Monte Carlo study of a kinetic lattice model with random diffusion of disorder

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We report Monte Carlo results for a nonequilibrium Ising-like model in two and three dimensions. Nearest-neighbor interactions J change sign randomly with time due to competing kinetics. There follows a fast and random, i.e., spin-configuration-independent *diffusion* of J's, of the kind that takes place in dilute metallic alloys when magnetic ions diffuse. The system exhibits steady states of the ferromagnetic (antiferromagnetic) type when the probability p that $J>0$ is large (small) enough. No counterpart to the freezing phenomena found in quenched spin glasses occurs. We compare our results with existing mean-field and exact ones, and obtain information about critical behavior.

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Much of the study of *impure* systems has focused on variations of the Ising model for the cooperative properties of pure systems. The latter [1] involves a periodic d-dimensional lattice, e.g., $\mathbb{Z}^d$, the spin configuration $\mathbf{s}\equiv\{s_x=\pm 1;\mathbf{x}\in\mathbb{Z}^d\}$, and the Hamiltonian

$$H(s)=-\sum_{\mathrm{NN}} J_{xy}s_x s_y \ , \tag{1}$$

where the sum is over all pairs of nearest-neighbor (NN) sites, and J_{xy} are exchange interactions. The spin system is in contact with a heat bath at temperature T that induces stochastic changes of $\mathbf{s}$ according to the master equation [2,3]

$$\frac{\partial\mu_t(\mathbf{s})}{\partial t}=\sum_{\mathbf{s}^x}[c(\mathbf{s}^x;\mathbf{x})\mu_t(\mathbf{s}^x)-c(\mathbf{s};\mathbf{x})\mu_t(\mathbf{s})] \ . \tag{2}$$

Here $\mu_t(\mathbf{s})$ is the probability of $\mathbf{s}$ at time t, and $c(\mathbf{s};\mathbf{x})$ is the probability per unit time for a transition from $\mathbf{s}$ to $\mathbf{s}^x$; the latter is obtained from $\mathbf{s}$ by flipping spin s_x. The detailed balance condition, i.e., $c(\mathbf{s};\mathbf{x})=c(\mathbf{s}^x;\mathbf{x})\exp[-\beta\Delta H]$, $\Delta H\equiv H(\mathbf{s}^x)-H(\mathbf{s})$, where $\beta=(k_BT)^{-1}$ is the inverse temperature, is sufficient to guarantee that the stationary solution of (2) is the Gibbs state corresponding to energy (1) and temperature T. This is satisfied by the Metropolis algorithm [4], $c(\mathbf{s};\mathbf{x})=\min\{1,\exp(-\beta\Delta H)\}$, for instance.

The spin-glass model of Edwards and Anderson [5] is a quenched random-exchange variation of the Ising model. Its simplest version, to be denoted EA model hereafter, is characterized by (1) but J_{xy} is to be interpreted then as a random variable distributed symmetrically around zero. It induces interesting macroscopic behavior, including freezing phenomena (i.e., extremely long relaxation times), within a wide, d-dependent temperature range. Freezing phenomena and other facts have seriously complicated both analytical and numerical work. The EA model has been used to interpret some *unusual* observations in disordered materials, namely, a series of macroscopic peculiarities related to a sort of glassy behavior not predicted by the Ising model. A widespread consensus exists that the EA model and its variations are a suitable representation of many realistic situations in physics and other fields, and it has motivated the development of new concepts and techniques. Nevertheless, some enigmas and controversy on basic issues persist, and the interpretation of laboratory experiments by models with quenched disorder is not quite satisfactory [6,7]. It thus seems interesting to examine further (impure) variations of the Ising model trying to capture some of the essential features in disordered systems in nature.

As previously pointed out [8–10], the EA model (as well as the familiar random-field and magnetically dilute Ising models with quenched impurities) neglects diffusion of magnetic ions. Diffusion makes the distance between pairs of spins change with time. One may model it allowing for variations of J_{xy}, both in space and time [10]. With that aim, we have studied by the Monte Carlo method the nonequilibrium model defined below; it is one of the possible explicit realizations of a system studied before both by exact methods for $d=1$ [8] and by mean-field theory [11]. Our study suggests that diffusion of disorder may affect macroscopic behavior significantly. In particular, the nonequilibrium system seems to exhibit some, but not all, of the macroscopic features that characterize the EA model. Numerical study of the nonequilibrium system, even though somewhat more involved than for the pure Ising model, seems feasible, in contrast to the difficulties revealed by the quenched case that seem related to the nature of the spin-glass phase. Results from a probabilistic cellular-automaton representation of the zero-temperature state of the model in which percolationlike phenomena occur [12] are very briefly described. Consequences of the interplay between

the latter phenomena and ordinary thermal fluctuations, as well as further questions, are discussed. A main conclusion in this paper is that a systematic investigation by different methods of lattice models in which disorder may diffuse is interesting.

