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Exact solution of an anisotropic centered honeycomb Ising lattice: Reentrance and partial disorder

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The exact phase diagram of an anisotropic centered honeycomb Ising lattice is obtained by transforming the system into a 32-vertex model that satisfies the free-fermion condition. We show that for a range of interaction parameters, a paramagnetic reentrant phase exists, on the temperature scale, between two ordered phases. The high-temperature ordered phase possesses partial disorder, in agreement with theoretical conjecture.

Frustrated-spin systems have been subjected to extensive studies during the last decade. The frustration, due to competing interactions between spins, is known to cause unexpected behavior. Examples are found in spin glasses, where the disorder in spin positions also plays an important role. We are interested here in frustrated Ising spin systems without disorder. These systems are interesting in statistical mechanics because they are periodically defined and thus subject to exact treatment. For a recent review, the reader is referred to Ref. 1. To date, very few frustrated systems have been exactly solved. They are limited to one and two dimensions.[1,2] A three-dimensional case has also been solved recently.[3] A few well-known systems include the centered-square[4] and the Kagomé[5] lattices. In a recent paper,[6] we obtained the exact solution of the Kagomé lattice with nearest-neighbor and next-nearest-neighbor interactions. The phase diagram shows a rich behavior with reentrance, coexistence of order and disorder, and a disorder line. The reentrance has been found also in the centered-square lattice[4] and its extended versions.[7] We have conjectured[6] that, in order to have a reentrant paramagnetic phase between two ordered phases, the necessary, but not sufficient, condition is that the system possesses a partial disorder in the high-temperature ordered phase to compensate for the loss of entropy. This feature is also found in the centered-square lattice[4,7,8] and other complicated cluster models.[9] Partial disorder is possible when a set of spins is free to flip, due to competing interactions. In three dimensions, a few systems such as the fully frustrated simple-cubic lattice,[10,11] the stacked triangular antiferromagnet,[12] and a body-centered-cubic (BCC) crystal[13] also exhibit this property, although evidence of reentrance is found only for the BCC case[13] and a complicated lattice model.[3]

In this paper, we study an anisotropic centered honeycomb 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 ($=\pm1$) is an Ising spin occupying the lattice site i, and the first, second, and third sums run over the spin pairs connected by heavy, light, and doubly light bonds, respectively (see Fig. 1). When $J_2=J_3=0$, one recovers the honeycomb lattice, and when $J_1=J_2=J_3$ one has the triangular lattice.

The phase diagram at temperature $T=0$ is shown in Fig. 2 for three cases ($J_1\neq J_2=J_3$), ($J_1\neq J_3$, $J_2=0$), and ($J_1\neq J_2$, $J_3=0$). The ground-state (GS) spin configurations are also indicated. Note that the phase diagram is symmetric with respect to the horizontal axis. In each case, there is a phase where the central spins are free to flip. Let us call this the partially disordered phase (PDP). In view of this common feature, one expects a reentrant phase occurring between the PDP and its neighboring phase at finite T. As it will be shown below, that though partial disorder exists in the GS, it does not in every case studied here yield a reentrant phase at finite temperature.

Now we proceed 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_6. The Boltzmann weight associated to the elementary cell is given by

$$W=\exp[K_1(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_5+\sigma_5\sigma_6+\sigma_6\sigma_1)+K_2\sigma(\sigma_1+\sigma_2+\sigma_4+\sigma_5)+K_3\sigma(\sigma_3+\sigma_6)]\,, \qquad (2)$$

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

$$Z=\sum_{\{\sigma\}}\prod_{\{C\}}W\,, \qquad (3)$$

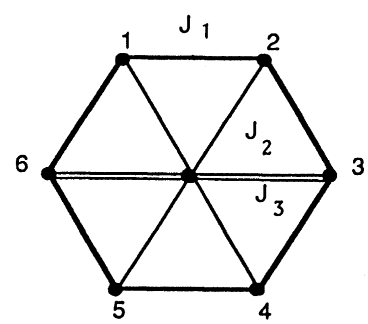

FIG. 1. Unit cell of the centered honeycomb lattice: heavy, light, and doubly-light bonds denote the interactions J_1, J_2, and J_3, respectively. The sites on the honeycomb are numbered from 1 to 6 for decimation.

