Finite-size scaling characterization of the $\pm J$ diluted Ising lattice

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Square lattices with $(\pm J)$ exchange interactions between nearest-neighbor spins have been analyzed by using an Ising Hamiltonian. The ground-state properties are numerically evaluated by computational techniques. The energy per bond, the site correlation parameter and the fraction of unfrustrated bond are averaged over 3000 samples randomly selected. The number of spin N considered were N= 16, 25, 36, 49, 64, 81, 100, and 144. After removing all the frustrated bonds from any of the ground-state, the remaining lattice, called diluted lattice, has been characterized by means of finite-size scaling. The percolation threshold h_{gc}, for the diluted lattice is $h_{gc} = 0.4$, which is less than the corresponding threshold for classical random percolation, *i.e.* $h_c = 0.5$. Critical exponents like the correlation lenght and the order parameter exponents, ν and β respectively, were also obtained for the diluted lattice. The results are compared with the well-known random percolation problem. Significant qualitative differences are shown and discussed.

Keywords: Ising lattice; frustration; percolation

Redes bidimensionales cuadradas con $(\pm J)$ interacciones mixtas a primeros vecinos son analizadas usando un Hamiltoniano de Ising. Las propiedades del nivel fundamental son evaluadas mediante técnicas computacionales. Energía por enlace y fracción de enlaces que nunca se frustran son promediadas sobre 3000 muestras al azar. El número de espines N considerado fue N= 16, 25, 36, 49, 64, 81, 100 y 144. Después de remover los enlaces frustrados de todos los estados del nivel fundamental, la red resultante (red diluida) es caracterizada por medio de técnicas de escaleo de tamaño finito. El umbral de percolación obtenido para la red diluida fue de $h_{gc} = 0.4$, el cual es menor que el umbral para el caso aleatorio ($h_c = 0.5$). Se obtuvieron los exponentes críticos ν y β, correspondientes a la longitud de correlación y parámetro de orden respectivamente. Los resultados son comparados con el conocido caso de percolación al azar. Diferencias cualitativas son mostradas y discutidas.

Descriptores: Red de Ising; frustración; percolación

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1. Introduction

The aim of this work is to evaluate and to characterize the more prominent features of the ground state at $T = 0$ for the well known $\pm J$ Ising problem [1–4]. This system is studied by using a square lattice with N spin sites built up with ferro- (F) and antiferromagnetic (A) nearest neighbor interactions, which are randomly distributed. It is assumed here that the concentration of A-bonds, (x_A), is numerically equal to the porcentage of F-bonds (x_F), *i.e.* $x_A = x_F = 0.5$. The Hamiltonian, H, which describes the problem presented above is given by

$$H = \sum_{(i,j)} J_{ij} S_i S_j \ , \qquad (1)$$

where S_i represents the third component of the spin in the i site; J_{ij} is the exchange interaction constant which can only take two values: $J_{ij} = -1$ (ferromagnetic) and $J_{ij} = 1$ (antiferromagnetic); and (i, j) indicates pairs of nearest neighbor sites. The complete solution for this Hamiltonian can be found by enumerating the 2^N states (or 2^{N-1} due to inversion symmetry of H). The presence of frustration is well known in this system and provides multiple degeneracy of ground state [1–4]. To reinforce the previous argument, Figs. 1a–1d show the ground state for a 3×3 square lattice, where the ferromagnetic (antiferromagnetic) bonds are plotted in simple (double) line, while the frustrated bonds are denoted by crosses. The same conclusions can be obtained via the topological approach, reported, *e.g.*, in Refs. 4–9. A new lattice is formed after removing all bonds that are frustrated in any of the ground state, Fig. 1e. This new lattice has been called in previous contributions the *diluted lattice*, and we notice that is one of the most important properties which characterizes the system under consideration.

