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Cluster analysis for percolation on a two-dimensional fully frustrated system

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Abstract. The percolation of Kandel, Ben-Av and Domany clusters for a two-dimensional fully frustrated Ising model is extensively studied through numerical simulations. Critical exponents, cluster distribution and fractal dimension of a percolating cluster are given.

1. Introduction

A two-dimensional fully frustrated (FF) Ising model is a model with Ising spins ± 1 where the interactions between nearest-neighbour spins have modulus $J > 0$ and sign ± 1 (ferro/antiferromagnetic interactions) and where the signs are chosen in such a way that every *plaquette* (i.e. the elementary cell of the square lattice) is *frustrated*, i.e. every plaquette has an odd number of -1 interactions so that the four spins of the plaquette cannot simultaneously satisfy all four interactions. In figure 1(1) we give an example of such a deterministic interaction configuration. In a plaquette of the FF model we can have only one or three satisfied interactions. The FF model has an analytical solution [1] and a critical temperature at $T_c = 0$.

Since single-spin dynamics for FF suffers critical slowing down, a fast-cluster dynamics was introduced by Kandel, Ben-Av and Domany (KBD) in [2].

The KBD clusters are defined by stochastically choosing, on each plaquette of a chequerboard partition of a square lattice, one bond configuration between the three shown in figure 1(2).

The probability of choice depends on spins configuration on the plaquette and it is a function of temperature (*correlated site–bond percolation* [3]). When there is only one satisfied interaction the zero-bond configuration is chosen with probability one. When three interactions are satisfied the zero-bond configuration is chosen with probability $P_0 = \mathrm{e}^{-4J/(kT)}$ (where k is the Boltzmann constant and T the absolute temperature), the bond configuration with two parallel bonds on two satisfied interactions is chosen with probability $P_1 = 1 - P_0$ and the third bond configuration has zero probability. Two sites are in the same cluster if they are connected by bonds. For the sake of simplicity from now on we choose $J/(kT) = 1/T$.

Reference [2] has stimulated several works [4, 5] that pay attention mainly to dynamics and to cluster numbers and cluster sizes. In [5] numerical simulations on relatively large FF lattice sizes (number of sites $N = 60^2$–120^2) supported the idea that the KBD clusters

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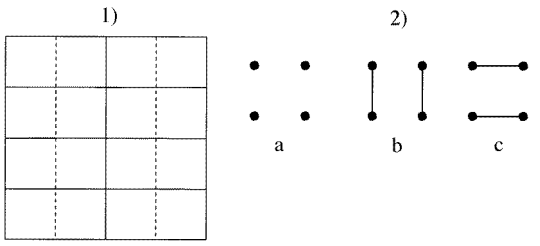

Figure 1. (1) Example of a two-dimensional FF lattice: the spin is on the vertices; full lines represent ferromagnetic interactions ($+J$) and broken lines antiferromagnetic interactions ($-J$). (2) Plaquette bond configurations: a, zero bond; b, two parallel vertical bonds; c, two parallel horizontal bonds.

