Successive reentrances and phase transitions in exactly solved dilute centered square Ising lattices

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We solve exactly several periodically dilute centered square Ising lattices by transforming the systems into eight-vertex models. We find that for a given set of interactions, there may be five transitions with decreasing temperature with *two* reentrant paramagnetic phases. These phases extend to infinity in the space of interaction parameters. Moreover, two additional reentrant phases are found, each in a limited region of phase space.

Frustration caused by competing interactions is known to cause unexpected and rich behavior in magnetic systems. Among its effects, the reentrant phenomenon is one of the most challenging problems. The reentrant phase is defined as a phase with short-range order (or no order at all) occurring below a more ordered phase on the temperature scale. A recent example is the reentrant spin glass.[1] We are interested here in the reentrance phenomenon occurring in a class of two-dimensional (2D) lattice models that are periodically defined, i.e., there is no bond disorder: the frustration caused by competing interactions will itself induce disorder in the spin orientations. The advantage of models without bond disorder is that they are subject to exact treatments,[2,3] and therefore represent possible applications in statistical physics. The 2D spin systems have recently attracted much attention due to their close relation to high-T_c materials.[4] Reentrance was found in a number of exactly solved models: centered square lattice,[5–7] Kagomé lattice,[8,9] centered honeycomb lattice,[10] and cluster models.[11] In a previous paper[8] we conjectured that the necessary condition for a reentrance to take place is the existence of a partially disordered phase (PDP) next an to an ordered phase in the ground state. This condition has been verified in all known cases.[5–11] However, we showed[10] that this is not a sufficient condition.

In this paper we study several 2D models defined from the centered square lattice by taking away one, two, or three centered spins in a periodic manner. These are shown in Figs. 1(a), 1(b), and 1(d). The model shown in Fig. 1(c) has been recently studied.[9] Our purpose is to examine the behavior of the phase diagram, in particular the existence of reentrant phases.

The Hamiltonian of the models shown in Fig. 1 is given by

$$H=-J_1\sum_i^j \sigma_i\sigma_j - J_2\sum_i^j \sigma_i\sigma_j - J_3\sum_i^j \sigma_i\sigma_j \ , \qquad (1)$$

where the first, second, and third sums run over the spin pairs connected by diagonal, vertical and horizontal bonds, respectively.

Let us show in Fig. 2 the phase diagrams at zero temperature in the space (a,b) where $a=J_2/J_1$ and $b=J_3/J_1$. The three-center case [Fig. 2(a)] has six phases (I to VI), five of which (I, II, IV, V, and VI) are PDP (with at least one centered spin being free), while the two-center case [Fig. 2(b)] has five phases, three of which (I, IV, and V) are PDP. Finally, the one-center case has seven phases with three PDP (I, VI, and VII). As will be shown later, in each model, *the reentrance occurs along most of the critical lines when the temperature is switched on.* This is a very special feature of the models shown in Fig. 1 which has not been found in other models.

The partition function is written as

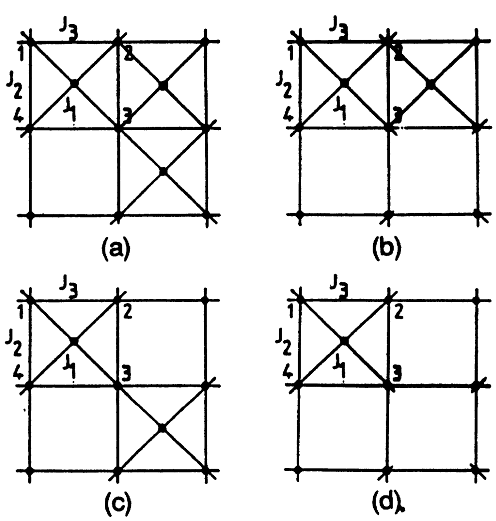

FIG. 1. Elementary cells of dilute centered square lattice: (a) three-center case, (b) two-adjacent-center case, (c) two-diagonal-center case, (d) one-center case. Diagonal, vertical, and horizontal bonds are J_1, J_2, and J_3, respectively.