The diluted lattice has been used to define the parameter associated to the bonds, h_g, given by

$$h_g = \frac{1}{2N} \sum_{i<j} \left\langle \sum_{\alpha}^{W} \frac{|S_i^\alpha S_j^\alpha - J_{ij}|}{2} \, divW \right\rangle \ , \qquad (2)$$

where the first sum extends over all pairs of nearest neighbor; α is a index that runs over the W ground state and div means

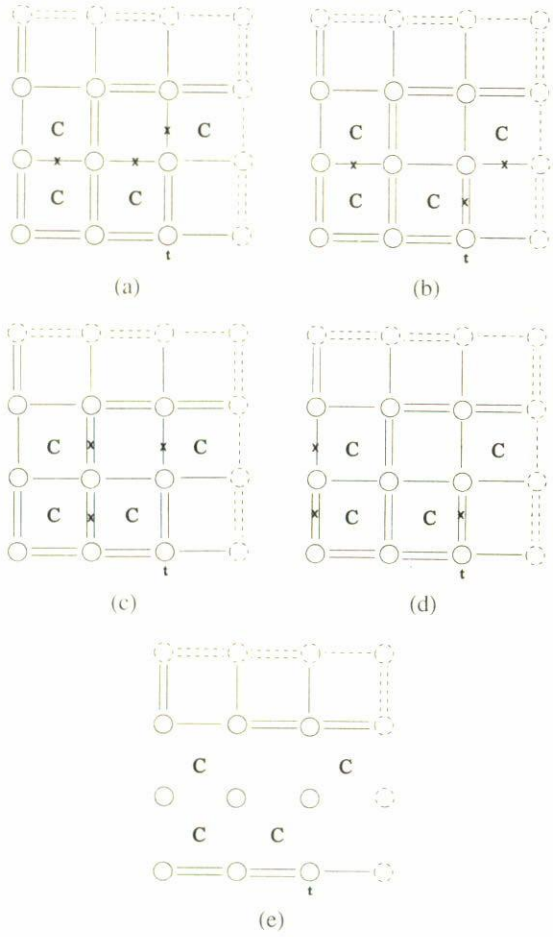

FIGURE 1. (a)–(d) Represent the four degenerated levels of the groud state for a given sample of 3×3. Single (double) lines represent a F (an A) bond; curved (frustrated) plaquettes are marked by the index C; frustration segment are shown by solid lines joining curved plaquettes; (e) shows the diluted lattice obtained after removing all bonds that frustrate in any of the ground state (a)–(d).

integer division. h_g can take values in the interval [0,1]. This parameter measure the fraction of the bonds that never are frustrated in all the W ground state. It is interesting to note that bonds in the diluted lattice have not been assigned at random, by the contrary they are distributed according to the topological rules which are inherent to the problem [3–6].

The diluted lattice undergoes a percolative phase transition and the main intention of the present work is to characterize such transition by using finite-size scaling theory.

2. Finite size analysis.

Algorithms have been dessigned in order to determine the multiple degeneracy of the ground state level. Such algorithms could need computer times that increase exponentially with N. This constrain restricts our analysis to samples up to 12×12. For each size (4×4, 5×5, 6×6, etc.), 3000 samples were randomly generated.

