PHYSICAL REVIEW B VOLUME 25, NUMBER 11 1 JUNE 1982

Ground states and the nature of a phase transition in a simple cubic fully frustrated Ising model

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(Received 13 April 1981; revised manuscript received 21 August 1981)

The ground state of a fully frustrated simple cubic lattice on N Ising spins is worked out. A degeneracy of the order $2^{N^{2/3}/4}$ is found. A possible phase transition is discussed within a Bethe-Peierls approximation and on the basis of symmetry arguments. The transition temperature is in good agreement with recent computer simulations.

I. INTRODUCTION

Recent investigations of spin-glasses[1] have aroused considerable interest in the fully frustrated Ising (FFI) spin systems.[2] Several two-dimensional fully frustrated models have been studied[3–8] so that now one has a fair understanding of the nature of the phase transition at zero temperature in two dimensions. For example, Southern, Chui, and Forgacs[7] showed that the square lattice can be mapped into the eight-vertex model. Forgacs[8] showed that the critical exponent η for this square lattice is equal to $\frac{1}{2}$, in agreement with the result of Stephenson[9] for the triangular lattice.

In three dimensions only one fully frustrated system has been systematically studied. This is the generalization of the triangular net to three dimensions which is the fcc antiferromagnet. The ground state of this system was first elucidated by Danielian.[10] The total number of ground states is of the order of $2^{N^{1/3}}$; hence there is no macroscopic entropy at zero temperature. Various calculations suggest that there is a first-order phase transition at a finite temperature.[11] It is amusing to note that if one takes away a quarter of the spins, a system with macroscopic entropy results.[12] Villain[2] has suggested some other fully frustrated three-dimensional (3D) systems. The generalization of the square lattice to three dimensions is the main focus of the present paper. The unit cell consists of eight smaller cubes, one of which is illustrated in Fig. 1, where a single (double) solid line indicates a ferromagnetic (antiferromagnetic) bond of absolute magnitude J. Figure 2(a) indicates how these smaller cubes are put together. In Fig. 2(b) we show a projection onto the xy plane. The ground state of this model is characterized in Sec. II. A phase transition is discussed in the Bethe-Peierls approximation in Sec. III. The nature of the phase transition is studied using symmetry arguments in Sec. IV. In Sec. V we discuss the nature of the phase transition and compare our results with recent computer simulations. The possible relevance to the existence of a phase transition in an Ising spin-glass will also be speculated.

II. THE FULLY FRUSTRATED CUBIC LATTICE

First the ground state of the cubic FFI lattice will be characterized. It is obvious that the lowest-energy configuration of the cube in Fig. 1 will be such that there is one wrong bond (i.e., a term in the Hamiltonian $-J_{ij}S_iS_j=+J$) on every face of the cube. This can be achieved by using three wrong bonds that do not touch each other. There are eight ways to arrange these bonds with each way having a net energy of $-12J$. This can be easily displayed with a projection of the cube on the xy plane as in Fig. 3, where one configuration of the wrong bonds is shown. In this projection, the location of the antiferromagnetic bonds is irrelevant and hence will no longer be shown. In

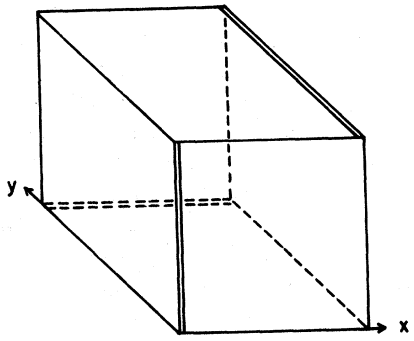

FIG. 1. $\frac{1}{8}$ of the unit cell of the FFI cubic lattice. Here the single (double) line indicate a ferromagnetic (antiferromagnetic) bond.

