Universality class of the two-dimensional site-diluted Ising model

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In this work, we evaluate the probability distribution function of the order parameter for the two-dimensional site-diluted Ising model. Extensive Monte Carlo simulations have been performed for different spin concentrations p $(0.70 \leq p \leq 1)$ on square lattices with linear sizes L $(20 \leq L \leq 100)$. The results indicate that the universality class of the diluted Ising model seems to be independent of the amount of dilution. Logarithmic corrections of the finite-size critical temperature behavior of the model can also be inferred even for such small lattices.

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The effects of impurities on the critical behavior of magnetic systems have been extensively investigated in both theoretical and experimental points of view [1–3]. The principal aim of these studies is certainly to know how the disorder changes the character of the phase transition and therefore its universality class. According to the Harris criterion [4], a weakly disordered system changes its universality class if the specific heat critical exponent—α_{pure}—of the corresponding pure system is greater than zero. Disorder does not affect the critical behavior of systems having negative α_{pure}. These results have been corroborated by several experiments [5] and theoretical analyses (e.g., renormalization group [6–8] and series expansions [9]). The two-dimensional diluted Ising model is particularly interesting, because it corresponds to a marginal case ($\alpha_{pure}=0$), at which the Harris criterion is inconclusive. Although this disordered model has been tackled via both computational [10] and theoretical [11] approximations, its universality class still remains not well defined and deserves special attention. Currently, there are two conflicting pictures about this subject: (a) the logarithmic corrections and (b) the weak universality. The former scenario (also known as strong universality) claims that the presence of weak dilution affects the critical properties of the model only through logarithmic corrections to the pure system behavior [12–14]. The latter picture is supported by numerical works [11,15,16] and suggests critical exponents varying with increasing disorder. A systematic finite-size scaling analysis [17] has shown that no unambiguous distinction between the strong and weak universalities is possible on the basis of the available finite-size data. Nevertheless, nowadays, there has been a general tendency to accept changes given by only logarithmic corrections to the pure system power-law singularities, though such corrections turn out to be very subtle to detect in numerical studies [18]. The present work attempts to go further in the direction of elucidating this dilemma, at least regarding the universality class of the model, by using extensive Monte Carlo simulations for different spin concentrations p on square lattices.

The system under investigation is the ferromagnetic spin-1/2 Ising model described by the Hamiltonian [19]

$$\mathcal{H} = -J\sum_{\langle ij \rangle} \epsilon_i \epsilon_j S_i S_j - H\sum_{i=1}^{N} \epsilon_i S_i, \tag{1}$$

where J is the exchange coupling, $S_i = \pm 1$ is the spin at site i, ϵ_i is 1 (0) if spin is present (absent) at site i, H is the external field, and N is the total number of sites. The first sum in Eq. (1) runs over nearest-neighbor spin pairs on a square two-dimensional lattice. Of course, one has $p=\langle \epsilon_i \rangle = (1/N)\Sigma_{i=1}^{N} \epsilon_i$, where p is the spin concentration. For $H=0$, it is well known that the pure infinite square system $(p=1)$ undergoes a second-order phase transition at a temperature $T_c = 2/\ln(1+\sqrt{2}) = 2.269\,185\ldots$ (in units of J/k_B, where k_B is the Boltzmann constant). Even this simple pure model has been shown to have detailed correspondence to specific real magnetic materials [20]. Regarding the diluted system, it is known that, as the spin concentration p decreases, the transition temperature also decreases. For $p < p_c$, where p_c is the percolation threshold on the corresponding lattice, there is no phase transition. For site dilution, one has $p_c = 0.592\,746\,21(13)$ [21].

