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Exact phase diagram of a generalized Kagomé Ising lattice: Reentrance and disorder lines

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We solve exactly a generalized Kagomé Ising lattice with three kinds of interactions by transforming the system into a 16-vertex model that satisfies the free-fermion condition. The phase diagram shows several interesting phenomena due to the frustration generated by the competing interactions: successive transitions with reentrance, partial disorder, and disorder lines. The reentrance region in the space of interaction parameters is found to be infinite, unlike previous exactly solved models. Two disorder solutions with interesting behavior are found.

The reentrance phenomenon has been experimentally observed in various magnetic systems including spin glasses.[1] The origin of the reentrance is the frustration generated by the competition between interactions. In general, the reentrance is so called when there exists a short-range-ordered phase below a long-range-ordered phase on the temperature scale. A well-known example is the spin-glass phase found below the ferromagnetic phase when disorder is introduced into a ferromagnetic (or antiferromagnetic) system.[1] In order to analyze the frustration effects, we are interested here in frustrated Ising spin systems that are periodically defined. These systems without disorder have their own interest in statistical mechanics because they are subject to exact treatment[2] and may have applications in different areas of physics wherever it is possible to map real systems into Ising spin language. For a recent review, the reader is referred to Ref. 3. To date, very few frustrated systems showing the reentrance phenomenon have been exactly solved.[3] A few well-known systems include the centered square (Union Jack) lattice[4] and its generalized versions,[5,6] the Kagomé[7] lattice, an anisotropic centered honeycomb system,[8] complicated cluster models,[9] and a three-dimensional case.[10] In general, the phase diagram shows a rich behavior with paramagnetic reentrance, coexistence of order and disorder, and disorder line. The partial disorder is possible when a set of spins are free to flip, due to competing interactions. In three dimensions, a few systems such as the fully frustrated simple-cubic lattice,[11,12] the stacked triangular antiferromagnet,[13] and a body-centered-cubic (bcc) crystal[14] also exhibit this property, although evidence of a reentrance is found only for the bcc case[14] and a complicated lattice model.[10]

In this paper, we study a generalized Kagomé lattice with Ising spins. The model is shown in Fig. 1 with the following Hamiltonian:

$$H=-J_1\sum_{(i,j)}\sigma_i\sigma_j-J_2\sum_{(i,j)}\sigma_i\sigma_j-J_3\sum_{(i,j)}\sigma_i\sigma_j\ , \qquad (1)$$

where σ_i ($=\pm 1$) is an Ising spin occupying the lattice site i, and the first, second, and third sums run over the spin pairs connected by diagonal, vertical, and horizontal bonds, respectively (see Fig. 1). When $J_2=0$ and $J_1=J_3$, one recovers the original nearest-neighbor (NN) Kagomé lattice,[15] having no transition at finite temperature. The effect of J_2 in the case $J_1=J_3$ has recently been investigated,[7] showing a reentrant phase in a small range of values of J_2.

The phase diagram at temperature $T=0$ is shown in Fig. 2 in the space ($\alpha=J_2/J_1$, $\beta=J_3/J_1$) for positive J_1. The ground-state (GS) spin configurations are also displayed. The hatched regions indicate the three partially disordered phases (I, II, and III) where the central spins are free. Note that the phase diagram is mirror symmetric with respect to the change of the sign of J_1. With negative J_1, it suffices to reverse the central spin in

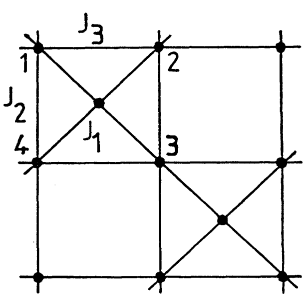

FIG. 1. A generalized Kagomé lattice: diagonal, vertical, and horizontal bonds denote the interactions J_1, J_2, and J_3, respectively. The sites on the corners are numbered from 1 to 4 for decimation.

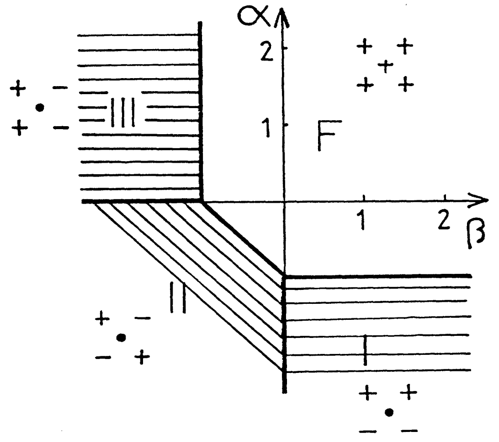

FIG. 2. Phase diagram of the ground state shown in the plane ($\alpha=J_2/J_1$, $\beta=J_3/J_1$). Heavy lines separate different phases and spin configuration of each phase is indicated (up, down, and free spins are denoted by $+$, $-$, and ●, respectively). The three kinds of partially disordered phases and the ferromagnetic phase are denoted by I, II, III, and F, respectively.

the spin configuration shown in Fig. 2. Furthermore, the interchange of J_2 and J_3 leaves the system invariant, since it is equivalent to a $\pi/2$ rotation of the lattice (see Fig. 1).