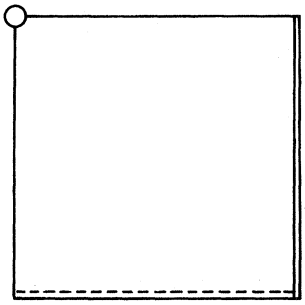

FIG. 3. A graph illustrating the location of the wrong vertical (circle) and horizontal (double line) bonds on the upper (solid lines) and lower (dotted-solid lines) faces.

Fig. 3 the circle denotes the location of the "vertical" wrong bond, the double solid line denotes the wrong horizontal bond on the upper face, and the dotted-solid line denotes the wrong bond on the lower face. The fact that the wrong bonds never meet requires that there be no wrong bonds on the lines connecting the circles. We show in Appendix A that the ground state is "dominated" (by this we mean that the other ground states are less numerous by a factor of $2^{N^{2/3}/4}$) by identical layers such that each layer is made up of a random mixture of the two unit cells as shown in Fig. 4. One such combination is shown in Fig. 5. (Note that the two unit cells of Fig. 4 can be mapped into each other by flipping a vertical line of spins.) Because of the randomness the total number of such states is of the order of $2^{N^{2/3}/4}$. The entropy per particle of the ground state is hence nonmacroscopic, similar to the fcc antiferromagnet. However, the total degeneracy of the fcc antiferromagnet is of the order of $2^{N^{1/3}}$ (Ref. 10) whereas in the present case it is of the order of $2^{N^{2/3}/4}$. This is because in the former case there is only a one-dimensional disorder whereas in the latter case there is a sublattice that possess two-dimensional disorder.

It is of interest to ask what the order parameter is. The choice of an order parameter is clearly not a unique procedure. An elegant choice has been discussed by Betts and Elliot[13] for the fcc antiferromagnet. We shall follow a simpler procedure

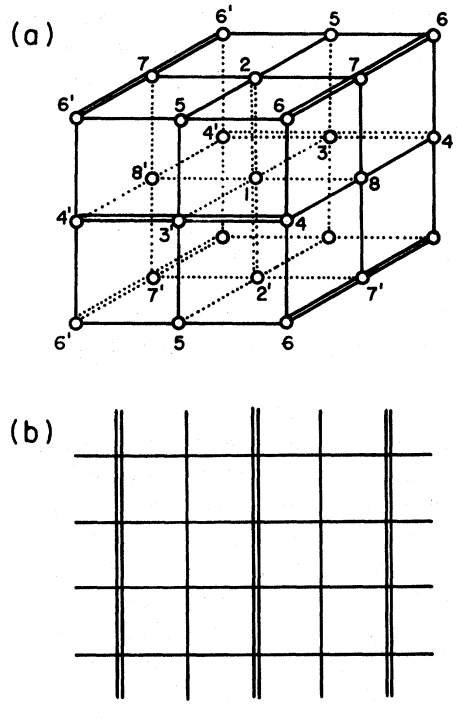

FIG. 2. (a) A unit cell of the FFI cubic lattice indicating how the sublattices in Fig. 1 are put together. (b) A projection of (a) onto the xy plane.

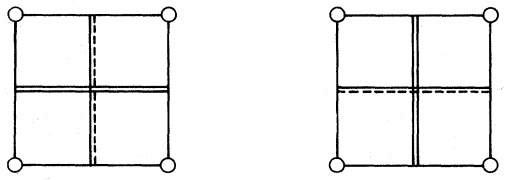

FIG. 4. A graph illustrating the possible ways of arranging the horizontal bonds in a unit cell.

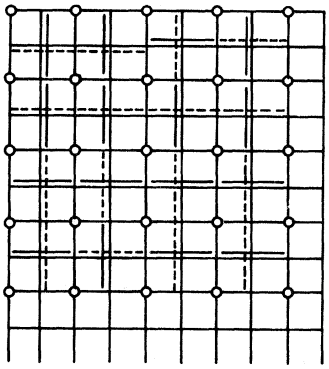

FIG. 5. A configuration of the wrong bonds.

here by specifying the magnetizations at individual sites. The ground state that we just discussed suggests that at $T=0$ there are 12 inequivalent configurations of local magnetizations obtained by specifying the dissatisfied "vertical" bonds with respect to the original lattice. The number 12 comes from the following consideration. One can call vertical the x, y, or z directions of the original lattice. This provides a factor of 3. Once the vertical direction is specified there are four positions at which the dissatisfied vertical bonds can be located with respect to the original lattice of ferro and antiferromagnetic bonds. Hence a total factor of 12.