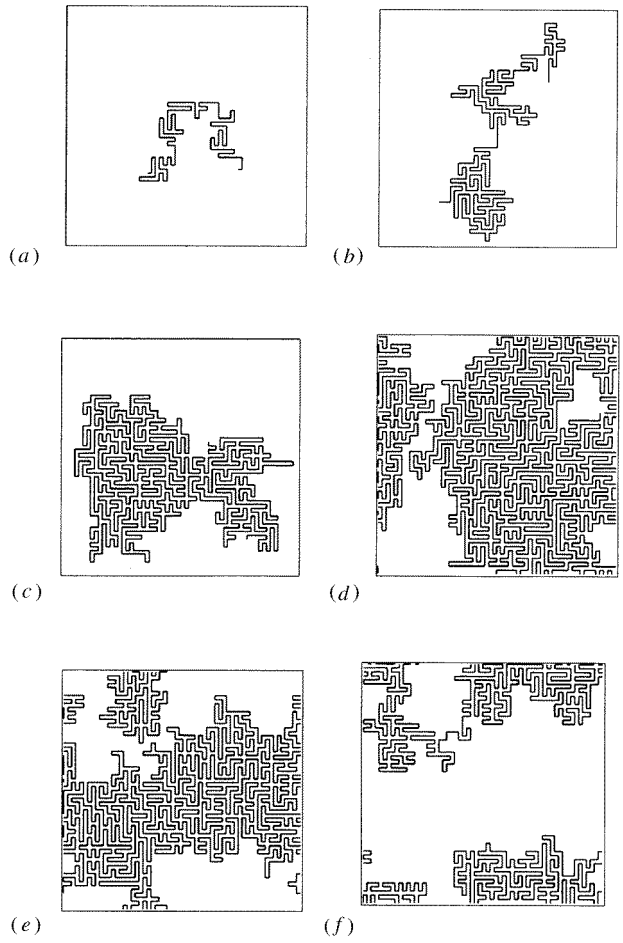

Figure 2. Typical KBD clusters on a FF lattice with size $L = 60$ with periodic boundary conditions: (a) at $T = 1$; (b) at $T = 0.65$; (c) at $T = 0.53$ slightly above $T_p(L) \simeq 0.52$; (d) at $T = 0.52 \simeq T_p(L)$; (e) at $T \simeq 0$ (largest cluster); (f) at $T \simeq 0$ (the second cluster).

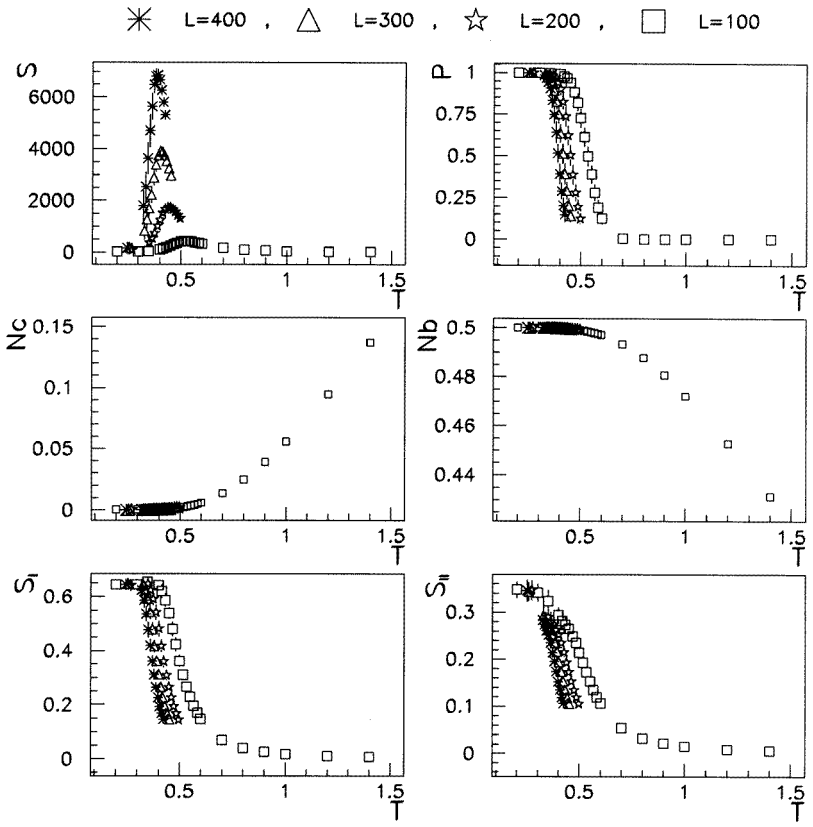

Figure 3. Mean cluster size S, percolation probability P, cluster number N_c, number of bonds per lattice site N_b, mean size of largest cluster S_{I} and mean size of second largest cluster S_{II} versus temperature T for lattice sizes $L = 100, 200, 300, 400$. The error bars (often included in symbols) are the statistical errors.

Table 1. Numerical estimates of $T_p(L)$ and $D(L)$ for $L = 60$–400. The way used to evaluate $T_p(L)$ and $D(L)$ give us confidence only on digits not in parentheses.