Let us consider the effect of the temperature on the phase diagram shown in Fig. 2. Partial disorder in the GS is known in some cases to give rise to the reentrance phenomenon in various systems.[4-10] Therefore, similar effects are to be expected in the present system. As it will be shown below, we find a new and richer behavior of the phase diagram: in particular, the reentrance region is found to be extended to infinity, unlike systems previously studied,[4-10] and for some given set of interactions, there exist two disorder lines which divide the paramagnetic phase into regions of different kinds of fluctuations with a reentrant behavior.

To solve our model, let us denote the central spin in a lattice cell shown in Fig. 1 by σ and number the other spins from σ_1 to σ_4. The Boltzmann weight associated to the elementary cell is given by

$$W=\exp[K_3(\sigma_1\sigma_2+\sigma_3\sigma_4)+K_2(\sigma_1\sigma_4+\sigma_2\sigma_3)+K_1\sigma(\sigma_1+\sigma_2+\sigma_3+\sigma_4)]\ , \tag{2}$$

where $K_i=J_i/kT$ ($i=1,2,3$), T being the temperature and k the Boltzmann constant. The partition function is written as

$$Z=\sum_{\{\sigma\}}\prod_{\{C\}}W\ , \tag{3}$$

where the sum is performed over all spin configurations and the product is taken over all elementary cells. Periodic boundary conditions are imposed. To obtain the exact solution, we decimate the central spin of each elementary cell of the lattice. We then obtain a checkerboard Ising model with multispin interactions. This resulting model is equivalent to a symmetric 16-vertex model which satisfies the free-fermion condition.[16-18] The 16-vertex model is soluble when the free-fermion condition is satisfied.[18] The explicit expression of the free energy as a function of interaction parameters K_1, K_2, and K_3 is lengthy to write down here. We give below only the explicit expression of the critical surface which enables us to analyze the reentrance phenomenon. The critical temperature of the model is given by

$$\cosh(4K_1)\exp(2K_2+2K_3)+\exp(-2K_2-2K_3)=2\cosh(2K_3-2K_2)\pm4\cosh(2K_1)\ . \tag{4}$$

Note that Eq. (4) is invariant when changing $K_1\rightarrow -K_1$ and interchanging K_2 and K_3 as stated earlier. The phase diagram in the three-dimensional space (K_1, K_2, K_3) is rather complicated to show. Instead, we show in the following the phase diagram in the plane $(\beta=J_3/J_1, T)$ for typical values of $\alpha=J_2/J_1$. To describe each case and to follow the evolution of the phase diagram, let us go in the direction of decreasing α.

(a) $\alpha>0$ (Fig. 3). Two critical lines are found with a paramagnetic reentrance having a usual shape [Fig. 3(a)] between the partially disordered (PD) phase of type III (see Fig. 2) and the ferromagnetic (F) phase with an end point at $\beta=-1$. The width of the reentrance region $[-1,\beta_1]$ decreases with decreasing α, from $\beta_1=0$ for α at infinity to $\beta_1=-1$ for $\alpha=0$ (zero width). Note that, as α decreases, the PD phase III is depressed and disappears at $\alpha=0$, leaving only the F phase [one critical line, Fig. 3(b)]. The absence of order at zero α for β smaller than -1 results from the fact that, in the GS, this region of parameters corresponds to a superdegenerate line separating the two PD phases II and III (see Fig. 2). So,