To illustrate a typical configuration of local magnetization let us consider Fig. 2(a) with the dissatisfied vertical bonds along the antiferromagnetic bonds $\ldots 212' \ldots$, etc. Since there is a degeneracy of the position of the horizontal bonds the average magnetization at $\ldots 646 \ldots$, $\ldots 6'4'6' \ldots$, etc., is zero; i.e., $\langle\sigma_4\rangle=\langle\sigma_6\rangle=\langle\sigma_4'\rangle=\langle\sigma_6'\rangle=0$. The rest of the magnetizations are all of the same average value, i.e., $\langle\sigma_2\rangle=\langle\sigma_1\rangle=\langle\sigma_8\rangle=\langle\sigma_{5'}\rangle=\langle\sigma_{3'}\rangle=\langle\sigma_7\rangle=\langle\sigma_{1'}\rangle=\langle\sigma_{2'}\rangle$ which is one at $T=0$. It is not difficult to write down the other eleven configurations but we shall not do it here.

III. BETHE-PEIERLS APPROXIMATION FOR THE 3D FULLY FRUSTRATED ISING MODEL

In this section we shall carry out a mean-field-type calculation for the 3D FFI model. In order to take into account the competition between the ferromagnetic and antiferromagnetic bonds and also to a certain extent fluctuations in the system, we shall apply an eight sublattice Bethe-Peierls approximation. In this approach the interactions within a given cluster of spins are treated exactly, while the effect of the remaining spins outside the cluster is treated in a mean-field approximation. The cluster we choose is a single spin with its six nearest neighbors. The self-consistency equation for spin 1, for example, on Fig. 2(a) is obtained as

$$m_1=\frac{1}{Z_1}\sum_{(\sigma)}\sigma_1\exp K[\sigma_1(-\sigma_2-\sigma_{2'}+\sigma_3+\sigma_{3'}+\sigma_8+\sigma_{8'})+(\sigma_3+\sigma_{3'})(m_1-2m_4+2m_5)$$
$$+(\sigma_2+\sigma_{2'})(2m_5+2m_7-m_1)+(\sigma_8+\sigma_{8'})(2m_4+m_1+2m_7)]\,. \tag{1}$$

Note that in Eq. (1) bonds such as $\sigma_1\sigma_3$ have not been double counted; this is why we have factors such as $m_1-2m_4+2m_6$. Here $m_i=\langle\sigma_i\rangle$ and Z_1 is the "partition function" of σ_1, i.e., the sum over the σ's of the exponential factor in (1). The other seven equations can be obtained in an analogous way, using Fig. 2(a). In (1) we assumed that $m_3=m_{3'}$, $m_2=m_{2'}$, and $m_8=m_{8'}$. This last approximation (together with similar ones for the other equations) is equivalent to assuming that the system can be divided into eight sublattices, within which the magnetization is the same for the corresponding spins. Since the model is periodic, if there is an ordered state it should also be periodic. Of course the periodicity of the ordered state is not necessarily the same as that of the underlying lattice. Our assumption about the eight sublattices is the simplest, nontrivial approximation which allows for analytical treatment. Note that this assumption does not contradict our previous discussion of the ground state. There are an infinite number of ground states divided into 12 classes. The interclass activation barrier is infinite whereas the intraclass barrier is finite. For equilibrium static properties, we feel that physical averages should be taken over states of one and only one class. The order parameter obtained this way has the same periodicity of the lattice.

