

## Spontaneous alignment of frustrated bonds in an anisotropic, three-dimensional Ising model

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The Ising model on a three-dimensional cubic lattice with all plaquettes in the  $x$ - $y$  frustrated plane is studied by use of a Monte Carlo technique; the exchange constants are of equal magnitude, but have varying signs. At zero temperature, the model has a finite entropy and no long-range order. The low-temperature phase is characterized by an order parameter measuring the  $\mathbb{Z}_4$  symmetry of lattice rotations which is invariant under Mattis gauge transformation; fluctuations lead to the alignment of frustrated bonds into columns and a fourfold degeneracy. An additional factor-of-2 degeneracy is obtained from a global spin flip. The order vanishes at a critical temperature by a transition that appears to be in the universality class of the  $D=3$ ,  $XY$  model. These results are consistent with the theoretical predictions of Blankschtein *et al.* This Ising model is related by duality to phenomenological models of two-dimensional frustrated quantum antiferromagnets.

### I. INTRODUCTION

Since the original suggestion by Villain and collaborators<sup>1-3</sup> much attention has been focused on the phenomenon of "order from disorder"—the ability of thermal or quantum fluctuations to produce long-range order in systems which have disordered classical ground states. Such ordering has been observed in many frustrated classical Heisenberg spin models<sup>4</sup> and in frustrated two-dimensional quantum antiferromagnets.<sup>5</sup> In this paper we shall study a three-dimensional frustrated Ising model, introduced by Blankschtein, Ma, and Berker (BMB),<sup>6</sup> which displays the phenomenon of order arising from disorder. We shall characterize the low-temperature phase by symmetry breaking in an order parameter  $\Psi$  which measures the  $\mathbb{Z}_4$  symmetry of lattice rotations. An important property of  $\Psi$  is that it is invariant under the Mattis gauge transformation<sup>7</sup>—the order parameter is thus independent of the particular realization of bonds producing the frustration. Our viewpoint is therefore different from that of BMB, who chose a particular realization of the signs and focused on the spatial ordering of the spins. Our final results on the universality class of the finite-temperature phase transition are in complete accord with their predictions.

Our interest in this Ising model arose from studies in frustrated quantum Heisenberg antiferromagnets.<sup>8</sup> Although we shall not pursue this connection further here, a synopsis of the mapping<sup>8</sup> runs as follows. The quantum disordered phases of unfrustrated antiferromagnets in two dimensions are known to be described by a  $(2+1)$ -dimensional compact  $U(1)$  gauge theory.<sup>9,10</sup> It has recently been shown<sup>5</sup> that frustration introduces a charge-2 Higgs scalar which reduces the underlying gauge symmetry down to  $\mathbb{Z}_2$ . The resulting  $\mathbb{Z}_2$  gauge theory is dual [in  $(2+1)$  dimensions] to the Ising model. The frustration in the Ising model is a consequence of the Berry phase of instantons and vortices in the Heisenberg antiferromagnets. The order in  $\Psi$  that we find in the low-temperature phase

of the Ising model corresponds to spin-Peierls ordering in the quantum antiferromagnet.<sup>9</sup>

### II. THE MODEL

We shall examine an Ising model partition function

$$Z = \sum_{\{s_i\}} \exp \left[ - \sum_{\langle ij \rangle} J_{ij} s_i s_j \right], \quad (1)$$

where the sites  $i, j$  extend over the vertices of a cubic lattice and  $J_{ij}$  is a nearest-neighbor interaction specified below. A crucial property of  $Z$  is its invariance under the Mattis gauge transformation<sup>7</sup>

$$s_i \rightarrow \varepsilon_i s_i, \quad J_{ij} \rightarrow \varepsilon_i \varepsilon_j J_{ij}, \quad (2)$$

where  $\varepsilon_i = \pm 1$ . Thus, after specification of the magnitudes of  $J_{ij}$ ,  $Z$  depends only upon the signs of gauge-invariant products of  $J_{ij}$ . We will choose these to be