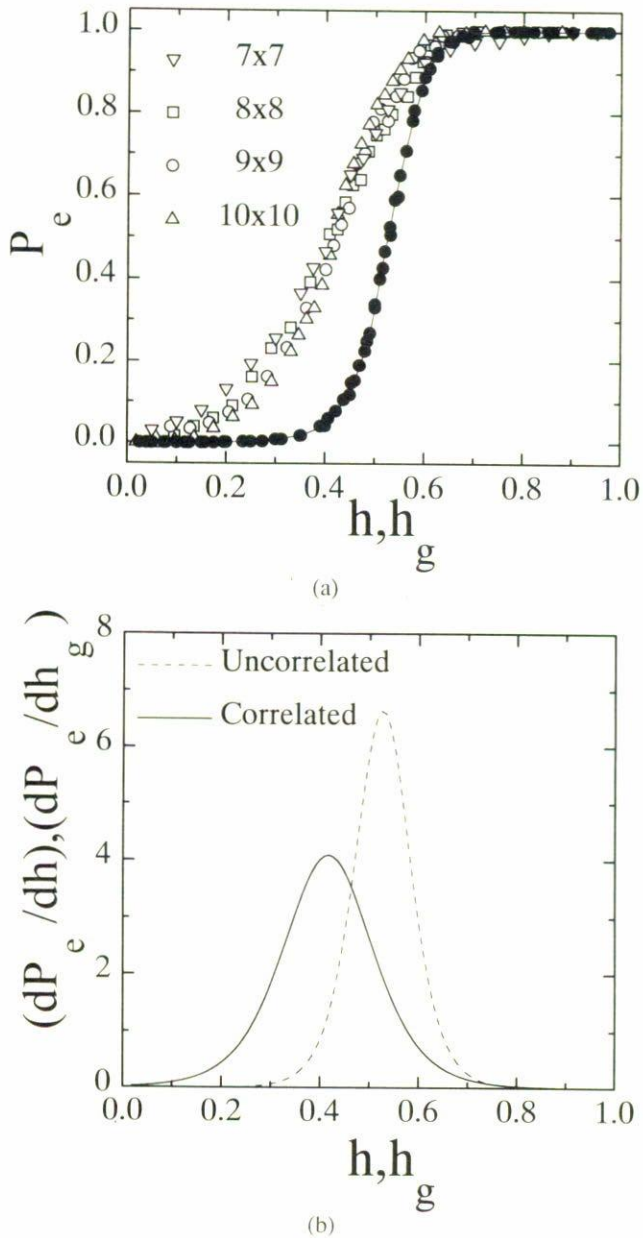

FIGURE 2. (a) Probability of percolation as function of the percolation variable h. Filled (empty) symbols represent the correlated (uncorrelated) case. (b) Shows the derivatives of the largest sizes considered in (a).

Our calculations were performed at $T = 0$ and all the bonds remain frozen in the lattice. Once the states are found, all physical properties of the lattices can be calculated. In particular, the bonds that frustrate each possible ground state can be identified and the diluted lattice for each sample can be determined. According to the well-known algorithms shown in Ref. 10 we meassure the probability of percolation, P_e.

Figure 2a shows the behavior of the probability of percolation P_e as a function of the order parameter associated to the bonds, h_g for different lattice sizes, L. The resulting percolation functions, $P_e(h_g)$ for the diluted lattices are represented by open symbols in Fig. 2a. It is interesting to note

that the larger is the lattice size the more pronounced is the step-wise behavior of the percolation functions, $P_e(h_g)$ at $h_g \sim h_{gc}$; where h_{gc} is the percolation threshold.

For purpose of comparison, diluted samples were prepared assigning the bond positions in a random way. Thus, the bond content, h, is fixed and correlations among bonds are completely ruled out. Such lattices will be called uncorrelated lattices and can be prepared at little cost in computer time. These systems are well known, so we will use their properties to compare with results for correlated lattices. As is expected, the analysis of the percolative behavior of these uncorrelated lattices deals to the classical bond percolation problem (filled symbols in Fig. 2b).

The derivatives of these functions show a sharp peak at $h_g \sim h_{gc}$. Upon increasing the lattice size, two characteristic features can be emphazised: (a) the maximum of the curves increases and (b) the maximum shifts to the percolation threshold. In Fig. 2b, we only show the derivatives corresponding to the largest value of L for uncorrelated lattices (dashed line) and for our diluted lattices (solid line).

From the inspection of these curves is clear that the slope of the curve for the correlated lattices at percolation threshold is notoriously larger than for the uncorrelated lattices. In other words, the transition from non-percolation to percolation is broader for correlated lattices as compared to uncorrelated ones. This fact is a consequence of the way in which the bonds in the uncorrelated lattice tend to cluster into regions free of frustration, as it was shown in Refs. 3 and 4.

The standard theory of finite size scaling [10–12] implies the following behavior of the probability of percolation near the percolation threshold, h_{gc}

$$P_e = L^{-\beta/\nu} \tilde{P}_e(\varepsilon L^{1/\nu}) \tag{3}$$

where $\varepsilon \equiv (h_g - h_{gc})$; β and ν are the critical exponent related to the order parameter and the correlation lenght respectively, in such a way that P_e behayes as $P_e \propto \varepsilon^{\beta}$ for $\varepsilon > 0^+$ and $L \to \infty$, and the correlation lenght ξ obeys to $\xi \propto \varepsilon^{-\nu}$ for $\varepsilon \to 0$ and $L \to \infty$. $\tilde{P}_e$ is the scaling functions for the probability of percolation which is the order parameter of the problem.

Figures 3a and 3b show the "data collapsing" plots towards a universal function according to the above equation for both the correlated and the uncorrelated lattices, respectively. We see that a reasonable fit is obtained in both cases by using $\beta = 0.125$ and $\nu = 4/3$. The agreement between the theory and our results for the uncorrelated lattices (Fig. 3b) was expected and the only justification to run numerical calculations for this case is to test our algorithm and the statistical accuracy of the sampling. These results for the uncorrelated case are very well-known and they are included here only for comparison with the uncorrelated one.