The model is defined as follows. Consider the kinetic Ising model mentioned above with N sites, say $\mathbf{x}=1,2,\ldots,N$. The time evolution of $\mathbf{s}$ is generated by (2) with $c(\mathbf{s};\mathbf{x})$ describing a competing process. The algorithm is as follows: a site $\mathbf{x}$ is selected at random; then, before a spin flip is to be attempted thereon (following Metropolis's rule), all exchange interactions with its $2d$ NN's are chosen to be all ferromagnetic of intensity $J_0>0$ with probability p, or all antiferromagnetic of intensity $-J_0$ with probability $1-p$. In other words, the master equation (2) is complemented with a competing transition rate given by

$$c(\mathbf{s};\mathbf{x})=p\min\{1,\exp(-\beta\Delta H_{J_0})\}+(1-p)\min\{1,\exp(-\beta\Delta H_{-J_0})\} \quad (3)$$

instead of the canonical Metropolis choice; here, $\Delta H_J=2Js_x\sum_{\mathrm{NN}}s_y$, where the sum is over all NN's of site $\mathbf{x}$. The following situation occurs under the action of (3): Let us assume that the system is characterized at $t=0$ by some spatial distribution of couplings, $P_0(\{J\})$, e.g., $J_{xy}=J_0$ for any pair of NN sites. This evolves with time into $P_t(\{J\})$ which (except for correlations between bonds ending at the same site) is random with J_0 occurring spatially with probability p and $-J_0$ occurring with probability $1-p$ for t large enough. Of course, the spatial distribution $P_t(\{J\})$ does not remain frozen in, but keeps changing with time. Moreover, $P_t(\{J\})$ and $P_{t+\Delta t}(\{J\})$ are uncorrelated for Δt large enough.

Several remarks are in order. Process (3) drives the system asymptotically towards a pure ferromagnetic (antiferromagnetic) equilibrium state for $p=1$ (0), but things are less simple otherwise. Competing interactions generate nonunique steady *nonequilibrium* states in general. In particular, the steady state depends on $c(\mathbf{s};\mathbf{x})$ given that (3) does not satisfy detailed balance and no single Hamiltonian characterizes the system. In addition to the specific motivation sketched above (i.e., to study the macroscopic consequences of diffusion of disorder), we find the consideration of a nonequilibrium impure model appealing because some *unusual* observations in disordered materials are consistent with the existence of nonequilibrium effects, e.g., dependence of the steady state on the past history. On the other hand, mathematically well-defined models with steady nonequilibrium states may help the development of theory. Furthermore, this model, which one may expect *a priori* to behave differently from the (equilibrium) EA model, essentially differs also from the annealed version [13] of the latter that involves an unrealistic representation of impurity diffusion. Namely, the J's in the annealed case are strongly correlated, which is not observed in nature in general. On the contrary, one may interpret that the impurities in the model here move as driven by infinite temperature, i.e., by a completely random mechanism in an appropriate time scale, as shown explicitly in Ref. [10].

The phase diagram is symmetric around $p=\frac{1}{2}$: Consider the evolution of two systems as in (1) and (2) with $J_{xy}=J$: (i) one with probability p that $J=J_0$, (ii) the other one with probability $1-p$ that $J=J_0$ (that is, with probability p that $J=-J_0$, since $J=\pm J_0$ only). Now, if the lattice can be decomposed into two sublattices (e.g., square and simple cubic (sc) lattices, but not the triangular one), let $\sigma_x=-s_x$ on all $\mathbf{x}$ on one of the sublattices. Then, the Hamiltonian for (ii) can be obtained from (1) by letting $Js_xs_y\rightarrow(-J)s_x\sigma_y$. Now, since the probabilities that $J=J_0$ for system (i) and that $J=-J_0$ for system (ii) are equal, it follows that a given evolution in time of (i) is equally probable as the corresponding evolution in (ii), which implies the mentioned symmetry. Thus we report for $p\geq\frac{1}{2}$ only.

We have studied the time evolution of square lattices of 128×128 sites for a range of p and T values. It requires about 10^6 Monte Carlo steps per lattice site to stabilize the system and to obtain good statistics. The magnetization m as a function of temperature and p is exhibited in Fig. 1(a). It suggests (a) a phase transition to a ferromagnetic state occurs at $T_C(p)$ for p large enough. (b) The parameter p has three main effects on the phase transition: (i) the degree of saturation decreases with p; (ii) the transition temperature also decreases with p, and (iii) there is no low-T ferromagnetic state for any $p\leq0.91$. (c) The indicated phase transition is qualitatively similar to the one in the pure system, i.e., to the Onsager one for the equilibrium case $p=1$. In particular, it is of second order, and a detailed analysis of data gives consistency with Onsager critical exponents. It is demonstrated, for instance, by the fact that all the data for $0.94\leq p<1$ can be made to lie together within experimental errors on the Onsager curve for $p=1$ by multiplying the quantity by the parameter in Table I and scaling temperatures by $T_C(p)$.