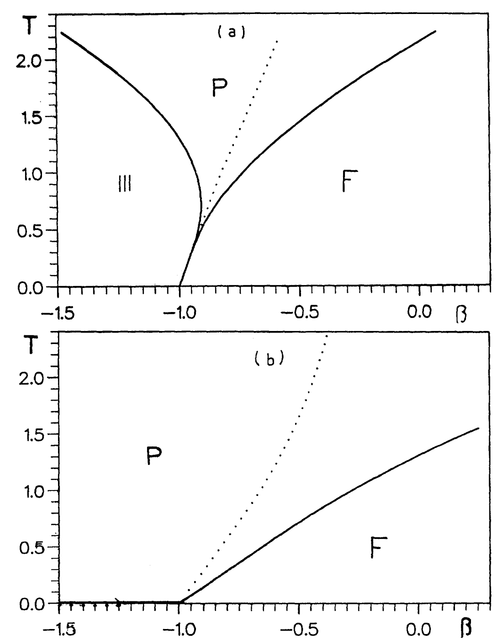

FIG. 3. Phase diagram in the plane ($\beta=J_3/J_1,T$) for positive values of $\alpha=J_2/J_1$: (a) $\alpha=1$, (b) $\alpha=0$. Solid lines are critical lines which separate different phases: paramagnetic (P), ferromagnetic (F), partially disordered phase of type III (III). Dotted line shows the disorder line. See text for comments.

along this line, the disorder contaminates the system for all T.

As for disorder solutions, for positive α we find, in the reentrant paramagnetic region, a disorder line with dimension reduction[19] given by

$$\exp(4K_3) = 2\cosh(2K_2)/[\cosh(4K_1)\exp(2K_2)+\exp(-2K_2)] . \quad (5)$$

This is shown by the dotted lines in Fig. 3.

(b) $0>\alpha>-1$. In this range of α, there are three critical lines. The critical line separating the F and P phases and the one separating the PD phase I from the P phase have a common horizontal asymptote as β tends to infinity. They form a reentrant paramagnetic phase between the F phase and the PD phase I for positive β between β_2 and *infinite* β (Figs. 4 and 5). An infinite region of reentrance like this has never been found before. As α decreases, β_2 tends to zero and the F phase is contracted. At $\alpha=-1$, the F phase disappears together with the reentrance [Fig. 6(c)].

In the interval $0>\alpha>-1$, the phase diagram possesses two disorder lines, the first being given by Eq. (5), and the second by

$$\exp(4K_3)=2\sinh(2K_2)/[-\cosh(4K_1)\exp(2K_2)+\exp(-2K_2)] . \quad (6)$$

These two disorder lines are issued from a point near $\beta=-1$ for small negative α; this point tends to zero as α tends to -1. The disorder line given by Eq. (6) enters the reentrant region which separates the F phase and the PD phase I (Fig. 4), and the one given by Eq. (5) tends to infinity with the asymptote $\beta=0$ as $T\rightarrow\infty$. The most striking feature is the behavior of these two disorder lines at low T: they cross each other in the P phase for $0>\alpha>-0.5$, forming regions of fluctuations of different nature. For $-0.5>\alpha>-1$, the two disorder lines no longer cross each other. The one given by (5) has a reentrant aspect: in a small region of negative values of β, one crosses this line three times in the P phase with decreasing T. This behavior of the disorder lines which cannot be seen in the scale of Figs. 4 and 5 is schematically shown in Figs. 6(a) and 6(b).

(c) $\alpha\leq-1$. For α smaller than -1, there are two critical lines and no reentrance (Fig. 7). Only the disorder line given by (5) survives with a reentrant aspect: in a small region of negative values of β, one crosses this line

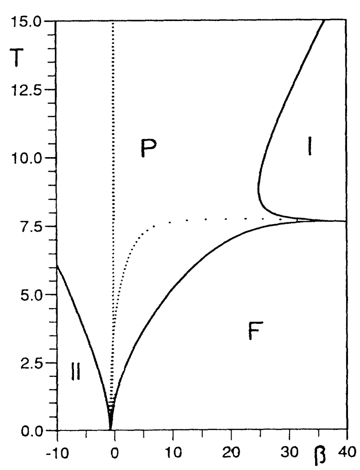

FIG. 4. Phase diagram in the plane ($\beta=J_3/J_1,T$) for a negative value of $\alpha=J_2/J_1=-0.25$. Solid lines are critical lines which separate different phases: paramagnetic (P), ferromagnetic (F), partially disordered phases of type I (I and III). Dotted lines show the disorder lines. See text for comments.

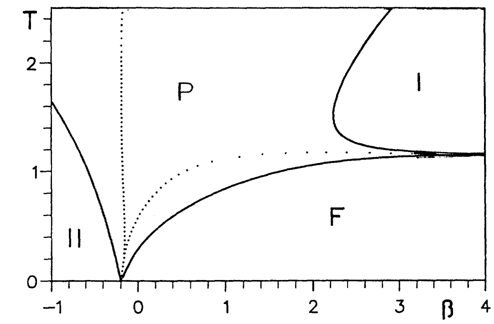

FIG. 5. The same caption as that of Fig. 4 with $\alpha=-0.8$.