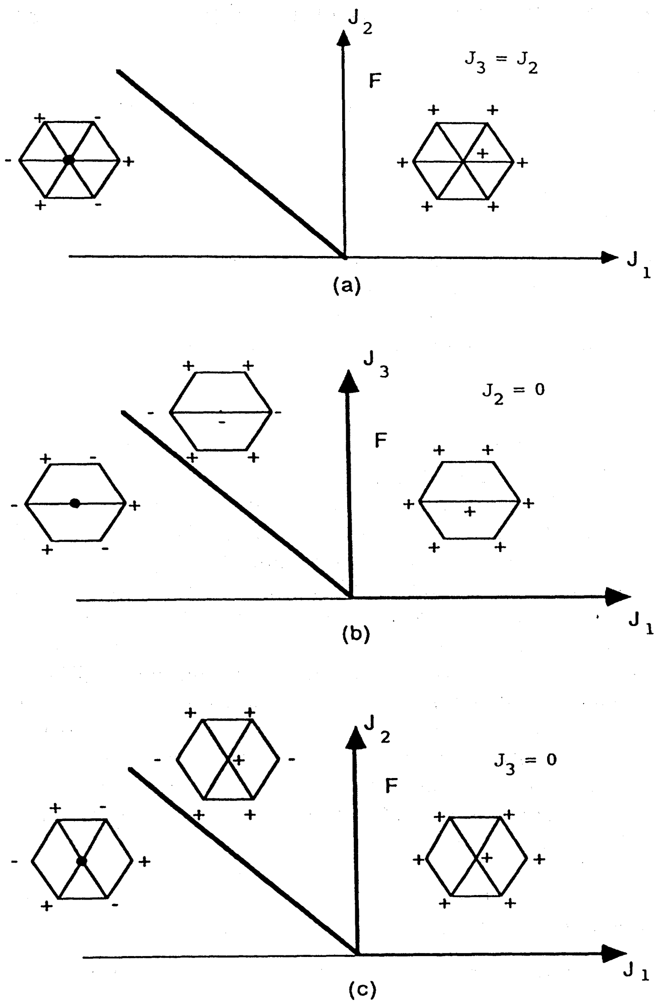

FIG. 2. Phase diagram of the ground state shown in the plane: (a) (J_1, $J_2=J_3$); (b) (J_1, J_3) with $J_2=0$; (c) (J_1, J_2) with $J_3=0$. Heavy lines separate different phases and spin configuration of each phase is indicated (up, down, and free spins are denoted by +, −, and ●, respectively).

where the sum is performed over all spin configurations and the product is taken over all elementary cells. Periodic boundary conditions are imposed. Since there is no crossing-bond interaction, the model is exactly solvable. 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 honeycomb Ising model with multispin interactions. This resulting model is equivalent to a special case of the 32-vertex model on a triangular lattice that satisfies the free-fermion condition.[2,14] The 32-vertex model is soluble when the free-fermion condition is satisfied, and the corresponding free energy has been calculated by Sacco and Wu.[14] Following the same method, we can obtain the free energy per spin of our model, and also the critical surface.

The explicit expression of the free energy as a function of interaction parameters K_1, K_2, and K_3 is very complicated. We give here only the explicit expression of the critical surface, which enables us to analyze the problem of reentrance. The critical temperature is determined by

$$\Omega_1+\Omega_2+2\Omega_3=2\max\{\Omega_1,\Omega_2,\Omega_3\} \tag{4}$$

where

$$\begin{aligned} \Omega_1 &= \exp(3K_1)\cosh(4K_2+2K_3)+\exp(-3K_1)\,, \\ \Omega_2 &= \exp(K_1)+\exp(-K_1)\cosh(4K_2-2K_3)\,, \\ \Omega_3 &= \exp(K_1)+\exp(-K_1)\cosh(2K_3)\,. \end{aligned} \tag{5}$$

The phase diagram in the three-dimensional space (K_1, K_2, K_3) is rather complicated to show. For simplicity, we consider the phase diagram in three particular planes ($K_1 \neq K_2 = K_3$), ($K_1 \neq K_3$, $K_2=0$), and ($K_1 \neq K_2$, $K_3=0$).

When $K_2=K_3$, the critical line obtained from (4) and (5) is

$$\exp(3K_1)\cosh(6K_2)+\exp(-3K_1) = 3[\exp(K_1)+\exp(-K_1)\cosh(2K_2)]\,. \tag{6}$$

In the case $K_2=0$, the critical line is given by

$$\exp(3K_1)\cosh(2K_3)+\exp(-3K_1) = 3[\exp(K_1)+\exp(-K_1)\cosh(2K_3)]\,. \tag{7}$$

The phase diagrams obtained from (6) and (7) are shown in Figs. 3(a) and 3(b), respectively. Note that the phase diagrams are symmetric with respect to the K_1 axis due to the invariance $K_2 \rightarrow -K_2$ [see Eq. (6)] and $K_3 \rightarrow -K_3$ [see Eq. (7)]. These two cases do *not* present the reentrance phenomenon. Let us consider first Fig.