$$\eta_p = \text{sgn}(J_{ij} J_{jk} J_{kl} J_{li}), \quad i, j, k, l \in p, \quad (3)$$

where  $p$  denotes an elementary plaquette of the cubic lattice with vertices  $i, j, k, l$ . We are now ready to specify the model of BMB.<sup>6</sup> We have

$$|J_{i, i+\hat{x}}| = |J_{i, i+\hat{y}}| = J$$

and  $|J_{i, i+\hat{z}}| = J'$  (our Monte Carlo simulations used  $J = J'$  for convenience, although the nature of the results is independent of this choice). We also choose  $\eta_p = -1$  for every plaquette in the  $x$ - $y$  plane and  $\eta_p = +1$  for all other plaquettes. (See Fig. 1.) The  $x$ - $y$  planes are copies of the "odd" model of Villain<sup>1</sup> or a degenerate limit of the "domino" models of André *et al.*<sup>2</sup> With this definition of the partition function, a crucial  $\mathbb{Z}_4$  symmetry is apparent:  $Z$  and all correlation functions of gauge-invariant quantities must be invariant under  $90^\circ$  rotations about the centers of plaquettes in the  $x$ - $y$  plane. Note, however, that any definite choice of the signs of  $J_{ij}$  satisfying (3) will not be invariant under such rotations—it will instead

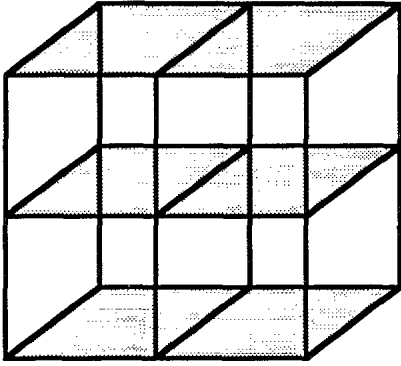


FIG. 1. Schematic of the Ising model. All the shaded (unshaded) plaquettes are frustrated (unfrustrated). All nearest-neighbor exchanges in the  $x$ - $y$  plane have magnitude  $J$  while those in the  $z$  direction have magnitude  $J'$ . We choose  $J=J'$  for convenience.

transform into a gauge-equivalent configuration.

At zero temperature ( $J \rightarrow \infty$ ) the model has an infinite number of degenerate ground states. These are discussed most simply in terms of the link field,

$$Q_{ij} = J_{ij} s_i s_j. \quad (4)$$

The most important property of  $Q_{ij}$  is its invariance under the transformations in Eq. (2). Links with  $Q_{ij} < 0$  ( $Q_{ij} > 0$ ) will be referred to as unfrustrated (frustrated). The ground state is obtained by minimizing the number of frustrated links. However, the values of  $\eta_p$  dictate that there must be an even (odd) number of frustrated links around every plaquette in the  $y$ - $z$  and  $x$ - $z$  planes ( $x$ - $y$  plane). Thus, every configuration of  $Q_{ij}$  with (i) one frustrated link around every plaquette in the  $x$ - $y$  plane and (ii) the identical configuration on every  $x$ - $y$  plane, will be a ground state. Two such configurations are shown in Figs. 2(a) and 2(b). Each configuration of the  $Q_{ij}$  can be associated with a dimer covering on the dual square lattice: the ground-state degeneracy therefore equals the number of such coverings. Correlation functions in the ground-state manifold can be calculated exactly and are found to decay by a power law to 0 in the  $x$ - $y$  plane<sup>2,11</sup> and are constant in the  $z$  direction. Thus, there is no long-range order at  $T=0$ .