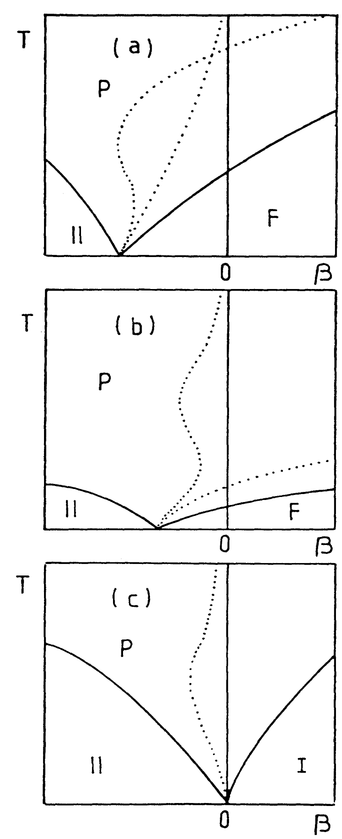

FIG. 6. The behavior of the disorder lines (dotted) is schematically enlarged in the case (a) $\alpha=-0.25$, (b) $\alpha=-0.8$, and (c) $\alpha=-1.5$. See text for comments.

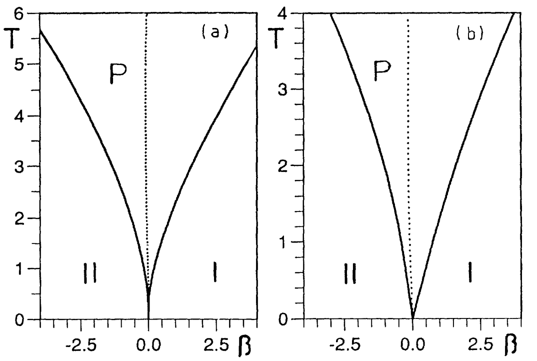

FIG. 7. The same caption as that of Fig. 4 with (a) $\alpha=-1$, (b) $\alpha=-1.5$.

twice in the P phase with decreasing T. This behavior, being undistinguishable in the scale of Fig. 7, is schematically enlarged in Fig. 6(c). The multicritical point where the P, I, and II phases meet is found at $\beta=0$ and $T=0$.

At this stage, it is interesting to note that, while reentrance and disorder lines occur along the horizontal axis $\alpha=-1$ and along the vertical axis $\beta=-1$ of Fig. 2 when the temperature is switched on, the most frustrated region ($\alpha<0$ and $\beta<0$) of the GS does not show successive phase transitions (see Fig. 7, for example). Therefore, the existence of a reentrance may require a sufficient frustration, but not overfrustration. Otherwise, the system may have either a PD phase (Fig. 7) or no order at all [Fig. 3(b)].

The origin of the reentrance phenomenon has been discussed in previous papers.[6–8] Let us summarize again here: The necessary condition for a reentrance to occur is the existence of a partial disorder in the GS next to an ordered phase. Starting from a point in the ordered phase at $T=0$, when the temperature is switched on, the entropy will work in favor of the partially disordered phase at high temperature. This phase is separated from the low-temperature ordered state by a paramagnetic reentrant phase which is necessary to keep a second-order character of the successive transitions. Note that a partial disorder alone is not sufficient to make a reentrance as shown by this model in some regions of parameters and in Ref. 8. Another ingredient which favors a reentrance may be the anisotropic character of the interactions. For example, the reentrant region is enlarged by anisotropic interactions of the centered square lattice,[6] and becomes infinite in the present model. It should be noted, however, that the occurance of a reentrance may also require an upper limit of frustration to avoid the disorder contamination of the whole system as shown above.

In conclusion, let us emphasize that we have obtained the exact phase diagram of the Ising model on a generalized Kagomé lattice. One of the most striking features is the existence of reentrance in an *infinite region* of parameters. For a given set of interactions in this region, successive phase transitions take place on the temperature scale, with a paramagnetic reentrant phase. Another interesting finding is the occurence of two disorder lines which divide the paramagnetic phase into regions of different kinds of fluctuations. Therefore, care should be taken in analyzing experimental data such as correlation functions, susceptibility, etc., in the paramagnetic phase. As a final remark, let us mention that, although the system studied here is a statistical physical model, we believe that the results obtained in this work have qualitative bearing on real frustrated spin systems, and in view of the new behavior of disorder lines found here, the model may have applications in the area of cellular automata.[20]

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