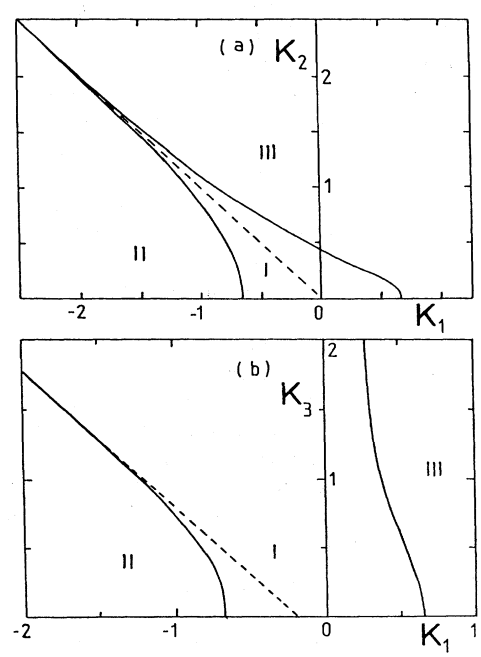

FIG. 3. Phase diagram in the plane (a) ($K_1=J_1/kT$, $K_2=K_3=J_{2,3}/kT$), (b) (K_1, K_3, $K_2=0$). Solid lines are critical lines which separate different phases I (paramagnetic), II (partially disordered), and III (ordered). Discontinued lines of slope −1 are the asymptotes. See text for comments.

3(a) for a given ratio K_2/K_1 ($K_3=K_2$), one crosses only one critical line at *finite* temperature (except at $K_2/K_1=-1$). In the ordered phase II, the partial disorder, which exists in the GS, remains so up to the phase transition. We have verified this by examining the Edwards-Anderson order parameter associated with the central spins in Monte Carlo (MC) simulations. When $K_2=K_3=0$ one recovers the transition at finite temperature found for the honeycomb lattice,[15] and when $K_2=K_3=K_1=-1$ one recovers the antiferromagnetic triangular lattice which has no phase transition at finite temperature.[16] The case $K_2=0$ [Fig. 3(b)] does not have a phase transition at finite temperature in the range $-\infty<K_3/K_1<-1$, and the ordered phase II has the same partial disorder as in Fig. 3(a).

Let us consider now the case $K_3=0$. The critical lines are determined from the equations

$$\cosh(4K_2)=\frac{\exp(4K_1)+2\exp(2K_1)+1}{[1-\exp(4K_1)]\exp(2K_1)}\,, \tag{8}$$

$$\cosh(4K_2)=\frac{3\exp(4K_1)+2\exp(2K_1)-1}{[\exp(4K_1)-1]\exp(2K_1)}\,. \tag{9}$$

The phase diagram obtained from (8) and (9) is shown in Fig. 4 where one observes a reentrant phase in the range $K_2/K_1=(-0.6,-0.5)$. For a given ratio of K_2/K_1 in this range, starting from the paramagnetic phase (I), with decreasing temperature one enters first an ordered phase (II) with a partial disorder due to free spins at the centered sites (we have verified this by MC simulations), then the reentrant paramagnetic phase before crossing the critical line to the low-temperature ordered phase III. Since this is not easily seen on the scale of Fig. 4, we show in Fig. 5 the phase diagram in the reentrant region in the space (T, $\alpha=K_2/K_1$). The reentrant paramagnetic phase goes down to zero temperature with an end point at $\alpha=-0.5$.

When K_3 is nonzero, the slope of the asymptote in Fig. 4 tends from -0.5 to -1 when K_3/K_2 varies from 0 to 1 [situation between Fig. 4 and Fig. 3(a)]. The reentrance exists in this range of K_3/K_2.

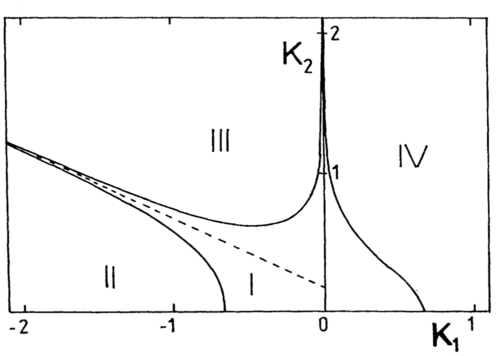

FIG. 4. Phase diagram in the plane ($K_1=J_1/kT$, $K_2=J_2/kT$, $K_3=0$). Solid lines are critical lines which separate different phases I (paramagnetic), II (partially disordered), III (ordered), and IV (ferromagnetic). Discontinued line is the asymptote with slope -0.5. The reentrant region is in the range $K_2/K_1=(-0.6,-0.5)$.