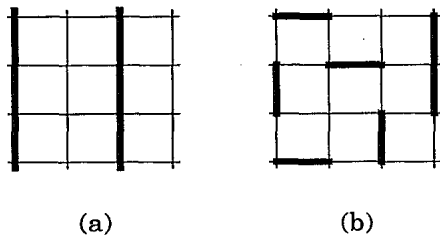


FIG. 2. Two possible ground-state configurations of the  $Q_{ij}$  field. Thick (thin) lines denote  $Q_{ij} > 0$  ( $Q_{ij} < 0$ ). The configurations are identical on all the  $x$ - $y$  planes. At finite temperatures we find a low-temperature phase in which the system breaks a  $Z_4$  lattice rotation symmetry and has the symmetry of (a) or the three other states related to  $90^\circ$  rotations.

### III. MONTE CARLO RESULTS

We now turn to finite temperatures. The model consisting of a *single*  $x$ - $y$  plane (a fully frustrated two-dimensional Ising model) has been solved exactly<sup>2</sup> and has no long-range order or phase transition at any finite, nonzero temperature. In contrast, the present three-dimensional model does have a finite-temperature phase transition.<sup>6,12</sup> We introduce an order parameter (which is the analog of the spin-Peierls order parameter of Ref. 9) associated with this transition:

$$\Psi = \frac{1}{N_s} \sum_{\langle ij \rangle} \phi_{ij} Q_{ij}, \quad (5)$$

where the sum extends over all the links of the cubic lattice and  $N_s$  is the number of sites in the lattice. The fixed field  $\phi_{ij}$  takes the values  $1, i, -1, -i$  on the links in the  $x$ - $y$  plane as shown in Fig. 3; on all  $z$ -directed bonds we have  $\phi_{ij} = 0$ . These values have been chosen such that, under a rotation about the center of a plaquette in the  $x$ - $y$  plane by an angle  $n\pi/2$ , we have

$$\Psi \rightarrow \Psi \exp \left[ \pm \frac{in\pi}{2} \right], \quad (6)$$

where the sign depends upon the sublattice of the plaquette. This result implies that, in the absence of any spontaneous symmetry breaking, we must have  $\langle \Psi \rangle = 0$ . Below we find a low-temperature phase with  $\langle \Psi \rangle \neq 0$ : this indicates that the frustrated links have aligned themselves into patterns with the symmetry of Fig. 2(a) [with  $\arg(\Psi) = -\pi/2$ ] or one of the three other states [ $\arg(\Psi) = 0, \pi/2, \pi$ ] that can be obtained by a  $Z_4$  rotation of Fig. 2(a). The state in Fig. 2(a) is entropically favored because the largest number of states in the ground-state manifold can be reached from it by a single spin flip.

We now present our Monte Carlo results for the phase transition. The standard Metropolis algorithm was used with  $7.5 \times 10^4$  time steps per site, complemented with the improved Monte Carlo method of Ferrenberg and Swendsen<sup>13</sup> near the critical regions. We worked with lattices with  $N_s = L^3$  sites, where  $L = 10, 20,$  and  $30$ . In Fig. 4 we show our results for  $\langle |\Psi|^2 \rangle^{1/2}$  for these three

	1	1	1	
-i	i	-i	i	
-1	-1	-1		
-i	i	-i	i	
1	1	1		
-i	i	-i	i	
-1	-1	-1		

FIG. 3. Values of the fixed link field  $\phi_{ij}$ . The same pattern is repeated on all the planes and  $\phi_{i, i+\hat{z}} = 0$ .

