s_{6} &= \left[ s^{2} \delta_{\sigma_{1} \sigma_{3}} \delta_{\sigma_{2} \sigma_{4}} - s \left( \delta_{\sigma_{1} \sigma_{3}} + \delta_{\sigma_{2} \sigma_{4}} \right) + 1 \right] . \end{split}$$

#### **Odd-spin interactions**

$$\begin{split} s_{7} &= \sum_{P} \left( s \delta_{\sigma_{1} 1} - 1 \right), \\ s_{8} &= \sum_{P} \left[ s^{2} \delta_{\sigma_{1} \sigma_{2} 1} - s \left( \delta_{\sigma_{1} 1} + \delta_{\sigma_{2} 1} \right) + 1 \right] - s_{1}, \\ s_{9} &= \frac{1}{2} \sum_{P} \left[ s^{2} \delta_{\sigma_{1} \sigma_{3} 1} - s \left( \delta_{\sigma_{1} 1} + \delta_{\sigma_{3} 1} \right) + 1 \right] - s_{2}, \\ s_{10} &= \sum_{P} \left[ s^{3} \delta_{\sigma_{1} \sigma_{2} \sigma_{3} 1} - s^{2} \left( \delta_{\sigma_{1} \sigma_{2} 1} + \delta_{\sigma_{2} \sigma_{3} 1} + \delta_{\sigma_{3} \sigma_{1} 1} \right) \right. \\ &+ s \left( \delta_{\sigma_{1} 1} + \delta_{\sigma_{2} 1} + \delta_{\sigma_{3} 1} \right) - 1 \right] - s_{3}, \\ s_{11} &= \frac{s}{6} \sum_{P} \left[ s^{2} \delta_{\sigma_{1} 1} \left( \delta_{\sigma_{2} \sigma_{3}} + \delta_{\sigma_{3} \sigma_{4}} \right) \right. \\ &- s \left( \delta_{\sigma_{2} \sigma_{3}} + \delta_{\sigma_{3} \sigma_{4}} + 2 \delta_{\sigma_{1} 1} \right) + 2 \right], \\ s_{12} &= \frac{s}{6} \sum_{P} \left[ s^{2} \delta_{\sigma_{1} 1} \delta_{\sigma_{2} \sigma_{4}} - s \left( \delta_{\sigma_{1} 1} + \delta_{\sigma_{2} \sigma_{4}} \right) + 1 \right], \end{split}$$

$$\begin{split} S_{13} &= \sum_{P} \begin{bmatrix} \frac{1}{4} S^{4} \delta_{\sigma_{1} \sigma_{2} \sigma_{3} \sigma_{4} 1} - S^{3} \delta_{\sigma_{1} \sigma_{2} \sigma_{3} 1} + S^{2} \\ &\times (\delta_{\sigma_{1} \sigma_{2} 1} + \frac{1}{2} \delta_{\sigma_{1} \sigma_{3} 1}) - S \delta_{\sigma_{1} 1} + \frac{1}{4} \end{bmatrix} - S_{4} ,\\ S_{14} &= \frac{S}{12} \sum_{P} \begin{bmatrix} S^{3} \delta_{\sigma_{1} \sigma_{2} \sigma_{3}} \delta_{\sigma_{4} 1} - S^{2} \\ &\times (\delta_{\sigma_{1} \sigma_{2} \sigma_{3}} + \delta_{\sigma_{1} \sigma_{2}} \delta_{\sigma_{4} 1} + \delta_{\sigma_{2} \sigma_{3}} \delta_{\sigma_{4} 1} + \delta_{\sigma_{1} \sigma_{3}} \delta_{\sigma_{4} 1}) \\ &+ S(2 \delta_{\sigma_{4} 1} + \delta_{\sigma_{1} \sigma_{3}} + \delta_{\sigma_{1} \sigma_{2}} + \delta_{\sigma_{2} \sigma_{3}}) - 2 \end{bmatrix} ,\\ S_{15} &= \sum_{P} \begin{bmatrix} S^{3} \delta_{\sigma_{1} \sigma_{2}} \delta_{\sigma_{3} \sigma_{4} 1} - S^{2} & (\delta_{\sigma_{3} \sigma_{4} 1} + \delta_{\sigma_{1} \sigma_{2}} \delta_{\sigma_{3} 1} + \delta_{\sigma_{1} \sigma_{2}} \delta_{\sigma_{4} 1}) \\ &+ S(\delta_{\sigma_{3} 1} + \delta_{\sigma_{4} 1} + \delta_{\sigma_{1} \sigma_{2}}) - 1 \end{bmatrix} - 2 S_{5} , \end{split}$$

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$$\begin{split} s_{16} = & \frac{1}{2} \sum_{P} \left[ s^{3} \delta_{\sigma_{1}\sigma_{3}} \delta_{\sigma_{2}\sigma_{4}1} - s^{2} (\delta_{\sigma_{2}\sigma_{4}1} + \delta_{\sigma_{1}\sigma_{3}} \delta_{\sigma_{2}1} + \delta_{\sigma_{1}\sigma_{3}} \delta_{\sigma_{4}1}) \right. \\ & + s (\delta_{\sigma_{2}1} + \delta_{\sigma_{4}1} + \delta_{\sigma_{1}\sigma_{3}}) - 1 \right] - 2s_{6} \,. \end{split}$$

Here,  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$ , and  $\sigma_4$  are the four ATP variables at the corners of the square;  $\sigma_1\sigma_2$ ,  $\sigma_2\sigma_3$ ,  $\sigma_3\sigma_4$ , and  $\sigma_4\sigma_1$  are nearest-neighbor pairs;  $\sigma_1\sigma_3$  and  $\sigma_2\sigma_4$  are next-nearest-neighbor pairs;  $\sum_P$  means a sum over all the four cyclic permutations of  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$ , and  $\sigma_4$ ; and

$$\delta_{A_1A_2\cdots A_n} \equiv \delta_{A_1A_2} \delta_{A_2A_3} \cdots \delta_{A_{n-1}A_n}.$$

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