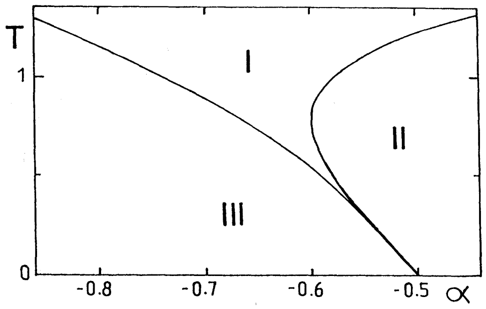

FIG. 5. Phase diagram in the plane (T, $\alpha=J_2/J_1$) in the reentrant region. I, II, and III denote the paramagnetic, partially disordered, and ordered phases, respectively.

Note that the model that we have studied in this work does not present a disorder solution with a dimensional reduction.

To investigate the kind of ordering in each phase, we have performed MC simulations. The sample sizes are up to 60×60 lattice sites with periodic boundary conditions. We discarded about 10000 MC steps per spin for equilibrating and averaged physical quantities over 10000 MC steps per spin. We show in Fig. 6 an example of ordering in the reentrant region. The order parameter in the low-temperature ordered phase is defined by an appropriate staggered magnetization [see the upper configuration on the left-hand side of Fig. 1(c)]. In the high-temperature phase, the order parameter of the sublattice containing the spins at centered sites is defined by the Edwards-Anderson order parameter q, and that of the other sublattice by the staggered magnetization m [see the lower configuration on the left-hand side of Fig. 1(c)]. As seen, the sublattice of centered spins stays disordered in the high-temperature (partially) ordered phase, while the other sublattice becomes disordered in the reentrant region and in the high-temperature paramagnetic phase. Note that due to the well-known problem encountered at low temperatures, the MC simulations overestimate the transition temperatures in the reentrant region when using the heating procedure.

Let us try now to analyze the origin of the reentrance

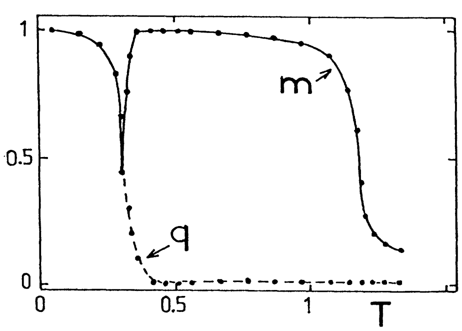

FIG. 6. Order parameters m (solid line as guide to the eye) and q (discontinued line) obtained from MC simulations (heating from the ground state) in the reentrant region with $\alpha=J_2/J_1=-0.514$. See text for the definitions of the order parameters and comments.

phenomenon. The necessary condition for reentrance to occur is the existence of partial disorder in the high-temperature ordered phase to compensate the loss of entropy, as has been conjectured.[6] But this partial disorder alone is not sufficient to make reentrance as shown in Figs. 3(a) and 3(b). So, the finite zero-point entropy due to the partial disorder of the ground state which is the same for three cases considered in Fig. 1, $S_0 = \frac{1}{3}\ln 2$ per spin, is not a sufficient condition. Another ingredient which favors reentrance may be the anisotropic character of the interactions. For example, the reentrant region of the centered-square lattice is enlarged by anisotropic interactions.[7] Finally, the presence of reentrance may require a coordination number at a disordered site to be large enough to influence the neighboring ordered sites. It may have an upper limit to avoid the disorder contamination of the whole system. A quantitative formulation has been suggested by Morita:[7] the effective multispin interactions which are functions of temperature and are generated by the decimation of the free spins at centered sites, may cancel the original pair interactions on the remaining sites at some temperature region, leading to the paramagnetic reentrant phase.

To conclude, we emphasize that we have solved exactly the Ising model on the anisotropic honeycomb lattice. We have found, in some region of parameters, successive phase transitions with a paramagnetic reentrant phase. The partial disorder in the GS remains up to the transition at finite temperature and plays a fundamental role in the occurrence of the reentrance.

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