The case $p=0.93$ in Fig. 1(a) suggests a departure from Onsager behavior for smaller values of p, however. That is, the scaling of $p=0.93$ to 1 is not satisfactory [and requires unexpectedly large values for $\alpha_1(p)$ or $\alpha_2(p)$ in Table I]; it corresponds to a qualitatively different behavior as suggested also by the plot in Fig. 1(a). It might indicate either that the phase transition becomes of first order as p is decreased, so that a (nonequilibrium) tricritical point exists for $p\approx0.93$, or else that critical exponents differ from the Onsager values for $p\approx0.93$. As we never observed discontinuities or metastable states, we favor the latter possibility, but no computation of critical indexes is attempted; it is beyond the scope of the present work. In fact, the above conclusions are supported by the data for the energy and specific heat and by the data in Figs. 1(b) and 1(c) also. Deviations shown for $p=0.93$ [small $T_C(p)$] in Figs. 1(a)–1(c) probably reflect influence of a different mechanism competing with thermal fluctuations, as argued below. We have defined the energy for this nonequilibrium system (which has no Hamiltonian) as the mean number of ±1 NN pairs as obtained starting from an arbitrary distribution of exchange interactions which is updated and stored at each Monte Carlo step.

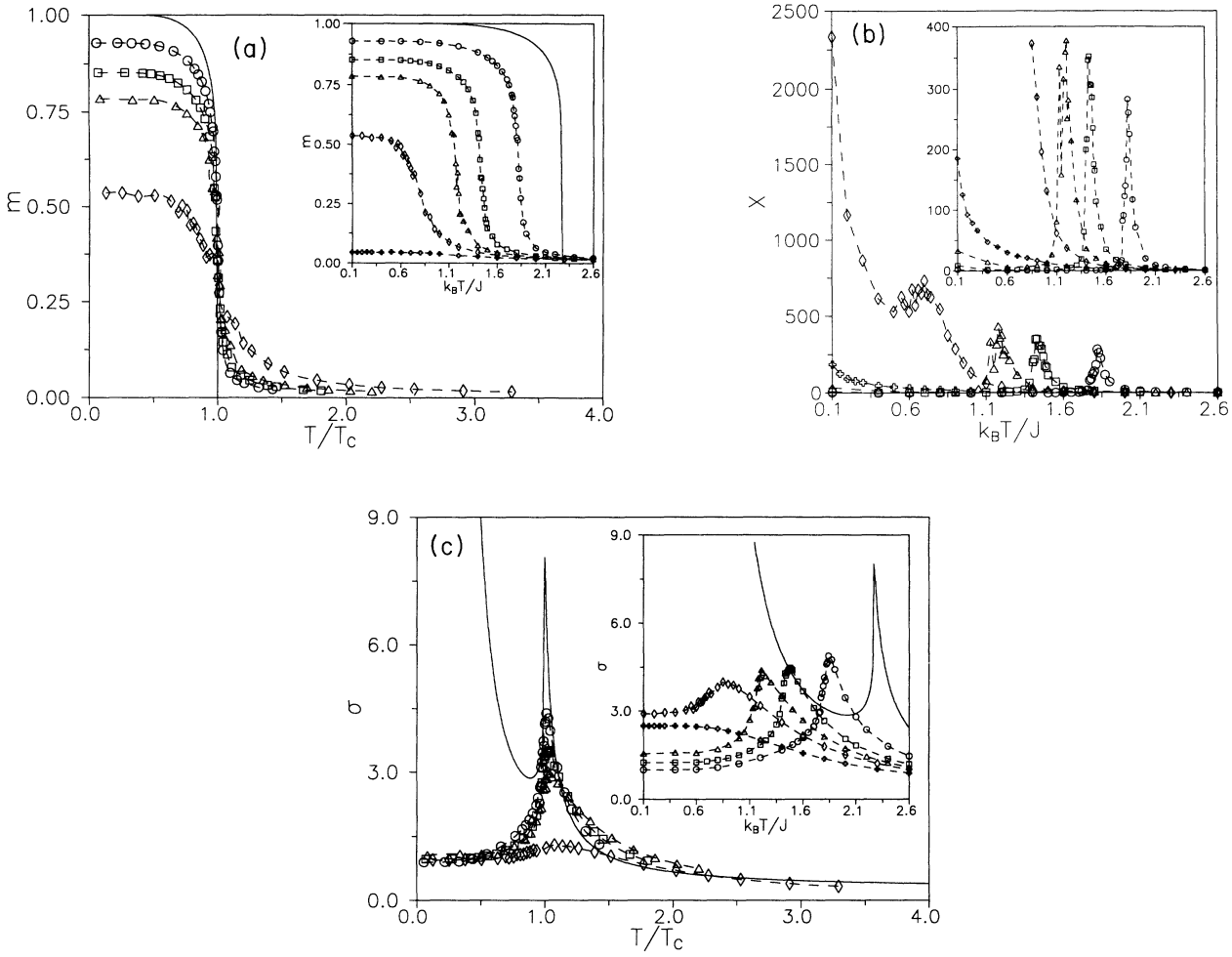

FIG. 1. (a) The magnetization versus temperature for the two-dimensional system for different values of p. From top to bottom: $p=0.97$ (circles), 0.95 (squares), 0.94 (triangles), 0.93 (rhombuses), and 0.91 (inset) (crosses). The solid line corresponds to the equilibrium, Onsager result for $p=1$. The inset shows the raw data with temperature in units of J_0/k_B. The temperature is in units of $T_C(p)$ in the main graph. The cases $1-p$ are similar to the ones here for p, i.e., there is symmetry around $p=\frac{1}{2}$. The size of the symbols here indicates approximately typical errors bars of the data. (b) Raw data for the magnetic susceptibility defined as the squared mean fluctuations of the magnetization. The same system and symbols as (a). The inset is a more detailed representation of some of the data. (c) The short-range order parameter, as defined by (4). The same system and symbols as in (a). The euqilibrium result (cf. the main text) is shown for comparison. The inset shows the raw data, while the data have been scaled in the main graph with $T_C(p)$ and $1/\alpha_1(p)$ as given in Table I.

The critical temperature $T_C(p)$ may be estimated from the data for the magnetic susceptibility [cf. Fig. 1(b)] and, sometimes more accurately, from analysis of short-ranged order [cf. Fig. 1(c)]. The latter may be measured by means of the parameter

$$\sigma \equiv \langle N_{++}N_{--}(N_{+-})^{-2} \rangle , \tag{4}$$

where N_{++}, N_{--}, and N_{+-} represent the number of NN pairs of $+1$ states, of -1 states, and of ± 1 states, respectively, and $\langle\ \rangle$ stands for the Monte Carlo average. The equilibrium result shown in Fig. 1(c) was obtained from the values for the magnetization and energy assuming that $\sigma = \langle N_{++}N_{--} \rangle \langle N_{+-} \rangle^{-2}$. One may prove [14] within the latter assumption that the critical