Note that the analysis given above is valid only for sufficiently large L and for ε in the asymptotic critical regime. However, it can be applied to the entire range of L and h if the data falls in the "domain of attraction" of a simple fixed point characterizing only one universality class of critical phenomena. In our case we observe that the critical exponents do not change and belong to the classical bond percolation universality class.

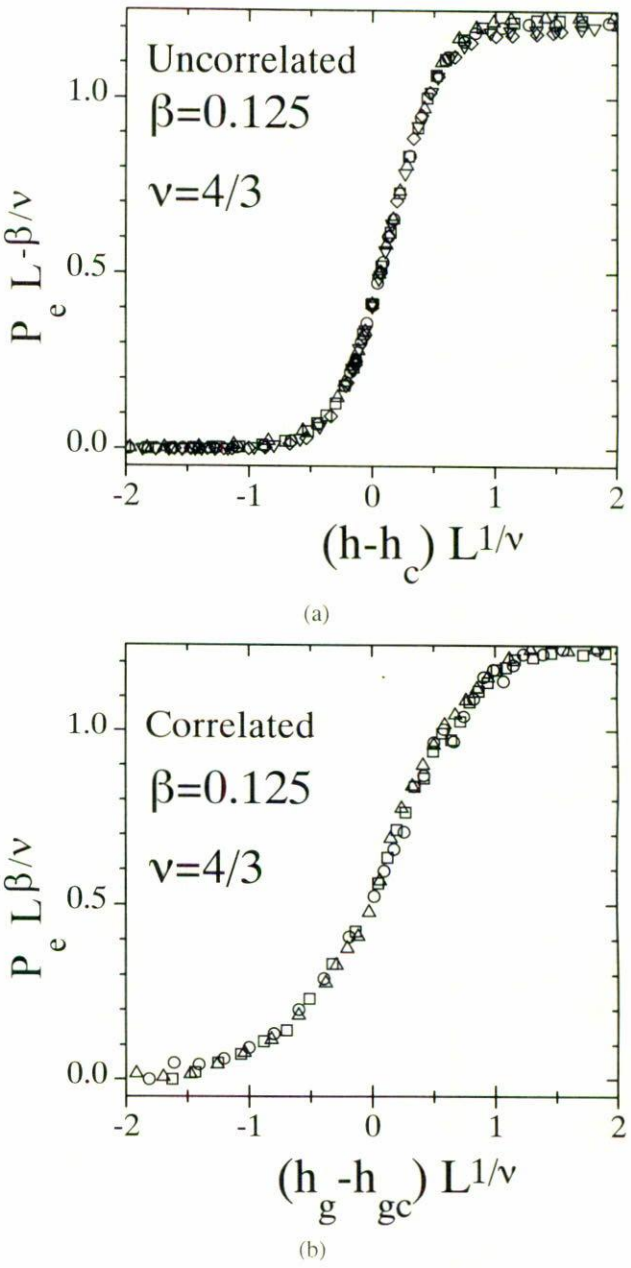

FIGURE 3. (a) Data collapsing plots according to Eq. (4) for the uncorrelated case. (b) Idem (a) for the correlated system.

It is very encouraging that the points coming from the numerical experiment follow a straight line given by

$$h_{gc}(L) = cL^{-\frac{1}{\nu}} + h_{gc}(\infty) \tag{4}$$

where $h_{gc}(L)$ is the percolation threshold for a lattice of size L; ν is the already mentioned critical exponent for the correlation lenght, c is a non-universal constant and $h_{gc}(\infty)$ is the extrapolation toward the thermodynamic limit of the percolation threshold.