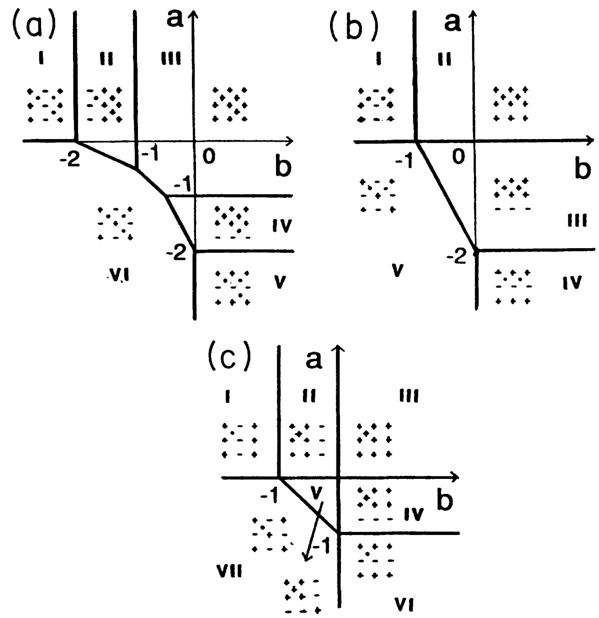

FIG. 2. Phase diagrams in the plane ($a=J_3/J_1$, $b=J_2/J_1$) at $T=0$ for (a) three-center case, (b) two-adjacent-center case, and (c) one-center case. Heavy lines are critical lines. Each phase is numbered and its spin configuration is indicated ($+,-$, and ● are up, down, and free spins, respectively). Degenerate configurations are obtained by reversing all spins.

$$Z=\prod_{(j)}\sum_{(\sigma)}W_j\ , \qquad (2)$$

where the sum runs over all spin configurations and the product over all elementary squares. W_j is the statistical weight of the jth square. If the centered site exists, W_j of the square is

$$W_j=\exp[K_1(\sigma_1\sigma_2+\sigma_3\sigma_4)+K_2(\sigma_1\sigma_4+\sigma_2\sigma_3)+K_3\sigma(\sigma_1+\sigma_2+\sigma_3+\sigma_4)]\ , \qquad (3a)$$

otherwise, it is given by

$$W_j=\exp[K_1(\sigma_1\sigma_2+\sigma_3\sigma_4)+K_2(\sigma_1\sigma_4+\sigma_2\sigma_3)]\ , \qquad (3b)$$

where $K_i=J_i/kT$ ($i=1,2,3$), k being the Boltzmann constant, and T the temperature.

To obtain the exact solution, we decimate the central spins of the centered squares. The resulting system is equivalent to an eight-vertex model on a square lattice, but with different vertex weights. Generally, we have to define different sublattices with different statistical weights. The problem has been studied by Hsue, Lin, and Wu for two different sublattices,[12] and Lin and Wang for four sublattices.[13] They showed that exact solution can be obtained provided that all different statistical weights satisfy the free-fermion condition.[2,12–14] This is indeed our case and we get the exact partition function in terms of interaction parameters. The critical surfaces of our models are then given by

$$\Omega_1+\Omega_2+\Omega_3+\Omega_4=2\max(\Omega_1,\Omega_2,\Omega_3,\Omega_4)\ , \qquad (4)$$

where Ω_i are functions of K_1,K_2, and K_3. Let us mention that the present models can also be solved by standard dimer and Pfaffian techniques.[2,15,16] Now, Eq. (4) can be written as a second-order equation of X, which is a function of K_2 only:

$$A(K_1,K_3)X^2+B(K_1,K_3)X+C(K_1,K_3)=0\ , \qquad (5)$$

with *a priori* four possible values of A, B, and C for each model.

For given values of K_1 and K_3, the critical surface is determined by the value of K_2, which satisfies Eq. (5) through X. X must be real positive. We give in the following the expressions of A, B, and C for which this condition is fulfilled:

(1) *Model with three centers* [Fig. 1(a)]:

$$X=\exp(4K_2)\ ,$$

$$A=\exp(4K_1)\cosh^3(4K_3)+\exp(-4K_1)-\cosh^2(4K_3)-\cosh(4K_3)\ ,$$

$$B=\pm\{1+3\cosh(4K_3)+8\cosh^3(2K_3)+[\cosh(4K_3)+\cosh^2(4K_3)]\times\exp(4K_1)+2\exp(-4K_1)\}\ ,$$