The eight self-consistency equations form a closed system of eight nonlinear equations. Assuming that there is an upper critical temperature above which all m_i's are zero and below which at

least one of them is different from zero, we can linearize the nonlinear equations around this temperature. We obtain

$$m_i=\gamma m_i, \quad i=1,2,\ldots,8 \tag{2}$$

where

$$\gamma=\frac{6K\sinh 2K}{1+\cosh 2K} . \tag{3}$$

Setting $\gamma=1$, for the critical temperature we get

$$K_c=0,42 . \tag{4}$$

This result is in good agreement (to within 5%) with recent Monte Carlo simulations.[14,15] It is interesting that Eq. (2) is a set of eight *independent* equations instead of a system of eight coupled equations. Had one applied a simple one-sublattice Weiss mean-field theory[14] one would get a *coupled* system of linear equations. We see that fluctuations in this fully frustrated system are very important. From (2) we get that any ordering is possible in our system in the linear approximation. If we expand Eq. (1) to third order in m we find that this degeneracy is partially but not completely lifted. In fact, although not every solution of (2) is a solution of the nonlinearized version of the self-consistency equation (1), even those nonlinear equations have a large number of solutions (see Appendix B). In order to decide which state is the true thermodynamically stable state at a given temperature, one should calculate the free energy and then minimize it with respect to the m_i's. Unfortunately this task is extremely complicated even for the small cluster we used and therefore we have not carried out the calculation of the free energy. Instead, we will use symmetry considerations for our guidance. The ground-state configurations discussed in the previous section provide one such clue. It is satisfying to note that the configuration discussed at the end of the preceding section is indeed one possible solution of the coupled nonlinear equations at any temperature below T_c.

IV. NATURE OF THE PHASE TRANSITION

The Bethe-Peierls approximation discussed in the preceding section suggests that there is a finite-temperature second-order phase transition in the cubic FFI model. It was, however, also pointed out that fluctuations are very important in this system; therefore, it is not clear how much one should trust a mean-field-type calculation.

In this section we wish to provide a Landau-type analysis[16] of the nature of the phase transition. A summary of the Landau arguments has been given by Mukamel and Krinsky.[17] We shall follow their language. The point group of the cubic FFI model can be identified with the point group T_h. It differs from the cubic group O_h in that the 90° rotation symmetry about the x, y, and z axis is missing.

If the periodicity of the ordered state is not the same as the underlying lattice then the full space group needs to be considered. As we discussed in the previous sections, we shall *assume* that the periodicity of the order is the same as that of the underlying lattice and so shall focus only on the point group here. This considerably simplifies the problem. In problems considered by the authors of Ref. 17, for example, the periodicity of the ordered state is not the same as that of the underlying lattice. Then one has to worry about the full space group of the problem. Even though we have arguments that suggest that the periodicity of the ordered state is the same as the underlying lattice, we have no rigorous proof that this is so. If the periodicity is different then the arguments below are inapplicable. As we discussed at the end of Sec. I, there are twelve inequivalent configurations of the magnetizations. These form a twelve-dimensional representation of the symmetry group. Now no point groups (in particular T_h) have irreducible representations with dimensions larger than three in three dimensions. Hence our twelve-dimensional representation must be reducible. Landau arguments would therefore suggest that this is a first-order phase transition.[18] We have then two methods for the study of the cubic FFI model, which lead to different results.

For two-dimensional FFI models it has been shown that there is no finite-temperature phase transition, but there are universal long-range correlations at $T=0$.[8] For a class of non-fully-frustrated systems studied in Ref. 19, there is a finite-temperature second-order phase transition and the models belong to the universality class of the ferromagnetic Ising model.[19] Consequently, in two dimensions, there is at least a universality class of fully frustrated systems and another one of non-fully-frustrated and nonfrustrated systems. This suggests that the fcc antiferromagnet and the model considered in this work have similar properties. Our Landau-type analysis certainly would be consistent with a first-order phase transition in the

cubic FFI model. This conclusion on the other hand seems to be in disagreement with the Monte Carlo calculations for the cubic FFI model. It should be emphasized, however, that the results of these Monte Carlo simulations for the cubic FFI model should be interpreted with great care.