L	60	80	100	120	200	300	400
$T_p(L)$	0.51(7)	0.48(1)	0.45(6)	0.43(7)	0.39(2)	0.36(1)	0.34(2)
$D(L)$	1.7(2)	1.7(5)	1.7(7)	1.7(9)	1.8(2)	1.8(5)	1.8(6)

represent spin-correlated regions (as Coniglio–Klein clusters [6] in the Ising model) and consequently percolation temperature T_p coincides with critical temperature T_c, percolation exponents coincide with critical ones and KBD-clusters at T_p are two-dimensional self-avoiding walks (SAW) at θ point [7].

In this paper we extensively study percolation features of KBD-clusters, considering very large lattice sizes ($N = 100^2$–400^2), and give numerical results on critical exponents, cluster distribution and fractal dimension at the percolation point.

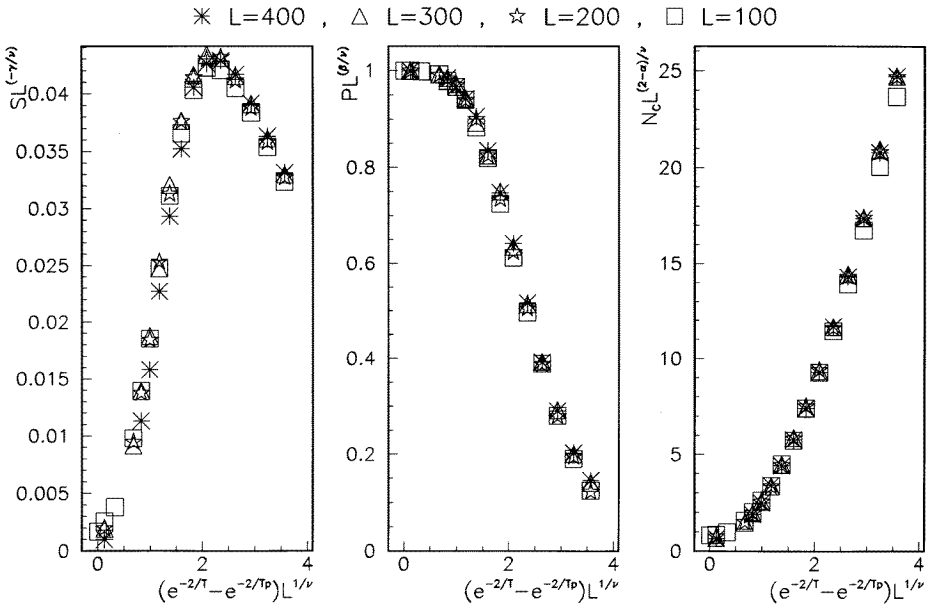

Figure 4. Scaling for S, P and N_c following assumptions (1), (2) and (3) for data of systems with sizes $L = 100, 200, 300, 400$. The parameters $e^{-2/T_p} = 0.0000 \pm 0.0001$, $\alpha = 0.1 \pm 0.1$, $\beta = 0.00 \pm 0.01$, $\gamma = 2.00 \pm 0.01$ and $\nu = 1.00 \pm 0.01$ are such that the data for different sizes L collapse on single curves (one for each graph). These curves are, respectively, the universal functions f_S, f_P and f_{N_c}. The errors are estimated observing the range of parameters within which the data points approximately collapse.

2. Critical exponents and the percolation point

We consider finite systems with increasing size ($L = 100$–400) with periodic boundary conditions.

A cluster percolates when it connects two opposed system sides. For every size L there is a percolation temperature $T_p(L)$. With T_p (without any argument) we mean the percolation temperature in the thermodynamic limit, i.e. $T_p(L) \to T_p$ for $L \to \infty$. In this limit percolating clusters are present at $T \leqslant T_p$ but not at $T > T_p$. In figure 2 we show typical clusters at several temperatures for a finite system with size $L = 60$.

For every L we have studied the mean cluster size $S = \sum_s s^2 n_s$ (where s is the cluster size, n_s the cluster number of sizes s per lattice site and the sum is extended over all finite clusters), the percolation probability $P = 1 - \sum_s s n_s$, the cluster number $N_c = \sum_s n_s$, the number of bonds per lattice site N_b, the mean size of the largest (percolating) cluster S_{I} and the mean size of the second largest (percolating) cluster S_{II}. These quantities are shown in figure 3 for $L = 100$–400. Note that for $T \to 0$ the bonds cover 50% of lattice interactions (that is the random-bond percolation threshold on the square lattice), S_{II} goes to a finite value (as predicted by KBD [2] and already verified in [4]) and occupies almost 35% of the lattice, and that S_{I} occupies almost 65% of the lattice. At $T = 0$ only two clusters survive, as shown in figures 2(e) and (f).