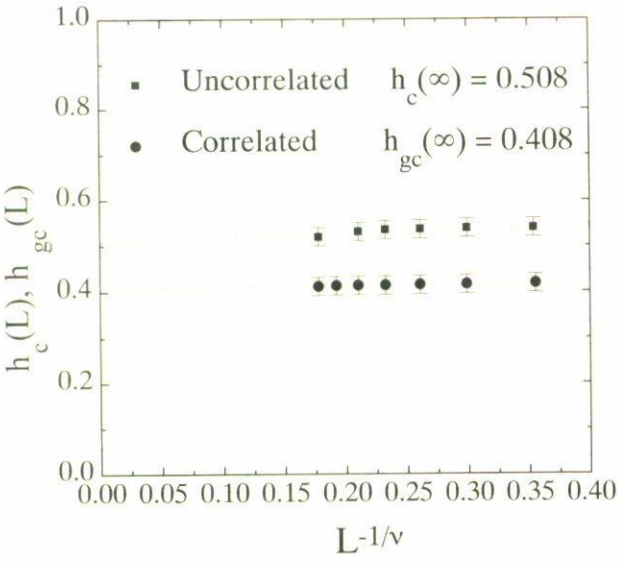

FIGURE 4. Application of scaling law (Eq. 5) to extrapolate the percolation threshold in the thermodynamic limit.

This relationship is plotted in Fig. 4 by using circles (squares) for the diluted (uncorrelated) lattices. The linear fit of the numerical data of $h_{gc}(L)$ according to Eq. (4) deals to the percolation threshold for the infinite lattice. For the standard bond percolation problem, this procedure provides $h_c(\infty) = 0.508$, which is in good agreement with the well known and exact value $h_c(\infty) = 0.5$ already predicted in the literature [10]. We notice that the percolation threshold for the diluted lattices is lower than 0.5. This fact can not be attributed to finite size effects. From Eq. (4) we determine that in the thermodynamic limit the percolation threshold for the diluted lattice, $h_{gc}(\infty) = 0.408$.

3. Conclusions

We deal with the problem of square lattices, with half the bond ferromagnetic and the other half antiferromagnetic. Equal strenght is assumed for all interactions that are restricted to nearest neighbors. Direct solution of the Hamiltonian looking for ground states leads to frustration due to the competing local field. When all bonds that frustrate in any ground state are removed we are left with a partially filled lattice that is called correlated diluted lattice. The name correlated is due to the tendency of unfrustrated bonds to group themselves in regions or islands free of frustration.

The main pourpose of this work was to determine the characteristic features of the percolative behavior of such lattices by using the standard scaling analysis. The most stricking finding is related with the different values of the percolation threshold in the thermodinamic limit for the diluted lattice [$h_{gc}(\infty) = 0.408$] and for the standard bond percolation problem [$h_c(\infty) = 0.5$] used here only for comparison. This change in the percolation threshold can be attributed to the existence of local correlations which control the formation of large magnetic domains.

The presence of such magnetic domains guide us to a different way to break the ergodicity. In fact, the ergodic separation can be done fixing the spins in the largest regions free of frustration in such a way to maximize the order parameter associated to the spins in the lattice which is defined in previous contributions [3–5].

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1. K. Binder and A.P. Young, *Rev. Mod. Phys.* **58** (1986) 801.
2. T. Klotz and S. Kobe, *J. Phys. A: Math. Gen.* **27** (1994) L95.
3. E.E. Vogel *et al.*, *Phys. Rev. B* **49** (1994) 6018.
4. A.J. Ramírez-Pastor, F. Nieto, and E.E. Vogel, *Phys. Rev. B* **55** (1997) 14323.
5. E.E. Vogel, S. Contreras, J. Cartes, and M.A. Osorio, in *Proceedings of the III Latin American Workshop on Magnetism, Magnetic Materials and their Applications*, edited by F. Leccabue and V. Sagredo, (World Scientific, Singapore, 1996), p. 152.
6. E.E. Vogel and W. Lebrecht, *Z. Phys. B* **102** (1997) 145.
7. G. Toulouse, *Communications on Physics* **2** (1977) 115.
8. I. Ono, *J. Phys. Soc. Japan* **41** (1976) 345.
9. J. Vannimenus and G. Toulouse, *J. Phys. C: Solid State Phys.* **10** (1977) 537.
10. D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd Edition, (Taylor & Francis, London, 1992).
11. V. Privman, *Finite Size Scaling and Numerical Simulation of Statistical Systems*, (World Scientific, 1990).
12. K. Binder, in : *Computational Methods in Field Theory*, edited by H. Gausterer and C.B. Lang, (Springer, Berlin, 1992), p. 59.
13. K.Binder and D.W. Heermann, *Monte Carlo Simulation in Statistical Physics. An Introduction*, (Springer, Berlin, 1988).