In what concerns physical thermodynamic quantities, the order parameter distribution function has been proved to be a powerful tool for studying not only magnetic systems [10,22–25], but also the liquid-gas critical point [26], the critical point in the unified theory of weak and electromagnetic interactions [27], and the critical point in quantum chromodynamics [28]. For the specific case of magnetic systems, the order parameter can be chosen as the magnetization per spin, namely, $m=(1/N)\Sigma_{i=1}^{N} \epsilon_i S_i$, where N is the total number of sites and S_i is the spin at site i. In finite-size systems, the magnetization m is a fluctuating quantity, characterized by the probability distribution $P(m)$ [22,29]. In Ising-like models undergoing a second-order phase transition, it is known that, at temperatures lower than the critical temperature T_c, the distribution $P(m)$ has a double peak, centered at the spontaneous magnetizations $+m$ and $-m$. At temperatures reasonably greater than T_c, $P(m)$ has a single peak at zero magnetization, and exactly at or close to T_c, a double-peak shape is observed [22]. In analogy to the usual finite-size scaling assumptions [30], one then expects that, for a

large finite system of linear dimension L at the critical point, $P(m)$ takes the form

$$P(m) = bP^*(\tilde{m}), \tag{2}$$

where $b=b_0L^{\beta/\nu}$, β and ν are the critical exponents of the magnetization and correlation length, respectively, $\tilde{m}=bm$, b_0 is a nonuniversal constant, and $P^*(\tilde{m})$ is a universal scaling function. Scaling functions, such as that given by Eq. (2), are characteristic of the corresponding universality class. Systems belonging to the same universality class share the same P^* scaling function. Thus, from the precise knowledge of $P^*(\tilde{m})$, one can characterize critical points and also identify universality classes. This is what has been done so far in the literature, with the distribution for the spin-1/2 Ising model being the standard P^* function [24,26] for this universality class. For instance, Fig. 10 of Ref. [31] shows the normalized distribution $P^*(\tilde{m})$ for the two-dimensional spin-1/2, spin-1, and spin-3/2 pure Ising models at criticality, where the universal aspect of these systems can be easily noted.

Monte Carlo simulations seem to be the most efficient method to obtain results like those discussed above, where the probability distribution $P(m)$ corresponds to the fraction of the total number of realizations in which the system magnetization is m, i.e.,

$$P(m) = \frac{N_m}{\mathcal{N}}, \tag{3}$$

where N_m is the number of times that magnetization m appears and $\mathcal{N}$ is the total number of Monte Carlo steps. To compute the normalized distribution $P^*(\tilde{m})$ via Eq. (2), one has to evaluate the prefactor b. This can be easily done by first normalizing the variance. In this way, one has $b=1/\sigma$, where σ is the square root of the magnetization variance $(\sigma^2=\langle m^2\rangle-\langle m\rangle^2)$. Thus, one obtains the universal function $P^*(\tilde{m})$ by simply rescaling the magnetization $\tilde{m}=m/\sigma$, and by using Eq. (2) to rescale the probability distribution $P^*(\tilde{m})=\sigma P(m)$. In this way, the desired probability distribution P^* turns out to be independent of any critical exponent, and is a hallmark of its universality class.

In general, the probability distribution function is used for studying models in which the critical temperature, or even the universal distribution function, is exactly (or very accurately) known. That is, in fact, what has been done in the study of several systems. When this distribution, as well as the critical temperature and critical exponents, are not known, one can of course first do a canonical simulation in order to get the critical values (universal and nonuniversal) and compute, afterward, the desired distribution. On the other hand, in Ref. [25], a different approach has been proposed, in the sense that it does use the order parameter distribution itself in order to obtain the criticality of the system. For a large L and a given temperature T_L near T_c, one can compute the corresponding probability distribution, which is considered a "reference" distribution. Lattices with different values of L have the same distribution as the reference one at different temperatures T_L. By using a set of T_L's, a finite-size scaling analysis can be done to estimate the critical temperature of the infinite system. For example, according to this approach, one gets $T_c=2.2693(1)$ for the two-dimensional Ising model [25], which is, in fact, quite close to the exact value. In the present case, however, we already have the standard universal distribution to be tested, and we will show that the estimates of $P^*(\tilde{m})$ for different spin concentrations p give the same distribution as that obtained for the pure system. Thus, the universality class of the two-dimensional site diluted Ising model is, in fact, unaffected by disorder.