Even though the macroscopic entropy is zero at $T=0$, the degeneracy is still extremely large. It is of the order of $2^{N^{2/3}/4}$ and $2^{N^{1/3}}$ for the present model and the fcc antiferromagnet, respectively. In order to have comparable accuracy, one would think that one needs to have $2^{N^{2/3}/4}/2^{N^{1/3}}$ samples more for the present model. For a $10\times10\times10$ system this number is $2^{25}/2^{10}=2^{15}$. If the simulations for the present model sampled 2^{15} more points than the fcc antiferromagnet we would feel more comfortable with the final result.

V. CONCLUSION

In this paper we have provided arguments that the fully frustrated cubic model is in many regards the same as the fcc antiferromagnet, another fully frustrated 3D system. They both possess zero macroscopic entropy at $T=0$ and they both undergo a phase transition at a finite temperature. As for the order of the phase transition, calculations for the fcc antiferromagnet suggest that it is of first order. For the cubic FFI model we think this question is not yet settled.

There has been interest in whether an Ising spin-glass possesses a phase transition at a finite temperature in 3D. It is thought that the effect of frustration is such as to destroy a possible finite-temperature phase transition. If, even in the worst case of a fully frustrated model, there is still a finite-temperature phase transition, it is not unreasonable to expect the 3D Ising spin-glass to have a phase transition as well. Our result suggests that the fcc antiferromagnet is not a singular case in three dimensions and that all 3D Ising spin-glasses may possess finite-temperature phase transitions. Real spin-glasses are disordered. The effect of disorder on the phase transition discussed here has not been explored.

ACKNOWLEDGEMENT

We have had helpful conversations with E. Fradkin, J. M. Kosterlitz, and J. Villain. We thank S. Kirkpatrick, E. Fradkin, and C. Jayaprakash for letting us know the results of their Monte Carlo calculation prior to publication. This work is partially supported by NSF Grant No.DMR77-23999 (G.F.).

APPENDIX A

We shall characterize the ground state in this appendix. First let us focus on the order for one layer of the cubes. We shall use the notation of Sec. II and exhibit our order by projecting it onto the xy plane. In every cube there can be one and only one wrong vertical bond. Thus no horizontal face connects two wrong vertical bonds (circle in our figures). Suppose there is a wrong vertical bond at the origin (0, 0). Then it is easy to see that we must have either situation (a) or (b) of Fig. 6 (where only the position of the vertical unsatisfied bond is displayed). The lines of circles continue indefinitely in the y direction. Clearly one may have an equivalent situation of lines of circles continuing in the x direction. Within the strip formed by the circles one now has to insert the wrong horizontal bonds. Within the square *ABCD* in Fig. 6(a) one can have two possible configurations as in Fig. 7. Furthermore there is no correlation between the position of the horizontal bonds from one square *ABCD* to another (e.g., *DCEF*) down the strip. The degeneracy of such configurations is of the order of $2^{N^{1/3}/4}$. On the other hand, the configuration corresponding to (b) is only doubly degenerate, as is shown in Fig. 8. Hence configuration (a) dominates configuration (b).

One might wonder if one can have mixtures of strips of type (a) and (b) in a plane. Perhaps the "entropy of mixing" gained in this way might

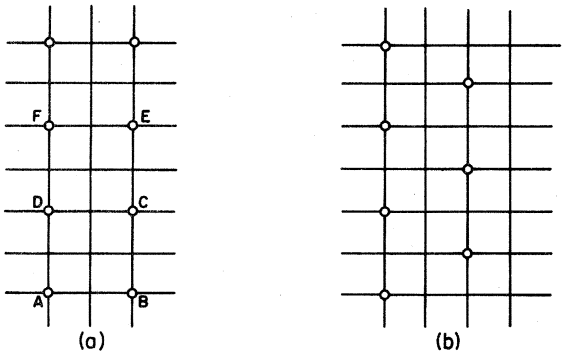

FIG. 6. Two possible ways that the vertical wrong bonds can be arranged.

