Coexistence of Order and Disorder and Reentrance in an Exactly Solvable Model

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(Received 10 August 1987)

We show in this Letter *exact* results for the Ising model on the two-dimensional *kagomé* lattice with nearest- and next-nearest-neighbor interactions J_1 and J_2. In some regions of phase space, we find a nonzero critical temperature despite a finite zero-point entropy. For a narrow range of J_2/J_1 we find successive transitions with a reentrance at low temperature. We studied the nature of order by Monte Carlo method and found that in these regions one sublattice remains disordered below the transition and down to zero temperature except in the reentrant region. Thus disorder can coexist with order at equilibrium.

PACS numbers: 05.50.+q, 75.40.Mg

One of the most striking features of frustrated systems is the high degeneracy of the ground state (GS). The questions which arise are whether or not such a degeneracy survives at finite temperatures and how it affects thermodynamic behavior. In the case of Ising spins, it has been[1,2] pointed out that thermal and quenched disorder may select a finite number of particular GS, leading to a well-defined ordered phase at low temperatures. Extension of this idea to XY and Heisenberg[3] systems has been carried out. Such conclusions rely on low-temperature expansions which require that the selected GS upon which low-temperature expansions are performed should differ from the other GS by an infinite number of spin orientations in the thermodynamic limit.[4] This condition is not always fulfilled in frustrated systems such as the fully frustrated simple cubic lattice with Ising spins[4] and systems with finite zero-point entropy. The high GS degeneracy often yields unexpected effects such as partial disordering in the ordered phase in the fully frustrated simple cubic Ising lattice[5] and particular type of excitations[6] observed in Monte Carlo (MC) simulations.

In this Letter, we study the Ising model on the *kagomé* lattice shown in Fig. 1. This system with nearest-neighbor interactions J_1 has been exactly solved a long time ago.[7] In the present work, next-nearest-neighbor interactions J_2 are taken into account. We have obtained the exact expression for the free energy from which exact results for the internal energy, specific heat, and entropy can be derived. The model has a finite zero-point entropy and undergoes a transition at a finite temperature. There are four critical lines in the space (K_1,K_2), where $K_{1,2}=J_{1,2}/k_BT$. One of the most striking points found here is the existence of a reentrant phase in a narrow range of J_2/J_1: As the temperature decreases, the system passes through the paramagnetic phase, an ordered phase, the *reentrant* paramagnetic phase, and the ferromagnetic phase. To investigate the nature of the ordering below the transition, we performed MC simulations. The results show that below the transition, one sublattice remains completely disordered and, except in the reentrant region, this partial disorder persists down to $T=0$. The coexistence of order and disorder thus gives rise to a new type of ordering. In the following we show and discuss our results in detail.

Let us consider the Ising spins σ_i on the *kagomé* lattice of N sites shown in Fig. 1. We take into account the nearest-neighbor interactions J_1 and next-nearest-neighbor interactions J_2. The partition function is written as

$$Z=\sum_{\{\sigma\}}\prod_{\{c\}}\exp[K_1(\sigma_1\sigma_5+\sigma_2\sigma_5+\sigma_3\sigma_5+\sigma_4\sigma_5+\sigma_1\sigma_2+\sigma_3\sigma_4)+K_2(\sigma_1\sigma_4+\sigma_3\sigma_2)], \tag{1}$$

where $K_{1,2}=J_{1,2}/k_BT$ and where the sum is performed over all spin configurations, the product is taken over all elementary cells, and periodic boundary conditions are imposed. Since there is no crossing bond interaction, our system in principle can be transformed into an exactly solvable free-fermion model.[8] Note that our model is somewhat similar to the brickboard Ising lattice recently studied by several authors.[9-11] To obtain the exact solution of our model, we decimate the central spin of each elementary cell of the lattice. In doing so, we obtain a checkerboard Ising model with multispin interactions. This resulting model is equivalent to a symmetrical sixteen-vertex model,[12-14] which satisfies the free-fermion condition.[14] In this case an exact solution can

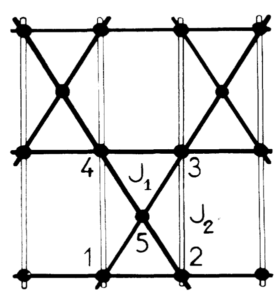

FIG. 1. *Kagomé* lattice. Interactions between nearest neighbors and between next-nearest neighbors, J_1 and J_2, are denoted by black and white bonds, respectively. The lattice sites in a cell are numbered for decimation.