We have performed Monte Carlo simulations [up to 10^7-10^8 Monte Carlo steps per spin after $(2.0-5.0)\times10^4$ steps were discarded for thermalization] on square $L\times L$ lattices with periodic boundary conditions for systems of characteristic length $20\leq L\leq 100$ and spin concentrations $p=0.99$, 0.97, 0.95, 0.93, 0.90, 0.85, 0.80, 0.75, and 0.70. For a given L and a given p, the simulation ran at a fixed temperature. We have evolved the system according to two different procedures: the standard single-spin flip Metropolis algorithm and the Wolff [32] cluster method. We have chosen the former because, although rather inefficient, it is the simplest to implement and one of the most used in Monte Carlo simulations. On the other hand, the latter approach has been used because its performance generally exceeds that of other methods such as the Swendsen-Wang procedure [33]. In these procedures, one Monte Carlo step corresponds to L^2 trials to flip a spin in the Metropolis case and to five attempts to flip a cluster in the Wolff algorithm. In both cases, we performed 200 random realizations for each value of p in order to compute averages over distribution of spins. A histogram reweighting technique [34,35] has been used to obtain thermodynamic information in the vicinity of the simulated temperature. For instance, for each concentration p and lattice size L, the temperature T (in units of J/k_B) has been tuned until its $P_L^*(p,T,\tilde{m})$ has the best match with the pure system probability distribution. We have generated the pure system probability distribution $P_L^*(\tilde{m})$ by simulating the Ising model on a lattice size $L=100$ at $T_c=2.269\,185\,3$ with the Wolff algorithm taking 10^8 Monte Carlo steps. We have also generated $P_L^*(\tilde{m})$ on a lattice size $L=64$ at $T_c=2.269\,185\,3$ with the Metropolis algorithm and 10^8 Monte Carlo steps. However, the difference between these two distributions for the pure system was not significant for our purposes.

Table I shows the temperatures for different spin concentrations, and different lattice sizes, in which the correspond-

TABLE I. Temperatures for different spin concentrations and different lattice sizes with the same probability distribution as that of the pure system. Simulations performed by using the single-spin flip Metropolis algorithm.

	p				
L	0.99	0.97	0.93	0.80	0.70
20	2.2362(5)	2.1675(5)	2.0260(5)	1.5390(10)	1.1280(20)
30	2.2350(5)	2.1647(5)	2.0212(4)	1.5280(10)	1.1075(15)
40	2.2345(5)	2.1636(5)	2.0189(4)	1.5220(6)	1.0965(10)
50	2.2343(3)	2.1630(3)	2.0180(4)	1.5175(6)	1.0880(6)
60	2.2341(2)	2.1627(5)	2.0175(4)	1.5150(6)	1.0820(6)

TABLE II. Temperatures for different spin concentrations and different lattice sizes with the same probability distribution as that of the pure system. Simulations performed by using the Wolff cluster algorithm.

	p				
L	0.95	0.90	0.85	0.80	0.75
20	2.0965(7)	1.9190(10)	1.7335(10)	1.5390(10)	1.3368(10)
30	2.0934(3)	1.9122(5)	1.7230(8)	1.5305(8)	1.3241(10)
40	2.0918(3)	1.9086(5)	1.7191(5)	1.5220(8)	1.3143(10)
50	2.0912(3)	1.9068(4)	1.7164(5)	1.5175(5)	1.3122(5)
60	2.0907(3)	1.9065(4)	1.7145(5)	1.5160(5)	1.3095(5)
70	2.0903(2)	1.9053(3)	1.7130(3)	1.5140(5)	1.3075(5)
100	2.0900(2)	1.9042(2)	1.7114(3)	1.5115(4)	1.3017(5)

ing probability distribution, obtained from the single-spin-flip Metropolis algorithm, matches well that from the pure system. Table II shows the same by employing the Wolff cluster algorithm.