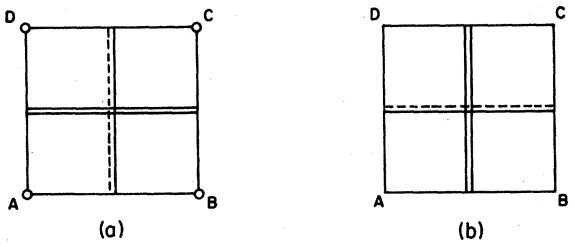

FIG. 7. The possible ways of arranging the horizontal bonds in a unit cell.

compensate for the entropy lost in putting a strip of type (b) in. An upper bound for this degeneracy factor is of the order of

$$D=\sum_{k=1}^{N^{1/3}/2}\begin{bmatrix}N^{1/3}/2\\ k\end{bmatrix}2^{-kN^{1/3}/2}2^k ,$$

where k indicates the number of strips of type (b). The first factor is the "degeneracy of mixing" gained; the second, the degeneracy lost. D can be simply summed and we get

$$D=(1+2^{1-N^{1/3}/2})^{N^{1/3}/2}-1 .$$

This is infinitesimally small for large N. We can thus continue down the x axis with strips of type (a) alone and obtain the situation shown in Fig. 5 for one layer.

Now we have to put in the next layer. If the horizontal wrong bonds are random as in Fig. 5 then one can only put the circles on top of each other. We thus conclude that the positions of the circles continue from layer to layer.

APPENDIX B

In this appendix, the nonlinear version of Eq. (1) will be discussed. Equation (1) can be simplified somewhat by doing the summation over σ_3,σ_3, σ_8,σ_8, and σ_2,σ_2; we write

$$m_i=\sum_{\sigma_i}\sigma_i Z_i(\sigma_i)\Big/\sum_{\sigma_i}Z_i(\sigma_i) , \tag{B1}$$

where

$$Z_i(\sigma)=2^3\prod_{\alpha=1}^{3}[1+\cosh 2K(\sigma+A_{\alpha i})] . \tag{B2}$$

A_{1i}, A_{2i}, and A_{3i} are given in Table I.

It is possible to expand the above to third power in m. One finds that, in contrast to the linear version, the equations are coupled. The equations are in general so complicated that a complete solution is not possible. Based on the symmetry of the ground state, we have found different solutions to these equations. This is sufficient to show that the solutions are still degenerate. We shall exhibit these solutions and show that they are indeed solutions of the full equations (B1) by direct substitution.

A solution suggested at the end of Sec. II is obtained by setting $m_4=m_6=0$, $m_2=m_1=m_8=m_5=m_3=m_7=m$. Then we have $A_{14}=4m$, $A_{24}=0$, $A_{34}=2m$, $A_{16}=-4m$, $A_{26}=4m$, $A_{36}=0$. From this, we get $Z_6(\sigma)=Z_4(\sigma)=2^3\{[1+\cosh 2K\times(\sigma+4m)][1+\cosh 2K(\sigma-4m)](1+\cosh 2K)\}$.

It is obvious that $Z_6(\sigma)$, $Z_4(\sigma)$ is independent of σ. Hence from (B1) we have $m_4=0=m_6$, in agreement with our assumption. We also have $A_{11}=3m$, $A_{21}=3m$, $A_{31}=-3m$. Hence $Z_1(\sigma)=2^3[1+\cosh 2K(\sigma+3m)]^2[1+\cosh 2K(\sigma-3m)]$ and we have

$$m=\frac{\sum_{\sigma}\sigma[1+\cosh 2K(\sigma+3m)]}{\sum_{\sigma}[1+\cosh 2K(\sigma+3m)]}=f_1(m) . \tag{B3}$$

It is easy to verify that identical equations are obtained for $i=2,3,5,7,8$, thus verifying that our starting assumption is valid.