TABLE I. Variation with p of the parameters that scale the data for $d=2$ (cf. the main text). The magnetization needs to be multiplied by $\alpha_1(p)$, the susceptibility and the short-range order parameter by $1/\alpha_1(p)$, the energy by $\alpha_2(p)$, and the specific heat by $1/\alpha_2(p)$; in any case, the temperature needs to be measured in units of $T_C(p)$. Then, all the data for $0.94 \le p < 1$ (but not for $p < 0.94$) scale within experimental errors (the comparison of different graphs gives an idea of error bars) onto the Onsager curve for $p=1$.

p	α_1	α_2
0.97	1.111	1.356
0.95	1.274	2.014
0.94	1.451	3.065
0.93	3.074	11.75

behavior of σ is determined by the critical indexes for the magnetization (b, say) and specific heat (α, say), namely,

$$\sigma \sim \sigma_C + a_1 \epsilon^{1-\alpha} - a_2 \epsilon^{2b} \text{ as } \epsilon \equiv |T - T_C| \to 0 ,$$

where σ_C is nonsingular, and a_1 and a_2 are both positive definite. Thus the trend towards a broader peak of σ near $T_C(p)$, which is observed in Fig. 1(c) for $p=0.93$, as compared to the cases where $p \geq 0.94$, suggests again a changeover of critical exponents from the Onsager values (it suggests—at least—the onset of some peculiar phenomenon as p is decreased). The study of σ for several lattice sizes, together with the rest of the data, leads to the phase diagram for the two-dimensional system in Fig. 2 (curve labeled $d=2$).

The above results are consistent with the exact solution for $d=1$ [8,10], and with a mean-field first-order study [11]. The latter gives a second-order phase transition at $T_C(p)$ for any $p > p_0 = \frac{32}{37}$ (as compared to $p_0 \approx 0.928$ here). It is remarkable that the mean-field approximation predicts a strong dependence of steady-state properties on the effective transition rate. Namely, the mean-field system may exhibit phase transitions of first order also (and tricritical points) when the rate is $c(\mathbf{s};\mathbf{x}) = \exp(-\frac{1}{2}\beta\Delta H_{J_0}) + (1-p)\exp(-\frac{1}{2}\beta\Delta H_{-J_0})$, which, as it occurs with the choice (3) here, does not satisfy the detailed balance condition. We refer to [10] for a more general discussion of the influence of the rate on properties of the steady state.

Further existing results (for $d=2$) are exact bounds for the region of the phase diagram in which the system is necessarily ergodic [8]. It is known that any sharp phase transition may only occur for $T < T_0$, where (T_0 is in units of J_0/k_B) $4T_0^{-1} \equiv -\ln(\frac{1}{3}\{2-8p+[4(4p-1)^2 + 3(16p-9)]^{1/2}\})$, $p > \frac{1}{2}$, as long as $p > \frac{9}{16}$. Therefore the existence of some sort of order at low temperatures that differs from the ferromagnetic one described in Fig. 2 cannot be excluded in principle for $0.562 < p < p_0$. In fact, the Monte Carlo simulations do not exclude such a possibility: the direct inspection of typical spin configurations suggests the existence of some sort of order for $p < p_0$. This is illustrated in Fig. 3. That is, the configurations in Figs. 3(a)–3(c) for $p=0.91$ differ from the disordered one (for $T=2.6$) in Fig. 3(d), and also from the ferromagneticlike ones in Figs. 3(e) and 3(f) for $p=0.93$ and 0.95, respectively. Furthermore, this sort of order seems independent of T (i.e., rather stable to thermal perturbations) as suggested by a comparison of Figs. 3(a)–3(c). The analysis of cumulants and other quantities also suggests the existence of intriguing phenomena at low temperature for $p < 0.93$. This is the case, for example, of the cumulants in Fig. 4, defined