Now we will give numerical estimates of critical exponents that characterize the KBD-cluster percolation.

We know [8] that in the thermodynamic limit the mean cluster size diverges for $T \to T_p$,

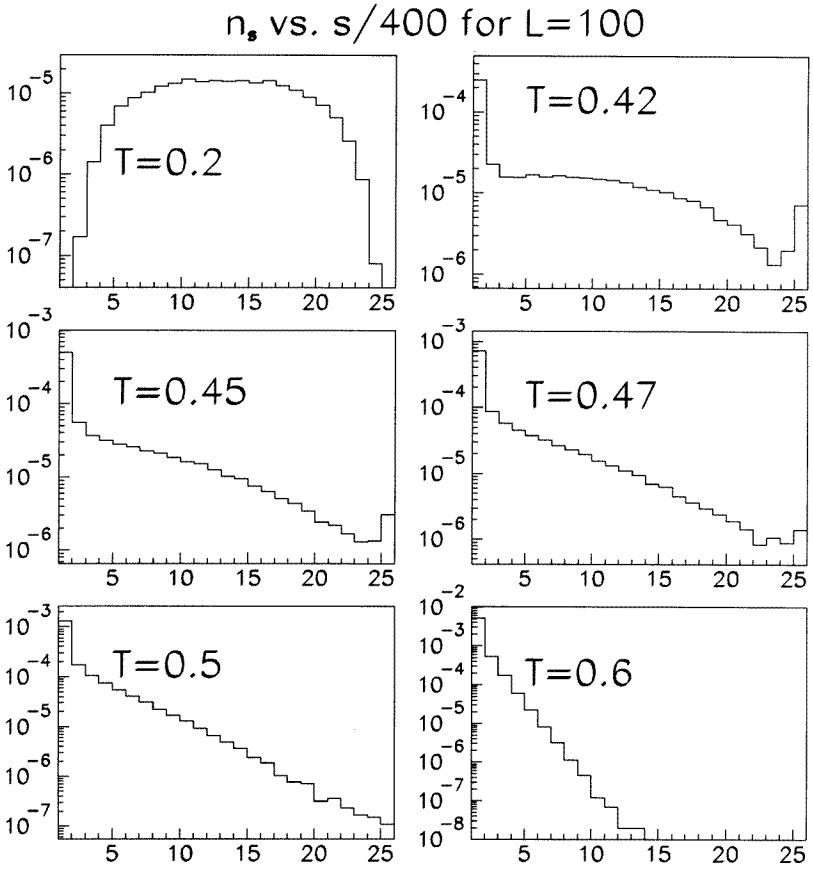

Figure 5. Cluster distribution n_s versus cluster size s for a system with size $L = 100$ at several temperatures T. Every bin is large 400 unities in cluster size. The percolation temperature for this system size is $T_p(L = 100) \simeq 0.46$ then for all $T \geqslant 0.47$, even if the highest bin is not empty, there are only no percolating clusters. Note that for all T above $T_p(L)$ it is $n_s \sim \mathrm{e}^{-s}$ and that the distribution become symmetric for $T \to 0$.

the percolation probability goes to zero in the limit $T \to T_p^-$ and the cluster number goes to zero for $T \to T_p^+$.

We assume that near T_p the *connectivity length* ξ (i.e. the typical linear cluster size) diverges as $\xi \sim |\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|^{-\nu}$, the mean cluster size diverges as $S \sim |\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|^{-\gamma}$, the percolation probability goes to zero as $P \sim |\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|^{\beta}$ and the cluster number goes to zero as $N_c \sim |\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|^{2-\alpha}$. The last relations are definitions of critical exponents α, β, γ and ν.

By standard finite-size scaling considerations [8] we can make the *ansatz*

$$S \sim L^{\gamma/\nu} f_S(|\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|L^{1/\nu}) \tag{1}$$

$$P \sim L^{-\beta/\nu} f_P(|\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|L^{1/\nu}) \tag{2}$$

and

$$N_c \sim L^{(\alpha-2)/\nu} f_{N_c}(|\mathrm{e}^{-2/T} - \mathrm{e}^{-2/T_p}|L^{1/\nu}) \tag{3}$$

where $f_S(x)$, $f_P(x)$ and $f_{N_c}(x)$ are *universal functions*, i.e. independent by L.