$$C=[\exp(2K_1)-\exp(-2K_1)]^2\ ,$$

$$A=\exp(4K_1)\cosh^3(4K_3)+\exp(-4K_1)+\cosh^2(4K_3)+\cosh(4K_3)\ ,$$

$$B=\{1+3\cosh(4K_3)+8\cosh^3(2K_3)-[\cosh(4K_3)+\cosh^2(4K_3)]\times\exp(4K_1)-2\exp(-4K_1)\}\ ,$$

$$C=[\exp(2K_1)+\exp(-2K_1)]^2\ .$$

(2) *Model with two adjacent centers* [Fig. 1(b)]:

$$X=\exp(2K_2)\ ,$$

$$A=\exp(2K_1)\cosh(4K_3)+\exp(-2K_1)\ ,$$

$$B=2[\exp(2K_1)\cosh^2(2K_3)-\exp(-2K_1)]\ ,$$

$$C=\exp(2K_1)+\exp(-2K_1)\ ,$$

$$A=\exp(2K_1)\cosh(4K_3)-\exp(-2K_1)\ ,$$

$$B=\pm2[\exp(2K_1)\cosh^2(2K_3)+\exp(-2K_1)]\ ,$$

$$C=\exp(2K_1)-\exp(-2K_1)\ .$$

(3) *Model with one center* [Fig. 1(d)]:

$$X=\exp(4K_2)\ ,$$

$$A=\exp(4K_1)\cosh(4K_3)+\exp(-4K_1)-2\cosh^2(2K_3)\ ,$$

$$B=\pm2\{[\cosh(2K_3)+1]^2+[\exp(2K_1)\cosh(2K_3)+\exp(-2K_1)]^2\}\ ,$$

$$C=[\exp(2K_1)-\exp(-2K_1)]^2\ ,$$

$$A = \exp(4K_1)\cosh(4K_3) + \exp(-4K_1) + 2\cosh^2(2K_3) ,$$

$$B = \pm 2\{[\cosh(2K_3)+1]^2 - [\exp(2K_1)\cosh(2K_3) - \exp(-2K_1)]^2\} ,$$

$$C = [\exp(2K_1) + \exp(-2K_1)]^2 .$$

Equation (4) defining the critical surface may have as much as five solutions for the critical temperature,[13] and the system may, for some given values of interaction parameters, exhibit up to five phase transitions. This happens for the model with three centers, when one of the interactions is large positive, the other slightly negative, and the diagonal one equals 1.

Before showing our results, we mention that all the critical lines shown below are of second order with standard two-dimensional Ising universality class. Furthermore, we emphasize that though the critical surfaces are obtained, it is not easy to calculate the order parameter as a function of temperature in each phase. To investigate the nature of ordering, we have performed Monte Carlo simulations in the same way we did in previous works.[8,10] The nature of ordering described below is thus a result of simulations that are tedious to show.

Let us describe now in detail the phase diagram of each model.

A. Three-center model [Fig. 1(a)]

For clarity, we show the phase diagram in the plane (a,T) for typical values of b, instead of displaying the three-dimensional space (a,b,T).

For $b<-1$, there are *two* reentrances. Figure 3(a) shows the case of $b=-1.25$ where the nature of the ordering in each phase is indicated using the same numbers of corresponding ground-state configurations (see Fig. 2). Note that phases I, II, and VI are PDP: the centered spins which are disordered at $T=0$ [Fig. 2(a)] remain so at all T. As seen, one paramagnetic reentrance is found in a small region of negative a [schematically enlarged in the inset of Fig. 3(a)], and the other on the positive a extending to infinity. The two critical lines in this region have a common horizontal asymptote.

For $-1<b<-0.5$, there are *three* reentrant paramagnetic regions as shown in Fig. 3(b): the reentrant region on the negative a is very narrow (inset), and the two on the positive a become so narrow while a goes to infinity that they cannot be seen on the scale of Fig. 3. Note that the critical lines in these regions have horizontal asymptotes. For a large value of a, one has five transitions with decreasing temperature: paramagnetic state–PDP I–reentrant paramagnetic phase–II–reentrant paramagnetic phase–ferromagnetic phase [Fig. 3(b)]. *This is the first time that such successive phase transitions with two reentrances are found in a simple model.*

For $-0.5<b<0$, there is an additional reentrance for $a<-1$: this is shown in the inset of Fig. 3(c). Note that as b increases, the ferromagnetic region (III) "pushes" the two PDP (I and II) toward higher T. Finally, at $b=0$, these two phases disappear at infinity. For positive b, there are thus only two reentrances remaining on a negative region of a, with endpoints at $a=-2$ and $a=-1$, at $T=0$ [Fig. 3(d)].