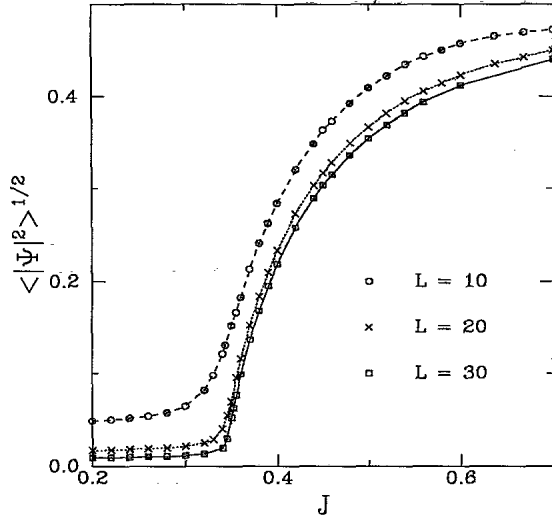


FIG. 4. Magnitude  $\langle |\Psi|^2 \rangle^{1/2}$  of the gauge order parameter  $\Psi$  as a function of the coupling strength  $J$ . The dashed, dotted, and solid lines are guides to the eye for  $L = 10, 20$ , and  $30$ , respectively.

lattice sizes as a function of  $J$ . The results are suggestive of a phase transition around  $J_c \approx 0.35$ . The existence of a phase transition can be more definitively settled by examining the invariant ratio

$$r = \frac{\langle |\Psi|^4 \rangle}{\langle |\Psi|^2 \rangle^2} \quad (7)$$

In an ordered phase we expect  $r \rightarrow 1$  as  $N_s \rightarrow \infty$ . In the disordered phase the fluctuations of  $\Psi$  are expected to be Gaussian around  $\Psi = 0$ . Because  $\Psi$  is a complex scalar, we therefore expect  $r \rightarrow 2$  as  $N_s \rightarrow \infty$ . The results in Fig. 5(a) are in complete accord with these expectations. We expect, moreover, that, for finite  $L$  and near  $J_c$ ,  $r$  will obey the scaling form

$$r = f((J - J_c)L^{1/\nu}) \quad (8)$$

The fit to such a scaling form is shown in Fig. 5(b) and we obtain a value of  $\nu = 0.63 \pm 0.05$  and  $J_c = 0.347$ .

The  $Z_4$ -lattice-symmetry-breaking pattern of the low-temperature phase suggests that the phase transition is in the universality class of the  $D=3$   $Z_4$  clock model or, equivalently, the two-color Ashkin-Teller model. The second-order transition in the latter model is  $XY$  like<sup>14</sup> and the exponent  $\nu_{XY} \approx \frac{2}{3}$  is consistent with our results; an  $XY$  transition was also predicted by BMB.<sup>6</sup> Further evidence for the  $XY$  nature of the transition can be obtained from the specific heat of the model which has also been measured by Grest.<sup>12</sup> Our measurements are shown in Fig. 6. There is a well-defined peak whose height increases logarithmically with  $L$  (inset of Fig. 6), consistent with the results of Grest.<sup>12</sup> Scaling suggests that this height should increase as  $L^{\alpha/\nu}$ —our results are thus consistent with the  $D=3$   $XY$  exponent of  $\alpha \approx 0$ . The asymmetry of the specific-heat peak is also consistent with that expected for the  $XY$  model:<sup>15</sup> the specific heat for  $J = J_c + \Delta J$  is greater than for  $J = J_c - \Delta J$ .