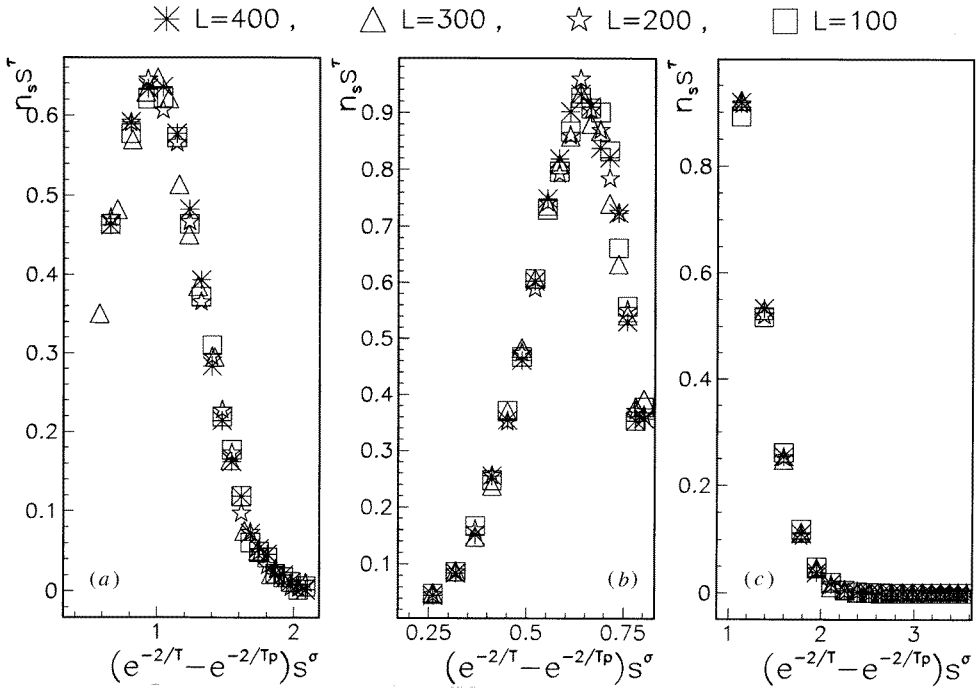

Figure 6. (*a*) Scaling for n_s following assumption (4) with parameter $\tau = 2.00 \pm 0.01$ and $\sigma = 0.50 \pm 0.01$ for data of systems with sizes $L = 100, 200, 300, 400$. Each set of data is chosen at a temperature near the corresponding $T_p(L)$. As a consequence for each temperature the quantity $(e^{-2/kT} - e^{-2/T_p})L^{1/\nu}$ with $T_p = 0$ and $\nu = 1$ is equal to 2.084. Every point in the graph is an average over 500 consecutive values of s for $L = 100$, 2000 for $L = 200$, 4500 for $L = 300$, 8000 for $L = 400$. (*b*) As in (*a*) but for $(e^{-2/T} - e^{-2/T_p})L^{1/\nu} = 0.823$ (below $T_p(L)$). (*c*) As in (*a*) but for $(e^{-2/T} - e^{-2/T_p})L^{1/\nu} = 3.567$ (above $T_p(L)$).

Via data collapse (see figure 4) we estimate the parameters $e^{-2/T_p} = 0.0000$, $\alpha = 0.1$, $\beta = 0.00$, $\gamma = 2.00$, and $\nu = 1.00$ with an error of one unit in the last given digit. Therefore, the scaling relation $\alpha + 2\beta + \gamma = 2$ and the hyperscaling relation $2 - \alpha = \nu d$ are satisfied with good approximation.

In table 1 we give numerical estimates of $T_p(L)$. The data are obtained taking for $L = 100, 200, 300, 400$ the values of $T_p(L)$ at which the S data in a log–log plot versus $|e^{-2/T} - e^{-2/T_p(L)}|$ follow two parallel straight lines (one above and one below $T_p(L)$) with slopes in good agreement with $\gamma = 2$ and then best-fitting these values as $e^{-2/T_p(L)} \sim 1/L$.