As another example we shall assume the satisfied vertical bonds are at 78.... We set $m_5=m_3=0$ and $m_7=m_8=-m_6=-m_4=m_2=m_1=m$; then $A_{13}=0$, $A_{23}=0$, $A_{33}=0$, $A_{15}=-4m$, $A_{25}=4m$, $A_{35}=0$. Hence both $Z_5(\sigma)$ and $Z_3(\sigma)$ are independent of σ and we get back from Eq. (B1) that $m_5=m_3=0$, consistent with our assumed order. Also, $A_{11}=m$, $A_{21}=3m$, $A_{31}=-m$; hence

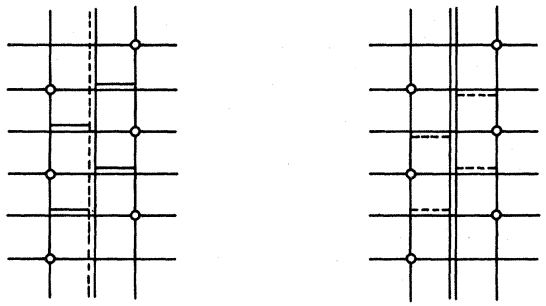

FIG. 8. Two ways of arranging the horizontal bonds when the vertical bonds are in the wrong configuration.

TABLE I. Coefficients used in Bethe-Peierls calculation of the transition.

i	A_{1i}	A_{2i}	A_{3i}
1	$2m_4+m_1+2m_7$	$m_1-2m_4+2m_5$	$-2m_5-2m_7+m_1$
2	$-2m_6+m_2+2m_8$	$2m_6+2m_3+m_2$	$-2m_8-2m_3+m_2$
3	$2m_6+2m_2+m_3$	$-2m_8-2m_6+m_3$	$2m_8+m_3-2m_2$
4	$2m_1+2m_7+m_4$	$2m_5-2m_7+m_4$	$-2m_1-2m_5+m_4$
5	$2m_4-2m_7+m_5$	$-2m_4+2m_1+m_5$	$-2m_1+2m_7+m_5$
6	$-2m_2-2m_8+m_6$	$2m_2+2m_3+m_6$	$-2m_3+2m_8+m_6$
7	$2m_1+m_7+2m_4$	$-2m_5-2m_4+m_7$	$2m_5-2m_1+m_7$
8	$-2m_6+2m_2+m_8$	$-2m_3+2m_6+m_8$	$-2m_2+2m_3+m_8$

$$m=\frac{\sum_\sigma \sigma[1+\cosh 2K(\sigma+3m)]}{\sum_\sigma [1+\cosh 2K(\sigma+3m)]} . \tag{B4}$$

This is the same as (B3). It is easy to verify that identical equations are obtained for $i=7,8,6,4,2,1$. It is easy to check that the other ten configurations discussed in Sec. II are also solutions to Eq. (B1).

These are not the only solutions, however. As an example, let us set $m_1=m_2=m_3=m_4=m_6=m_7=0$ and $m_5=m_8=m^*$. Then $A_{11}=0$, $A_{21}=+2m^*$, $A_{31}=-2m^*$. Hence $Z_1(\sigma)$ is independent of σ and the Eq. (B1) for $i=1$ is satisfied. In the same way, the equations for $i=2,3,4,6,7$ can be verified. We also get $A_{15}=A_{25}=A_{35}=m=A_{18}=A_{28}=A_{38}$. Hence we get for both $i=5$ and 8

$$m^*=\frac{\sum_\sigma \sigma[1+\cosh 2K(\sigma+m^*)]^3}{\sum_\sigma [1+\cosh 2K(\sigma+m^*)]^3}$$

$$=f_2(m^*) . \tag{B5}$$

The linearized version of (2.7) is the same as that of Eq. (B5). The full nonlinearized version is different, however.

By direct numerical evaluation, one can show that $f_2(m)\geq f_1(m)$ for $K>K_c$. Hence the solution m^* of (B5) is always less than the solution m of (B3). This is consistent with our expectation that m^* is not the state of lowest energy of the system. This calculation suggests that even though the linearized version is highly degenerate, the degeneracy is indeed lifted when the nonlinear equations are considered.

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