be obtained and the free energy per spin is given by

$$F=-\frac{k_B T}{24\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}d\theta\, d\phi \ln[A+2B\cos\theta+2C\cos\phi+2D\cos(\theta-\phi)+2E\cos(\theta+\phi)], \quad (2)$$

with $A=\omega_1^2+\omega_2^2+\omega_3^2+\omega_4^2$, $B=\omega_1\omega_3-\omega_2\omega_4$, $C=\omega_1\omega_4-\omega_2\omega_3$, $D=\omega_3\omega_4-\omega_7\omega_8$, and $E=\omega_3\omega_4-\omega_5\omega_6$, where

$$\begin{aligned}
\omega_1&=\exp(2K_2+2K_1)\cosh(4K_1)+\exp(-2K_2-2K_1)+\exp(2K_2-2K_1)+\exp(-2K_2+2K_1)+4\cosh(2K_1),\\
\omega_2&=\omega_1-8\cosh(2K_1),\\
\omega_3=\omega_4&=\exp(2K_2+2K_1)\cosh(4K_1)+\exp(-2K_2-2K_1)-\exp(2K_2-2K_1)-\exp(-2K_2+2K_1),\\
\omega_5=\omega_6&=\exp(2K_2+2K_1)\cosh(4K_1)-\exp(-2K_2-2K_1)+\exp(2K_2-2K_1)-\exp(-2K_2+2K_1),\\
\omega_7=\omega_8&=\exp(2K_2+2K_1)\cosh(4K_1)-\exp(-2K_2-2K_1)-\exp(2K_2-2K_1)+\exp(-2K_2+2K_1).
\end{aligned} \quad (2a)$$

The critical condition[14] for this model is

$$\begin{aligned}
&\tfrac{1}{2}[\exp(2K_1+2K_2)\cosh(4K_1)+\exp(-2K_1-2K_2)]+\cosh(2K_2-2K_1)+2\cosh(2K_1)\\
&\quad=2\max\{\tfrac{1}{2}[\exp(2K_1+2K_2)\cosh(4K_1)+\exp(-2K_1-2K_2)];\ \cosh(2K_2-2K_1);\ \cosh(2K_1)\},
\end{aligned} \quad (3)$$

which is decomposed into four critical lines depending on the values of J_1 and J_2. The singularity of F is everywhere logarithmic. Furthermore, our model possesses a disorder line[15,16] for $J_2<0$ and $T>T_c$, where T_c is the critical temperature. Along the disorder line, the partition function is zero dimensional and the correlation functions behave as in one dimension. The internal energy U, the specific heat C_v, and the entropy S can be obtained from Eq. (2) by successive differentiations. In Fig. 2 we show the phase diagram in (K_1,K_2) space. Several important remarks are in order.

(i) In the frustrated regions I, II, and III, the system has a finite zero-point entropy which is $S_0=\frac{1}{3}\ln 2$. This can also be seen directly by considering the structure of the GS: The spins on the elementary squares (sublattice A) can be arranged to satisfy all horizontal and vertical bonds, whatever the signs of J_1 and J_2 are, while the central spins (sublattice B) have zero energy and therefore are freely flipping. Since the total number of spins on sublattice B is $N/3$, the GS degeneracy is $2^{N/3}$, in agreement with S_0 given above. Note that in region III there is one particular GS where the spins on sublattice A are up and those on sublattice B are down. However, this single GS does not contribute to the zero-point entropy in the limit $N\rightarrow\infty$.

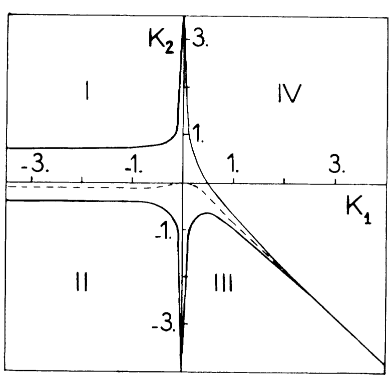

FIG. 2. Phase diagram in the (K_1,K_2) space. The solid curves are critical lines and the dashed curve is the disorder line. The regions numbered I, II, III, and IV are the low-temperature ordered phases.