3. Fractal dimension and cluster distribution

Let us now consider the fractal dimension D of the percolating cluster. From the scaling invariance hypothesis [8] we know that $P \sim \xi^{D-d}$, then we obtain $D = d - \beta/\nu$ (hyperscaling). In the present case we have $\beta = 0$, then $D = d = 2$. The same result is obtained from the scaling relation $\beta + \gamma = D\nu$.

This is confirmed by the analysis of cluster distribution (see figure 5). The scaling invariance hypothesis [8, 9] gives for $T \to T_p$ and $s \to \infty$

$$n_s = s^{-\tau} f_{n_s}(|e^{-2/T} - e^{-2/T_p}|s^\sigma) \tag{4}$$

with $\tau = 1 + d/D$, $\sigma = 1/(\nu D)$ and $f_{n_s}(x)$ the universal function.

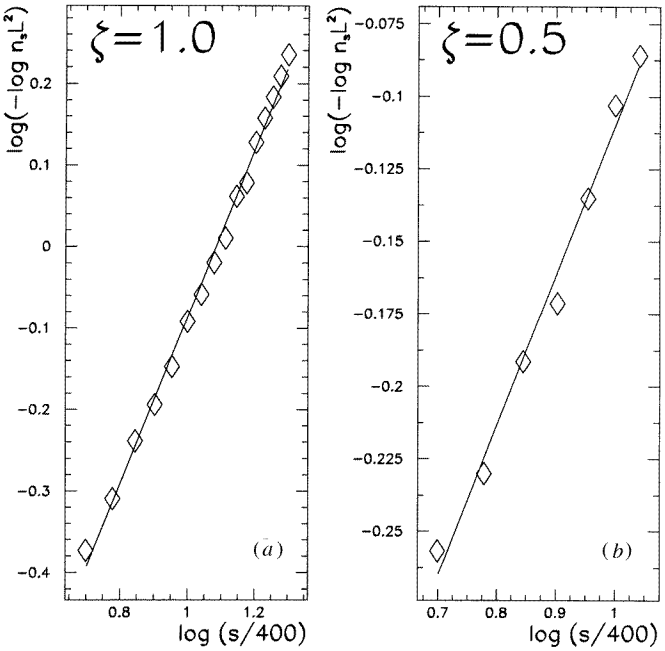

Figure 7. Fit of $\log(-\log n_s L^2)$ versus $\log(s/400)$ for a system with $L = 100$ and $T_p(L) \simeq 0.46$. (*a*) At $T \simeq 0.47 > T_p(L)$ the slope is $\zeta \simeq 1$, (*b*) at $T \simeq 0.45 < T_p(L)$ the slope is $\zeta \simeq \frac{1}{2}$.

From data collapse for n_s near T_p (see figure 6(*a*)) we obtain numerical estimates of parameters. The data in figure 6(*a*) are chosen in such a way that the quantity $(e^{-2/T} - e^{-2/T_p})L^{1/\nu}$ (with $e^{-2/T_p} = 0$ and $\nu = 1$) is a constant with $T \simeq T_p(L)$ for every considered L. The results are $\tau = 2.00$ and $\sigma = 0.50$ (with error of one unit in the last digit), that, with the definitions of τ and σ, give $D = 2$ and $\nu = 1$. On the other hand these values of τ and σ satisfy the relation $\sigma(2-\alpha) = \tau - 1$, $\sigma\beta = \tau - 2$, $\sigma\gamma = 3 - \tau$ [8].

From figure 6(*a*) we see that the universal function $f_{n_s}(x)$ is a bell-shaped curve for $T \simeq T_p(L)$. For temperatures slightly below $T_p(L)$ (figure 6(*b*)) $f_{n_s}(x)$ is shifted, while for temperatures slightly above $T_p(L)$ (figure 6(*c*)) $f_{n_s}(x)$ dramatically changes its shape.