$$U_\kappa = 1 - \tfrac{1}{3}\langle \kappa^4 \rangle / \langle \kappa^2 \rangle^2 , \tag{5}$$

where κ refers either to the magnetization m or to the short-range order parameter σ (before Monte Carlo averaging). For an infinite system, one has $U_\kappa \to \frac{2}{3}$ as long as $\langle \kappa^n \rangle \to \langle \kappa \rangle^n$, i.e., for *nonpathological* distributions, as long as $\langle \kappa \rangle \neq 0$, while $U_\kappa \to 0$ when $\langle \kappa^4 \rangle \to 3\langle \kappa^2 \rangle^2$, that occurs (e.g.) for a Gaussian distribution symmetrically distributed around zero. The data for U_m in Fig. 4(a) are as expected for $p=0.91$ ($m=0$ then) and $p > 0.93$ for $T < T_C(p)$, while there is a slight deviation for $p=0.93$. The behavior exhibited by U_σ in Fig. 4(b) is rather puzzling (e.g., it suggests that the phase transition is not of second order, apparently against all other evidence). The behavior in Fig. 4(c) of the cumulant of the *energy* (see above) is also interesting.

In three dimensions, we have studied lattices of $L \times L \times L$ sites for $L \leq 64$, for up to near 10^6 Monte Carlo steps per lattice site, by using the algorithm (3). As predicted by mean-field theory [11], it behaves qualitatively similarly to the two-dimensional lattice above. Consequently, we shall avoid any repetition. The corresponding phase diagram is indicated in Fig. 2 (curve labeled $d=3$). We get $p_0 = 0.835$, as compared to the mean-field result $p_0 = 0.786$. The finite-size analysis of the data (which was performed precisely by the procedure that is familiar for the pure Ising model) for several values of p leads to exponents that are consistent with (equilibrium) critical indexes of the pure case, but we cannot exclude the possibility of a crossover when p decreases as described above for $d=2$. On the other hand, the exact results in Ref. [8] do not bar the possibility of an ordered phase for $T < T_0$ with $[1-4(2p-1)]e^{-12T_0} + 30e^{-8T_0} + [15+60(2p-1)]e^{-4T_0} - 56(2p-1) - 14 = 0$, $p \geq \frac{1}{2}$. Such a possibility is suggested again by direct inspection of typical configurations corresponding to steady states outside the ferromagneticlike region near the corresponding transition temperature. Concerning this sort of order, we observe that (i) it is less pronounced for $d=3$ than for $d=2$. (ii) It tends to be washed out as one approaches $p=0.5$. (iii) It is quite likely related to the behavior of the magnetic susceptibility (Fig. 5). Namely, the peak of the latter quantity at $T_C(p)$ tends to disappear as p is decreased and one approaches p_0, while the background increases significantly for $p \lesssim p_0$ between

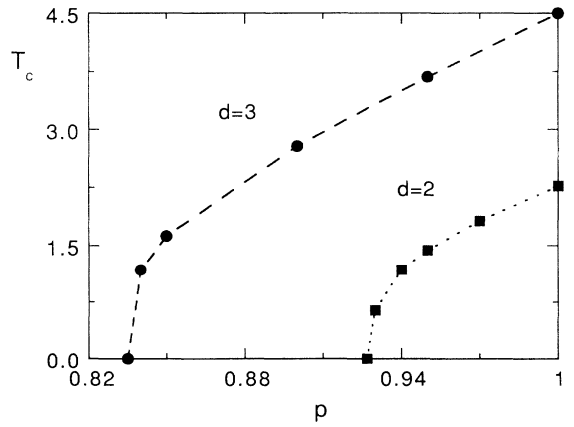

FIG. 2. Monte Carlo estimate of the transition temperature T_C as a funtion of p for the two-dimensional system with $N=128\times128$ sites and for the *infinite* ($N \to \infty$) three-dimensional system, the latter from a (standard) finite-size scaling analysis, as indicated. There is a similar situation within the antiferromagnetic, $p < \frac{1}{2}$ region.