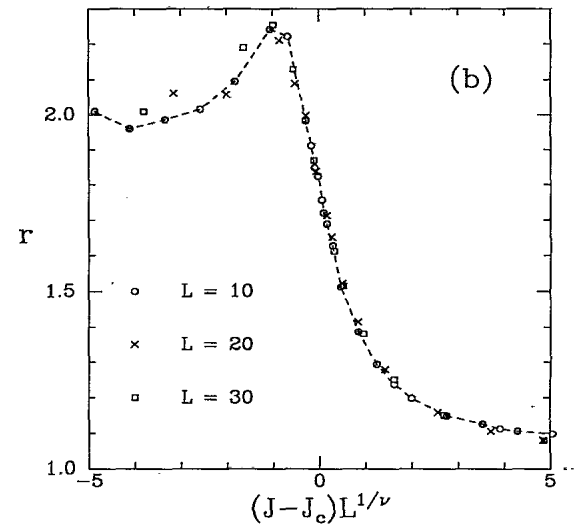
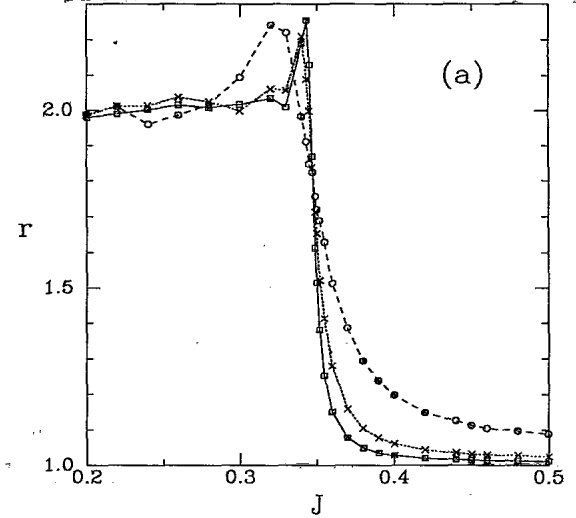


FIG. 5. (a) Invariant ratio  $r$  [Eq. (7)] vs the coupling strength. The three lines cross at  $J_c \approx 0.35$ . The peak structure below  $J_c$  is due to finite-size effects. (b) Scaling plot of the invariant ratio  $r$ . Notice the data collapsing in the critical region. The fitting parameters are  $\nu = 0.63$  and  $J_c = 0.347$ . The dashed line is a guide to the eye through the points with  $L = 10$ .

After a given choice of gauge for the  $J_{ij}$  satisfying (3) and the specification of given configuration of  $Q_{ij}$ , there is still a global twofold degeneracy in the possible values of  $s_i$ . The possibility exists, therefore, that this symmetry is also broken in the low-temperature phase. To discuss this further we have to make a specific choice of gauge. We make the choice that  $J_{ij} = -J$  for all the links except for the thick lines in Fig. 2(a) for which  $J_{ij} = J$ . Let us assume that, of the four low-temperature phases, the system is in the one in which the frustrated bonds are also lined up as in Fig. 2(a), i.e.,  $Q_{ij} > 0$  on the thick lines and  $\arg(\Psi) = -\pi/2$ . The values of  $s_i$  associated with this state are simply  $s_i = 1$  for all  $i$  or  $s_i = -1$  for all  $i$ . For this ordering in this *specific choice of gauge*, we therefore introduce the magnetization

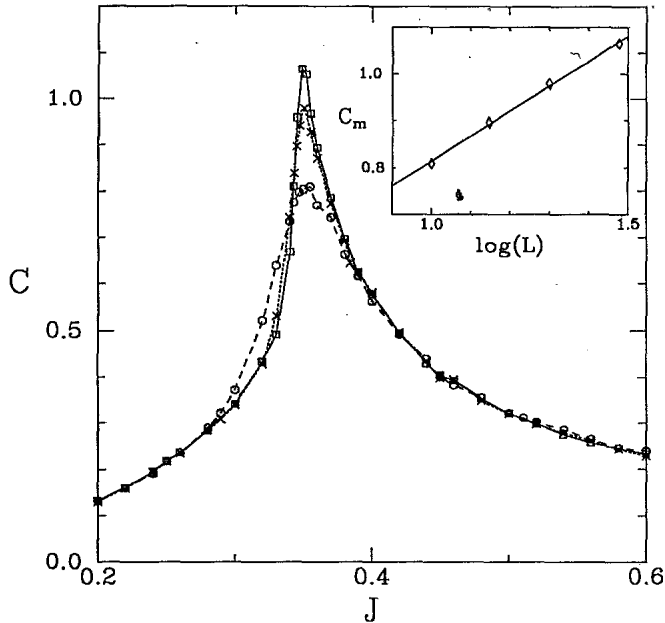


FIG. 6. Specific heat as a function of the coupling strength for  $L = 10$  (circles),  $20$  (crosses), and  $30$  (squares). Inset: height of the specific heat vs the logarithm of the system size  $L$ . The error bars are smaller than the symbol size. The straight line is the best fit through the points for  $L = 10, 14, 20$ , and  $30$ .