In Fig. 1 we have the plot of the normalized distribution function for each lattice size, according to the data from Table II, and the standard one for the pure model. One can see that the agreement among them is excellent (note that, in fact, in each figure we have eight different distributions, seven coming from the matching of the data from Table II and one for the pure model). Similar figures showing the distribution collapse for various p and the pure distribution, like those depicted in Fig. 1, are obtained from the data of Table I, which employed the Metropolis algorithm. However, with the Wolff procedure we are able to increase the lattice size up to $L=100$. We can also see that, from the values at $p=0.80$ in Tables I and II, both algorithms give almost the same result for the tuned temperatures.

We are now in position to obtain the extrapolated critical temperature T_c from the values of T_L given in Tables I and II. For pure models, one has the finite-size scaling

$$T_L = T_c + AL^{-(1+\theta)/\nu} = T_c + AL^{-x}, \tag{4}$$

where ν is the correlation length critical exponent, θ is the corresponding correction to scaling exponent, and A is a non-

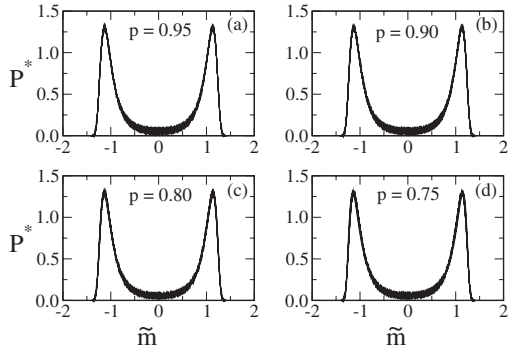

FIG. 1. Normalized distribution $P^*(\tilde{m})$ for systems with lattice sizes and temperatures shown in Table II. Each figure has a superposition of eight different distributions, taking the data from this table and for the pure model.

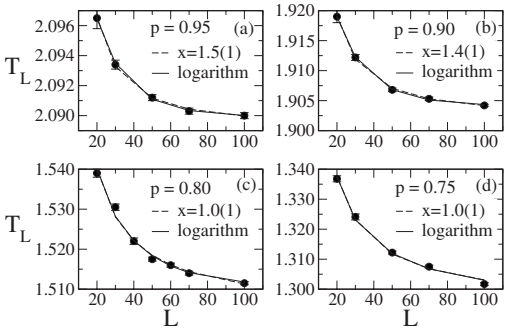

FIG. 2. Dependence of the temperatures T_L on the lattice size L. Dashed lines are obtained by varying the exponent x in Eq. (4). Solid lines take into account logarithmic corrections as in Eq. (6) and keep the exponent x constant ($x=3$). Critical temperatures T_c in the thermodynamic limit obtained from both methods are listed in Table III.

universal constant [22]. This works rather well for $p=1$ [25]. Instead, for $p<1$ the above scaling seems not to be valid for the exact values $\nu=1$ and $\theta=2$ for the two-dimensional Ising model. In fact, log-log plots of the data do not reproduce a linear curve as p varies. Nevertheless, rather good fittings to the value of T_L can be obtained by varying the exponent $x=(1+\theta)/\nu$ instead, as can be seen for some values of p by the dashed lines in Fig. 2. The corresponding extrapolated results for T_c are shown in Table III.

However, in the light of the results from Fig. 1, we expect the diluted model to have the same critical exponents as the pure model [22,23,29]. Although the scaling relation (2) depends on the ratio β/ν, from [22,23,29] we do not expect to have the same P^* for different universality classes, which preserves only the ratio β/ν. In addition, renormalization group arguments also show that the correction to scaling exponent should be the same for a given universality class. Therefore, one also expects to have the same universal exponent $x=(1+\theta)/\nu=3$ for any value of the concentration p.