Away from $T_p(L)$ we know [8] that the valid relation is

$$\log n_s \sim -s^{\zeta} \tag{5}$$

for $s \to \infty$, with $\zeta = 1$ above $T_p(L)$ and $\zeta = 1 - 1/d = \frac{1}{2}$ below $T_p(L)$. This relation is confirmed with reasonable approximation by our numerical simulations, as shown in figure 7. Note that, while the exponent $\zeta = 1$ above $T_p(L)$ is good for a wide range of s ($s = 2000$–8000 for $L = 100$), the exponent $\zeta = \frac{1}{2}$ below $T_p(L)$ is good for a smaller s range ($s = 2000$–4400 for $L = 100$) since finite-size effect becomes more important below $T_p(L)$. The smaller the T, the smaller is the s range.

A direct way to estimate the fractal dimension D is given through its definition

$$s \sim R^D \tag{6}$$

for $T = T_p$, with R radius of gyration of the cluster of size s. We know [8] that cluster dimension deviates from D away from T_p, becoming the Euclidean dimension d below T_p and a value smaller than D above T_p. This is true because (6) is valid within the

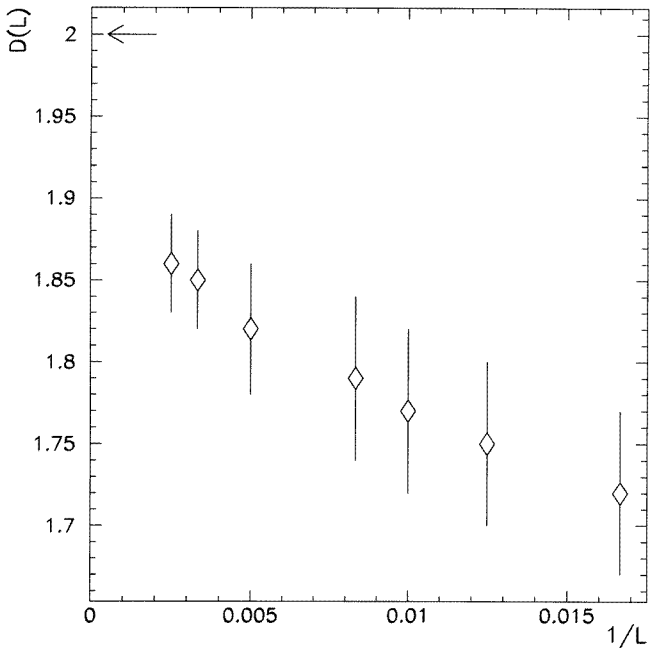

Figure 8. Estimate of D from definition (6) versus $1/L$ (see table 1): at $T = 0.517$ for $L = 60$, at $T = 0.481$ for $L = 80$, at $T = 0.450$ for $L = 100$, at $T = 0.437$ for $L = 120$, at $T = 0.389$ for $L = 200$, at $T = 0.360$ for $L = 300$ and at $T = 0.343$ for $L = 400$. The error bars are probably underestimated. The arrow heads for the asymptotic value of D.

connectivity length ξ for all temperatures, but ξ goes to zero away from T_p. Unfortunately data about this relation are difficult to analyse. Indeed near $T_p(L)$ for every finite system with $L \leqslant 120$ it seems that D is almost $\frac{7}{4} = 1.75$ (the fractal dimension of a SAW at θ point), but for larger L (see figure 8 and table 1) the fractal dimension D grows slowly to the asymptotic value 2.

4. Conclusions

We have numerically investigated the KBD-cluster percolation problem in two-dimensional FF Ising model. From our simulation we found that, within numerical errors, this correlated site–bond percolation satisfies scaling and hyperscaling relations and have, in the thermodynamical limit, a percolation temperature $T_p = 0$ and the exponents $\alpha = 0$, $\beta = 0$, $\gamma = 2$, $\nu = 1$, $\tau = 2$, $\sigma = \frac{1}{2}$, $\zeta(T > T_p(L)) = 1$, $\zeta(T < T_p(L)) = \frac{1}{2}$. Moreover, at T_p, clusters are compact (fractal dimension $D = 2$). Therefore, we can now correct the conclusion of [5] and say that, since $T_p = T_c$ and ν is equal to the spin-correlation exponent†, the site connectivity length ξ equals the spin-correlation length diverging at zero temperature. Although the exponent γ is different the coincidence between ξ and correlation length is enough to give an efficient Monte Carlo cluster dynamics [10].

† As for clusters of parallel spin in the two-dimensional Ising model [6].

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