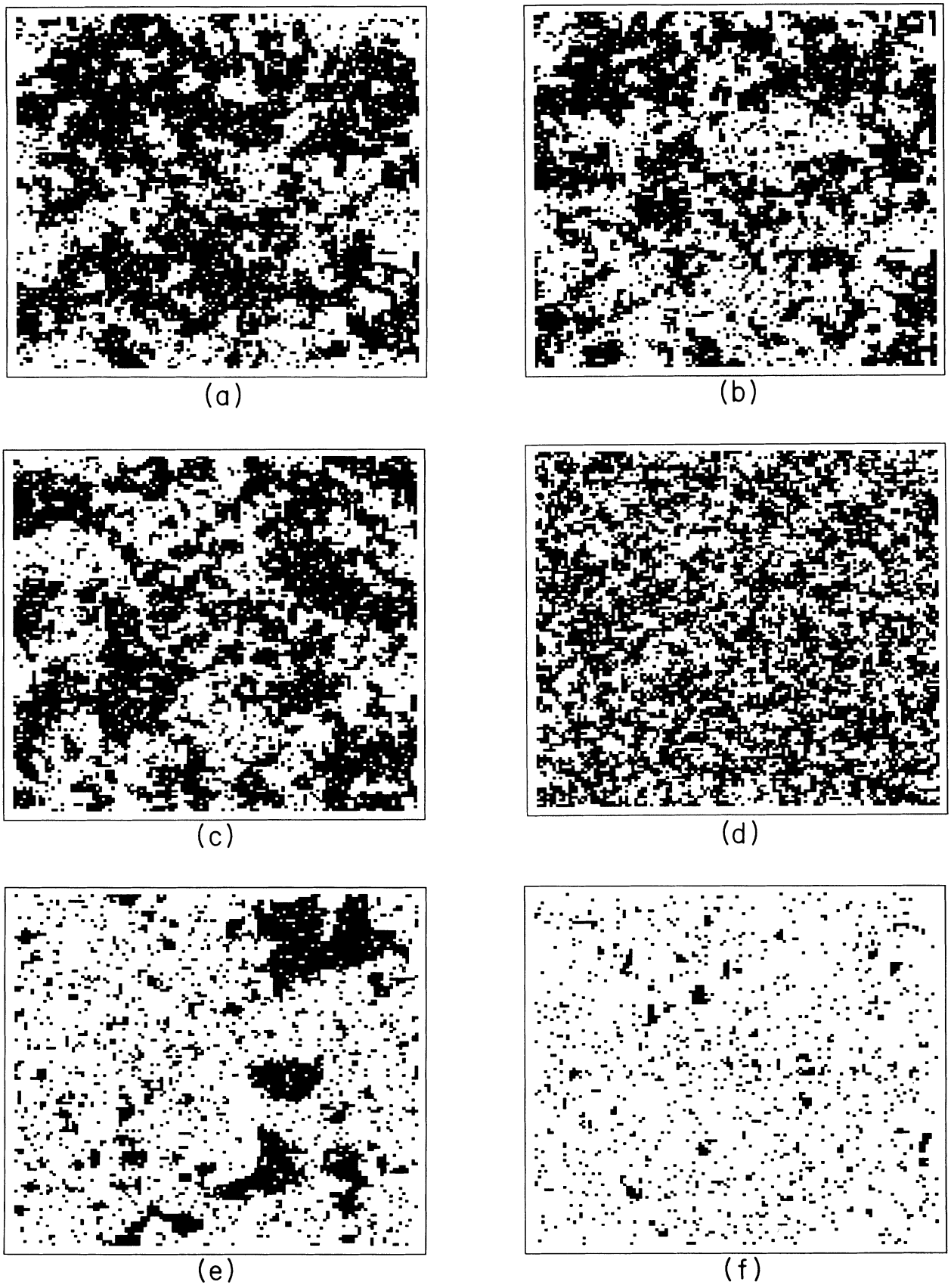

FIG. 3. Typical configurations with zero mangetization for the two-dimensional system: (a) $p=0.91$ and temperature $T=0.10$, (b) the same for $T=0.30$, (c) the same for $T=0.60$, (d) the same for $T=2.60$, (e) the same for $p=0.93$ and $T=0.10$, and (f) the same for $p=0.95$ and $T=0.10$.

$T_C(p)$ and $T=0$, as remarked above about short-range order. It seems remarkable also that the susceptibility for $p \lesssim p_0$ depends strongly on the lattice size; cf. Fig. 5(b).

The present system has a simple representation for $T=0$ which is convenient for numerical analysis. That is, (2) and (3) reduce for $T=0$ to the following rule to attempt the flip of spin s_x: Compute $\epsilon_x \equiv s_x \sum_{\mathrm{NN}} s_y$, where the sum extends over the $2d$ NN's of site $\mathbf{x}$; the flip is performed with probability p or $1-p$ according to whether ϵ_x is negative or positive, respectively; the flip is performed anyway if ϵ_x is zero. This rule is similar but not identical to the one in some majority vote models considered before [12,15]. The ensuing steady state for $d=2$ and 3 is described elsewhere [12]. A main observation is that, in the absence of thermal fluctuations (i.e., $T=0$), the system exhibits a (nonequilibrium) second-order *percolative* phase transition. It occurs for $p=p_0(d)$ (as estimated above), and the corresponding critical exponents happen to be the ones for the ordinary Ising model. This is a different phenomenon than the phase transition described above which is governed by the conflict between two values of the exchange interaction and the thermal bath. But the latter transition is influenced by the *percolation* phenomena at low enough T, namely, if one crosses the transition curve by keeping p constant such that $p \gtrsim p_0$ while varying T. We claim that such an influence may explain our observation above about an apparent departure of critical behavior from the Ising class as one describes the transition curves in Fig. 2 by decreasing p. It may be mentioned that the (peculiar)