(ii) There is a finite critical temperature for a given value of J_2/J_1 except in a very narrow range of J_2/J_1 given below where there are several transitions, and when $J_2=0$ and $J_1<0$ where there is no transition as found earlier.[7] Besides, for our model the Hoever-Wolff-Zittartz conjecture[17] does not apply: Though any two GS's in our model are connected by a succession of purely local transformations, a phase transition *does* occur at finite temperature.

(iii) In a very narrow range of J_2/J_1 which is $[-0.91,-1]$ with $J_1>0$, there are successive transitions with decreasing temperature: A trajectory defined by $K_2/K_1=\alpha$, where $\alpha\in[-0.91,-1]$ with $K_1>0$, will cross the critical line of region III twice before crossing the disorder line and then critical line of region IV. These multiple crossings cannot be seen on the scale of Fig. 2. We represent in Fig. 3 these successive transitions in the space (α,T), where $\alpha=J_2/J_1$. One observes that for $\alpha\in[-0.91,-1]$ there are the following successive phases with decreasing temperature: the paramagnetic phase (P), an ordered phase (X), the reentrant P phase, and a ferromagnetic (F) phase. We note that the critical line of Fig. 3 has a vertical tangent and there is an end point at $\alpha=-1$ and $T=0$ where the two critical lines and the disorder line meet. The inset of Fig. 3 shows this region schematically enlarged. The reentrance observed here may be related to the nature of ordering.

In view of the GS structure in the regions I, II, and III of Fig. 2 (in region IV, the GS is ferromagnetic), one may ask the question what is the nature of the ordering

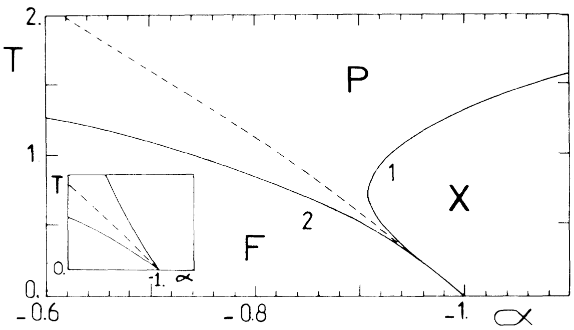

FIG. 3. Phase diagram in the reentrant region ($J_1>0$) of the space (α,T), where $\alpha=J_2/J_1$. T is measured in units of J_1/k_B. Curves 1 and 2 correspond respectively to critical lines of regions III and IV of Fig. 2, dashed line is the disorder line. P, F, and X stand for paramagnetic, ferromagnetic, and an ordered phase, respectively. Inset: Schematically, enlarged region of the end point.

below the transition. To answer this, we performed extensive MC simulations using the sample size of $\frac{4}{3}\times 60\times 60$ sites with periodic boundary conditions. The MC procedure has been described in detail elsewhere (see, e.g., Ref. 5). We discarded 10000 MC steps/spin for equilibrating the system before averaging physical quantities over the next 10000 MC steps/spin. The MC results for internal energy U and specific heat C_v per spin are shown in Fig. 4, where exact results are also presented for comparison. An excellent agreement with exact results is observed (for example, U is identical up to the fifth figure). We show in Fig. 5 the MC result for the Edwards-Anderson sublattice order parameters q_A and q_B as functions of temperature in the case $J_1=-1$ and $J_2=-0.5J_1$. As is seen, sublattice A is ordered up to the transition at T_c while sublattice B stays disordered at

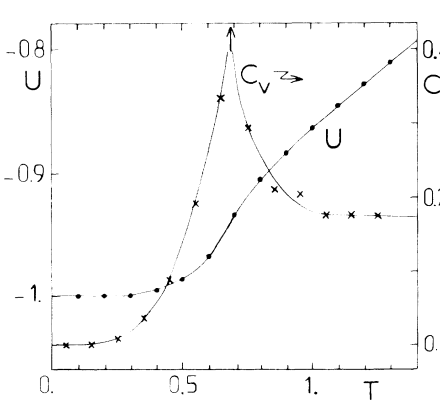

FIG. 4. Internal energy U and specific heat C_v, per spin, as functions of temperature T, for $J_1=-1$ and $J_2=-0.5J_1$. Circles and crosses are Monte Carlo results for U and C_v, respectively. Curves are results from exact solution. Divergence of C_v is indicated by vertical arrow.

all temperatures. This result is remarkable enough; it shows that order and disorder can coexist in an equilibrium state (the equilibrium in MC simulations has been verified not only by comparing U and C_v with the exact results but also by looking at the time dependence of q_A and q_B). The same behavior is seen in the three frustrated regions I, II, and III of Fig. 2 except in the reentrant zone. A similar situation was also numerically observed in some range of temperature in another model.[5] In our opinion, the coexistence of order and disorder occurs each time the GS possesses unconnected freely flipping sets of spin.