$$M = \frac{1}{N_s} \sum_{i=1}^{N_s} s_i. \quad (9)$$

We are interested in exploring the question whether the symmetry  $M \leftrightarrow -M$  is broken. As before, we investigate this question by examining the ratio

$$r_M = \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}. \quad (10)$$

In the high-temperature phase, it can be shown that  $r_M \rightarrow 3$  as  $N_s \rightarrow \infty$ . To calculate  $r_M$  in the low-temperature phase we assume (i) ordering of the  $M$  and (ii) the system samples all four phases with different values of  $\Psi$  equally and does many global spin flips. An additional complication is that the magnetizations associated with the four possible  $\Psi$  phases are not orthogonal. Using all these facts, a simple calculation shows that  $r_M \rightarrow 1.75$  in the low-temperature phase. Our results are shown in Fig. 7 for  $L = 20$ . The high-temperature value is close to 3 and there is an abrupt jump at  $J = J_c$  to a value consistent with 1.75. The extra noise on the low-temperature side is presumably due to the long relational times associated with tunneling between the four  $\Psi$  states and global spin flips.

#### IV. CONCLUSIONS

We have examined a frustrated three-dimensional Ising model shown in Fig. 1, introduced by BMB,<sup>6</sup> by Monte

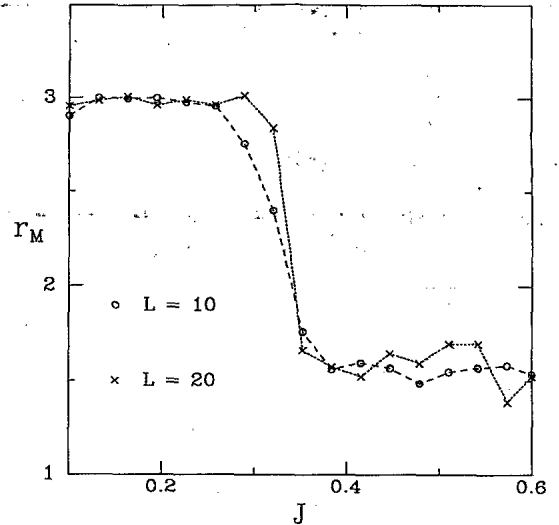


FIG. 7. Invariant ratio  $r_M$  [Eq. (10)] for the magnetization  $M$  vs the coupling strength.

Carlo simulations. At zero temperature the model has no long-range order and an infinite ground-state degeneracy. At finite temperature we find a low-temperature phase with a fourfold degeneracy and long-range order associated with the breaking of the  $Z_4$  symmetry of lattice rotations about the centers of plaquettes in the  $x$ - $y$  plane. The order parameter associated with this phase is one that measures the alignment of frustrated bonds: states of the type shown in Fig. 2(a) (and the three other states that can be obtained by lattice symmetry) are entropically favored as one can reach a maximum number of low-energy states from them by single spin flips. An important property of this order parameter is that it is invariant under Mattis gauge transformation and thus independent of the particular signs chosen for the  $J_{ij}$  to realize the frustration. At a finite temperature we find a transition at which the symmetry is restored; the transition appears to be in the universality class of the  $D = 3$  XY model. If one makes a specific choice of gauge, and allows examination of gauge-dependent quantities, one finds an additional twofold degeneracy in the low-temperature state associated with global spin flips. These results on the universality class of the transition and the degeneracy of the low-temperature phase are in accord with the theoretical predictions of BMB.<sup>6</sup>

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