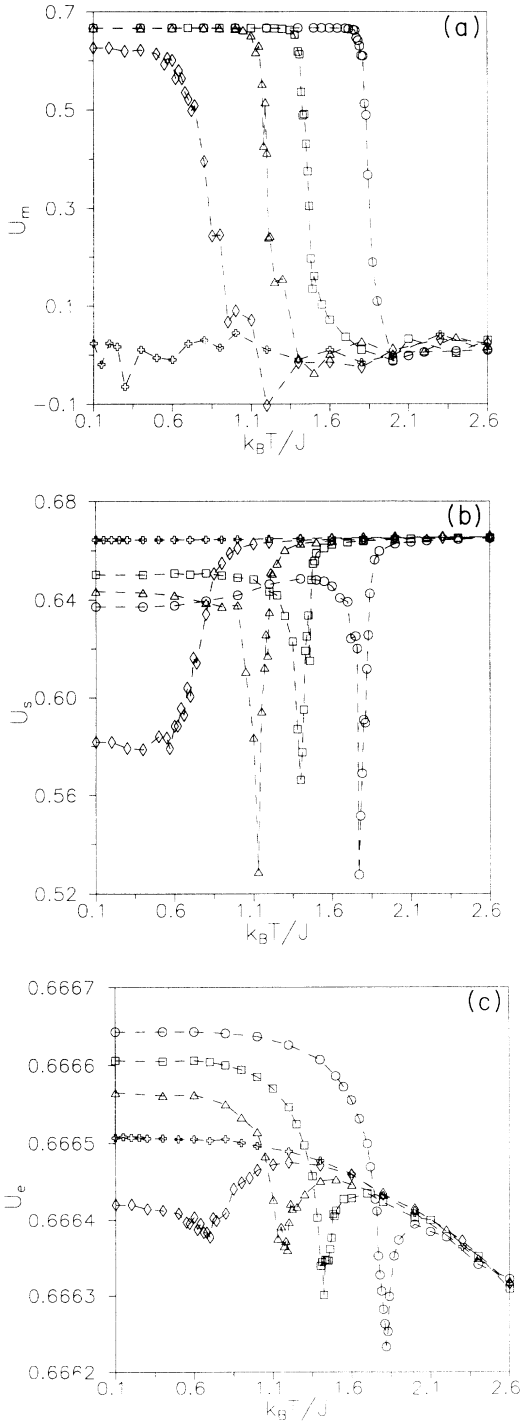

FIG. 4. Temperature variation of the cumulants, as defined in (5), of the magnetization, (a), short-range order parameter, (b), and *energy* (cf. the main text), (c). The same system and symbols as in Fig. 1(a).

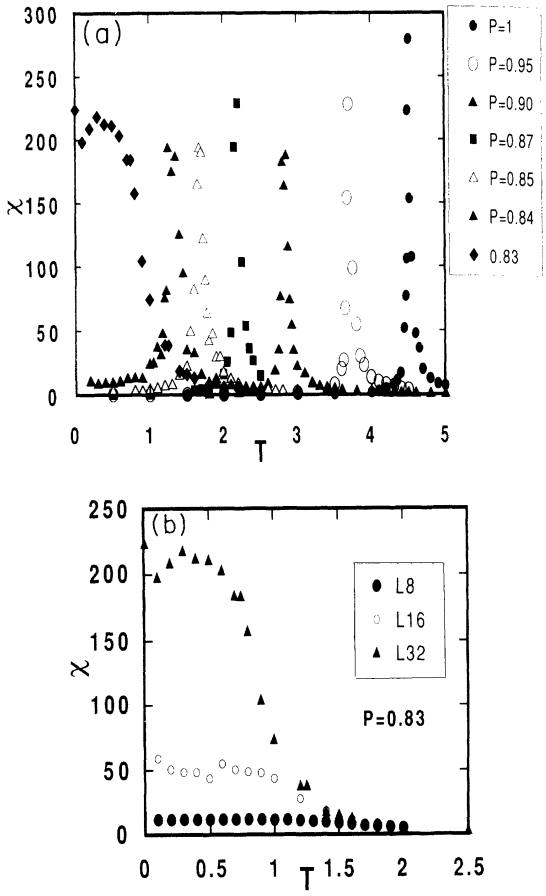

FIG. 5. Temperature dependence of the magnetic susceptibility for the three-dimensional system. (a) As a function of p for the L^3, $L=32$, lattice. (b) As a function of L for $p=0.83$.