B. Two-adjacent-center model [Fig. 1(b)]

For $b<-1$, this model shows only one transition for a given value of a, except when $a=0$ where the paramagnetic state goes down to $T=0$ [Fig. 4(a). However, for

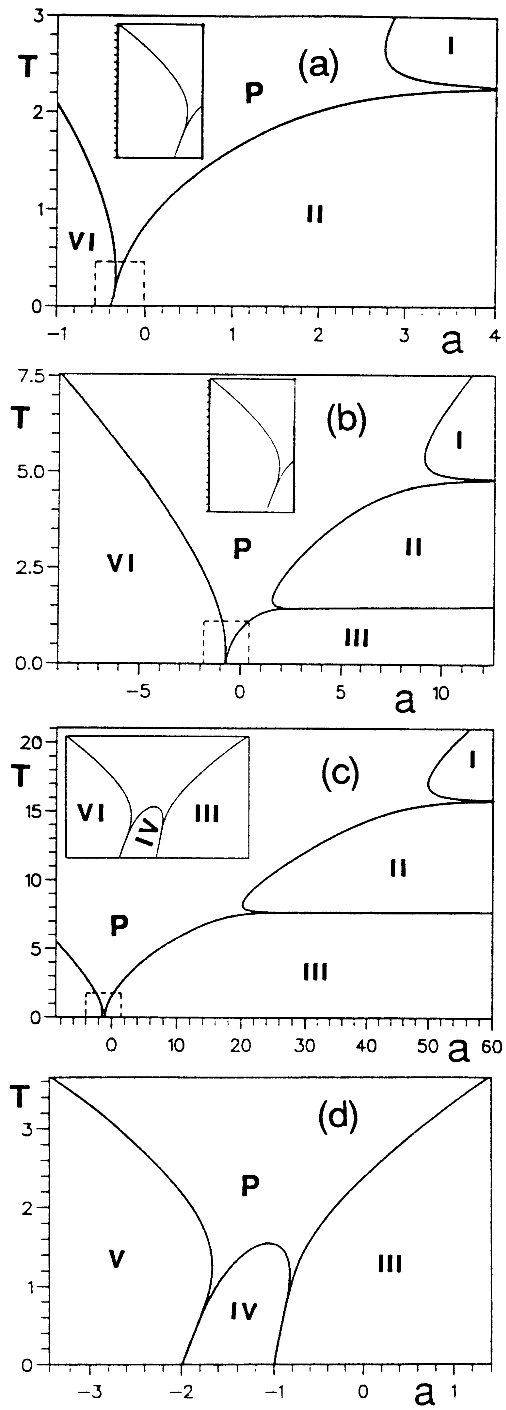

FIG. 3. Three-center case: phase diagram for typical values of b: (a) $b=-1.25$, (b) $b=-0.75$, (c) $b=-0.25$, (d) $b=0.75$. Reentrant regions on negative side of a (limited by discontinued lines) are schematically enlarged in the insets. The nature of ordering in each phase is indicated by a number which is referred to the corresponding spin configuration in Fig. 2. P is paramagnetic phase.

$-1<b<0$, two reentrances appear, the first one separating phases I and II goes to infinity with increasing a, and the second one exists in a small region of negative a with an endpoint at ($a=-2-2b$, $T=0$). Note that the slope of the critical lines at $a=0$ is vertical [inset of Fig. 4(b)]. As b becomes positive, the reentrance on the positive side of a disappears [Fig. 4(c)], leaving only phase III (ferromagnetic).

C. One-center model [Fig. 1(d)]

The phase diagram of this model is shown in Fig. 5. It is very similar to that of the two-center model shown in Fig. 4 in the regions $b<-1$, $-1<b<0$, and $b>0$. This is not surprising if one examines the ground-state phase diagrams of the two cases [Figs. 2(b) and 2(c)]: their common point is the existence of a PDP next to an ordered phase. The difference between the one- and two-center cases and the three-center case shown above is that the latter has, in addition, two boundaries, each of which separates two PDP's [Fig. 2(a)]. It is along these boundaries that the two additional reentrances take place at finite temperatures.