We have also calculated by MC simulations the staggered susceptibility and spatial correlation functions from which the critical exponents associated with the transition are computed. The universality class is that of the pure Ising model in two dimensions. The details of MC results, specially in the reentrant region, will be reported elsewhere.

We now discuss the connection between our model and the random-field problem. Since the B spins are free to flip in the frustrated regions as discussed above, they act on their neighboring A spins as an annealed random field. It is easy to see that the probability distribution of this random field at an A site is given by

$$P(H)=\tfrac{1}{4}[2\delta(H)+\delta(H+2J_1)+\delta(H-2J_1)], \quad (4)$$

namely, the random field is *diluted.* Moreover, this field distribution is correlated because each B spin acts on four A spins. Since the B spins are completely disordered at all temperatures it is reasonable to consider this effective "random"-field distribution as quenched. In addition to possible local annealed effects, the phase transition in our model at $T\neq 0$ may be thus a consequence of the above-mentioned dilution and correlation of the random-field distribution. We recall that such a transition is absent in the two-dimensional random-field Ising model.[18]

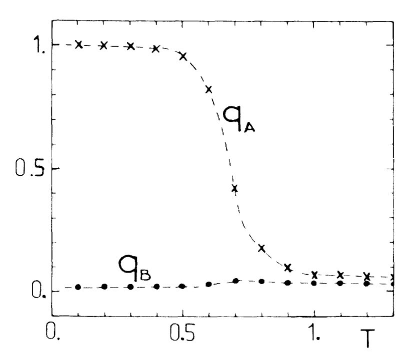

FIG. 5. Monte Carlo results for temperature dependence of sublattice Edwards-Anderson order parameters q_A and q_B (crosses and circles, respectively) in the case $J_1=-1$ and $J_2=-0.5J_1$. Dashed lines are drawn as guides to the eye. Note that exact solution gives the critical temperature T_c for this case at $\simeq 0.693|J_1|/k_B$.

Before concluding, we emphasize that the present solvable model contains one of the most interesting and fundamental aspects of physics of frustrated systems, that is the reentrant phenomenon which has been experimentally observed in various systems. We believe that the necessary, but not sufficient, condition for the occurrence of reentrance at low temperature is the existence of partial disorder in a high-temperature ordered phase (see Fig. 3). The partial disorder just compensates the loss of entropy due to the partial ordering of the high-temperature phase. Finally, we note that the existence of the disorder line in the reentrant paramagnetic phase (see Fig. 3) may also be necessary for the change of ordering from the high-temperature ordered phase to the low-temperature one. In the narrow reentrant paramagnetic region, preordering fluctuations with different symmetries exist near each critical line; they are separated by the disorder line: The system needs to forget the memory of its past.

In conclusion, let us mention that frustrated Ising spin systems with infinite GS degeneracy have been subject to extensive studies.[19] The existence of a phase transition at finite temperature depends on the connectedness of the different GS's. When it is possible to make a low-temperature expansion one may show that the system can eventually select the GS for which the density of low-lying excited states is maximum. This process has been called order by disorder.[1] On the other hand, zero-temperature disorder may contaminate the whole system at finite temperature leading to no phase transition at all.[20] In this Letter, we have shown that a third alternative is possible, namely, the one where partial order coexists at finite temperature with partial disorder below the transition. This possibility can be called *order with disorder.* This new type of ordering may shed light on the understanding of reentrant phenomena.

One of us (H.G.) is supported by a fellowship of Consejo Nacional de Investigaciones, Científicas y Técnicas (Argentina). Discussions with S. Galam, A. Ghazali, and W. Saslow are gratefully acknowledged. One of us (P.A.) wishes to thank Dr. Finn Geipel for encouragement. The simulations have been carried out on the FPS-164 computer of the Groupemente de Recherches Coördonnées "Expérimentation Numérique" at the Ecole Normale Supérieure.

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