TABLE III. Critical temperatures T_c for different spin concentrations p. $T_c(x)$ in the third column is the extrapolated value assuming that the exponent $(1+\theta)/\nu=x$ changes with dilution in Eq. (4). The last column gives the corresponding critical temperature assuming a logarithmic correction as in Eq. (6) and keeping $x=3$. The data come from the results using the single-spin-flip Metropolis algorithm (Table I) and Wolff algorithm (Table II).

p	$(1+\theta)/\nu=x$	$T_c(x)$	$T_c(3)$
1.00	3.0(1)	2.2693(1)	2.2693(1)
0.99	1.8(1)	2.2338(1)	2.23397(3)
0.97	1.6(1)	2.1617(2)	2.16235(4)
0.95	1.5(1)	2.0893(2)	2.08989(8)
0.93	1.5(1)	2.0153(3)	2.01677(4)
0.90	1.4(1)	1.9025(5)	1.9042(3)
0.85	1.2(1)	1.7077(6)	1.7104(4)
0.80	1.0(1)	1.5046(10)	1.5102(4)
0.75	1.0(1)	1.2955(10)	1.2990(10)
0.70	1.0(1)	1.0609(12)	1.0729(10)

This means, indeed, that Eq. (4) should no longer be valid for diluted systems. On the other hand, according to the strong universality scenario, close to criticality, the correlation length is predicted to behave as [12,13]

$$\xi \sim t^{-\nu}[1 + C \ln(1/t)]^{\tilde{\nu}}, \tag{5}$$

where $\tilde{\nu}=1/2$ and C is a concentration-dependent constant. Since for a finite system one has $\xi_{max}=L$, from the above relation one can suggest the following scaling for the temperature T_L in diluted systems:

$$T_L = T_c + AL^{-1/\nu}[L^{\theta/\tilde{\nu}} + C' \ln(L)]^{-\tilde{\nu}/\nu}, \tag{6}$$

where C' depends on p and vanishes for $p=1$. Figure 2 also shows the fittings of the data according to the above scaling relation (6), keeping the critical exponents ν and θ constant (namely, $x=3$). The corresponding extrapolated values for the critical temperature are given in Table III. Although both solid and dashed lines in Fig. 2 are quite similar, as the dilution increases, the difference between the critical temperatures, obtained from both approaches in Table III, becomes more significant. In addition, for $p<0.85$ the unexpected $\theta=\nu-1$ limit is achieved by using Eq. (4).

The reduced limiting slope $S \equiv (1/T_c)(dT_c/dp)|_{p=1}$, obtained by using the temperatures for $p=0.99$ and 1.00 expressed in Table III with logarithmic corrections, give $S=1.557(6)$, in quite good accord with the expected value $S=1.565$ [1].

One has to note that spin concentrations $p<0.70$ were not included in this work. For $0.60 \lesssim p < 0.70$, a large amount of computational time is required to compute averages over distribution of spins because many configurations do not have a percolating cluster of spins. Furthermore, near the percolation threshold, one expects a crossover phenomenon. We believe that, for spin concentrations herein considered ($p \geq 0.70$), crossover is not relevant, although Fig. 1(d) (even though it is printed on a very small scale) does show observable thickening of the line at the maxima.

Hence, one can say in summary that the present results seem to be in good agreement with the strong universality scenario, which predicts only logarithmic corrections to the critical behavior, as can be seen from Fig. 2 for the finite-size scaling of the critical temperature, even for the small lattices considered herein. The weak universality scenario, in which critical exponents vary with dilution, appears unlikely, because it should lead to different order parameter distribution functions, in contrast to what is seen in Fig. 1, even if the ratio β/ν is the same. As a result of the logarithmic corrections, we believe that a definite and more complete answer can be achieved only by increasing the size of the lattices.

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