In conclusion, we have found two reentrant phases occurring on the temperature scale at a given set of interaction parameters in very simple models. Another

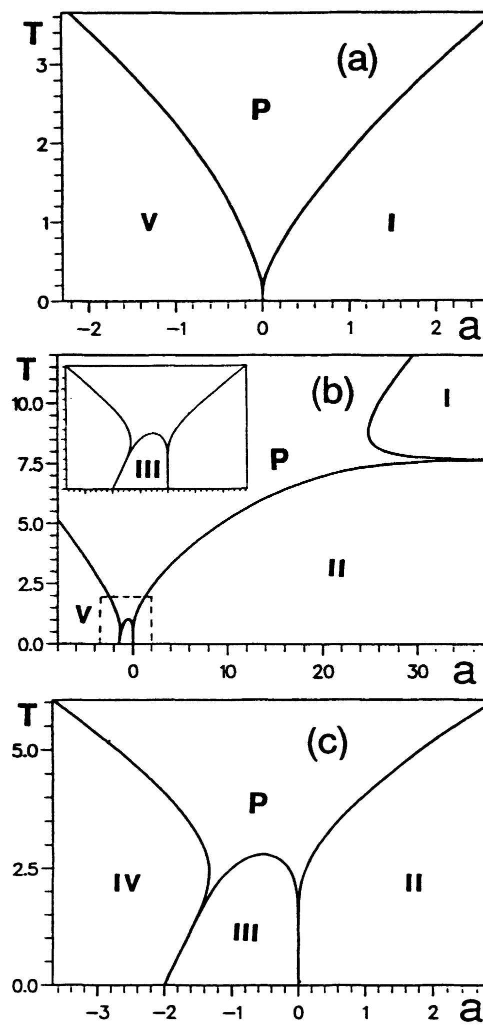

FIG. 4. Two-center case: the same as that of Fig. 3 with (a) $b=-1.25$, (b) $b=-0.25$, (c) $b=2$.

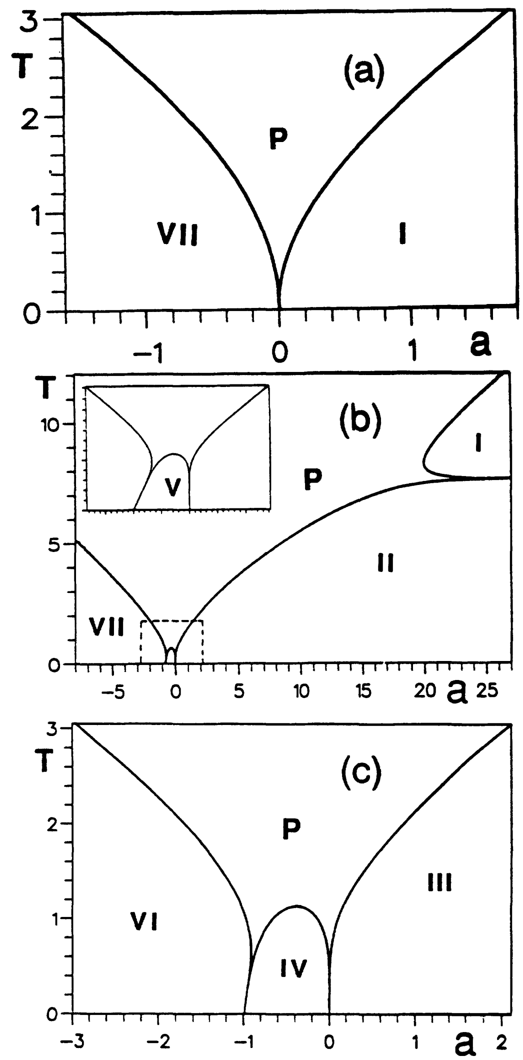

FIG. 5. One-center case: the same as that of Fig. 3 with (a) $b=-1.25$, (b) $b=-0.25$, (c) $b=0.5$.

striking feature is the existence of a reentrant phase between two PDP's which has not been found so far in any other model (we recall that previous works found a reentrant phase only between an ordered phase and a PDP). Therefore, the conjecture on the occurrence of a reentrance[8] should be modified as follows: the necessary condition for a reentrant phase to take place between two phases at finite temperatures is at least one of them being a PDP in the ground state. Finally, let us mention that simple models like those studied here can possess complicated phase diagrams. In particular, very narrow reentrant regions can exist on the temperature scale. Therefore, care should be taken while analyzing experimental data in frustrated systems. In view of the simplicity of our models, we hope that the results found here will have applications in statistical physics.

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