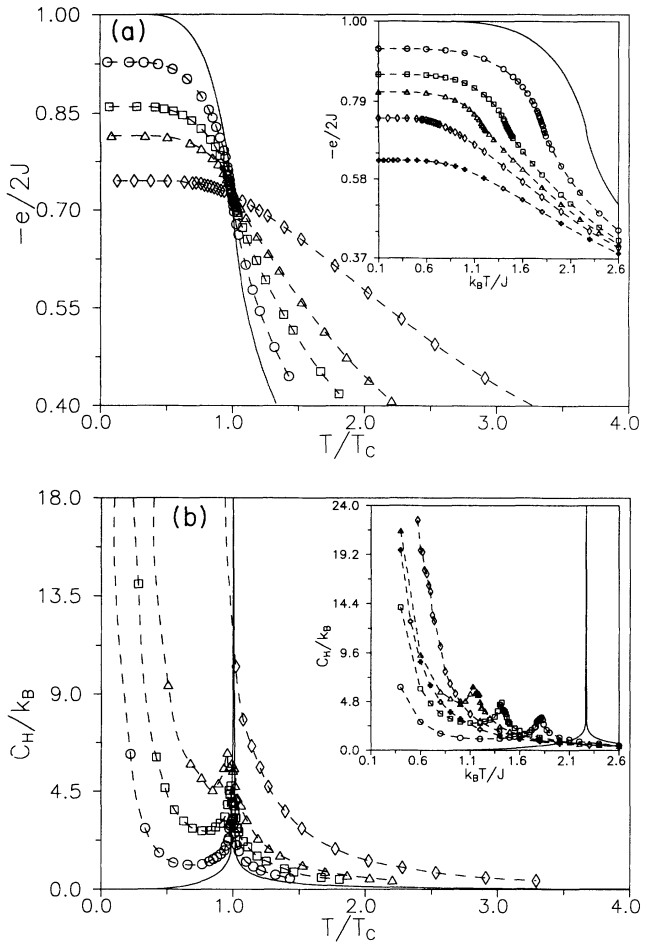

FIG. 6. (a) The *energy* (cf. the main text) for the two-dimensional system plotted as in Fig. 1(a). (b) The corresponding square mean fluctuations or "specific heat."

behavior reported in Ref. [12] for the variation with $p<p_0$ of the cumulant U_m for $T=0$ also supports that the corresponding region might not be simply paramagnetic, as suggested by some observations above.

Summing up, diffusion of magnetic ions in spin-glass materials is neglected in the standard models in which spatial disorder is quenched. However, atomic diffusion produces time variations of the spin exchange interactions, which may lead to interesting nonequilibrium effects. This motivates one to study kinetic Ising-like models that involve diffusion of impurities [10]; moreover, the models allow for a systematic study of nonequilibrium steady states and phase transitions. A nonequilibrium spin-glass model with competing kinetics that simulates a fast random diffusion of impurities, which is independent of the spin configuration, has been solved exactly for $d=1$ (under certain restrictions) [8] and in a mean-field approximation [11]. We report in the present paper some Monte Carlo results for $d=2$ and 3 of the simplest realization of the same model. This confirms that the model is interesting, and also more amenable to numerical analysis than the quenched case. The main findings and several problems raised which deserve further study may be summarized as follows.

In agreement with the mean-field solution [11], phase transitions of second order occur on the solid lines in Fig. 2 for $d=2$ and 3. The low-T states are ferromagneticlike for $p>\frac{1}{2}$ and antiferromagneticlike for $p<\frac{1}{2}$ below $T_C(p)$. The diffusion of disorder induced by competing kinetics seems to have the following effects on the transitions: (i) the degree of saturation in $m(T)$ curves as $T\to 0$ decreases with$p$, (ii) the transition temperature $T_C(p)$ decreases with p (both effects are expected on simple grounds), and (iii) a low-T ordered state is prevented below some value of p, say p_0. Near (e.g.) $p=1$ there is an approximately linear behavior that may be represented by the phenomenological fits $T_C(p)=T_C(1)(11p-8)/3$ for $d=3$ and $T_C(p)=T_C(1)(7p-6)$ for $d=2$. The critical exponents that characterize the phase transition are quite likely the same as for the equilibrium system for $p=1$ or 0, at least for p large enough. We found, however, some evidence of a departure from that behavior, perhaps evidencing a crossover towards new values as p goes to p_0 from above; cf. Figs. 1 and 6 for instance. Such a departure from the Ising behavior (as well as the peculiar behavior that evidences most of the figures at low temperature) is probably due to the influence of the nonequilibrium percolation phenomena that undergoes the system at $T=0$ [8,12]. It should be remarked also that the mean-field approximation predicts the existence of discontinuous phase transitions and tricritical points when the effective rate $c(\mathbf{s};\mathbf{x})$ in (2) is implemented by means of competing algorithms that differ from the Metropolis one involved by (3) [11]. Further systematic study of some of the most interesting features we have found is called for. Sharper quantitative results require much computer time. We intend to do that in the near future.

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