Cluster Analysis for Percolation on Two Dimensional Fully Frustrated System

Giancarlo Franzese

Dipartimento di Scienze Fisiche, Università di Napoli, Mostra d’Oltremare Pad.19 I-80125 Napoli

Italy

and INFM - unità di Napoli

(October 15, 2018)

Abstract

The percolation of Kandel, Ben-Av and Domany clusters for 2d fully frustrated Ising model is extensively studied through numerical simulations. Critical exponents, cluster distribution and fractal dimension of percolative cluster are given.
I. INTRODUCTION

A 2d fully frustrated (FF) Ising model is a model with Ising spins ±1 where the interactions between nearest neighbor 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 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 Fig.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 Ref. \[2\].

The KBD-clusters are defined by choosing stochastically on each plaquette of a checkerboard partition of a square lattice one bond configuration between the three shown in Fig.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 $P_0 = e^{-4J/(kT)}$ (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 sake of simplicity from now on we choose $J/(kT) = 1/T$.

Ref. \[2\] has stimulated several works \[4,5\] that pay attention mainly to dynamics and to number of clusters and clusters sizes. In \[5\] numerical simulations on relatively large FF lattice sizes (number of sites $N = 60^2 \div 120^2$) supported the idea that the KBD-clusters represent spin correlated regions (like Coniglio-Klein clusters \[6\] do in 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 2d self-avoiding walks.
In this paper we extensively study percolative features of KBD-clusters, considering very large lattice sizes \((N = 100^2 \div 400^2)\), and give numerical results on critical exponents, cluster distribution and fractal dimension at percolation point.

II. CRITICAL EXPONENTS AND PERCOLATION POINT

We consider finite systems with increasing size \((L = 100 \div 400)\) 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. \(T_p(L) \rightarrow T_p\) for \(L \rightarrow \infty\). In this limit percolating clusters are present at \(T \leq T_p\) but not at \(T > T_p\). In Fig.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 \(S = \sum s^2 n_s\) (where \(s\) is the cluster size, \(n_s\) the number of cluster of size \(s\) per lattice site and the sum is extended over all finite clusters), the percolation probability \(P = 1 - \sum s n_s\), the number of cluster \(N_c = \sum s n_s\), 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 Fig.3 for \(L = 100 \div 400\). Let’s note that for \(T \rightarrow 0\) the bonds cover 50% of lattice interactions (that is the random-bond percolation threshold on square lattice), \(S_{II}\) goes to a finite value (like predicted by KBD [2] and already verified in Ref. [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 Fig.2 e) and f).

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

We know [3] that in the thermodynamic limit the mean cluster size diverges for \(T \rightarrow T_p\), the percolation probability goes to zero in the limit \(T \rightarrow T_p^-\) and the number of cluster goes
to zero for $T \to T_p^+$.

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

By standard finite-size scaling considerations we can make the ansatz

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

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

and

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

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

Via data-collapse (see Fig.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 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 Tab.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 vs. $|e^{-2/T} - e^{-2/T_p(L)}|$ 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 $e^{-2/T_p(L)} \sim 1/L$.

III. FRACTAL DIMENSION AND CLUSTER DISTRIBUTION

Let’s now consider the fractal dimension $D$ of the percolating cluster. From the scaling invariance hypothesis we know that $P \sim \xi^{D-d}$, then we obtain $D = d - \beta/\nu$ (hyperscaling).
In 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 Fig.5). The scaling invariance hypothesis \[8,9\] gives for $T \to T_p$ and $s \to \infty$

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

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

From data-collapse for $n_s$ near $T_p$ (see Fig.6.a) we obtain numerical estimates of parameters. The data in Fig.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 $\tau$ and $\sigma$, give $D = 2$ and $\nu = 1$. On the other hand these values of $\tau$ and $\sigma$ satisfies the relation $\sigma(2 - \alpha) = \tau - 1$, $\sigma\beta = \tau - 2$, $\sigma\gamma = 3 - \tau$. \[8\]

From Fig.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 $T_p(L)$ (Fig.6.b) $f_{n_s}(x)$ is shifted, while for temperatures slightly above $T_p(L)$ (Fig.6.c) $f_{n_s}(x)$ changes dramatically its shape.

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

$$\log n_s \sim -s^\zeta$$

for $s \to \infty$, with $\zeta = 1$ above $T_p(L)$ and $\zeta = 1 - 1/d = 1/2$ below $T_p(L)$. This relation is confirmed with reasonable approximation by our numerical simulations, as shown in Fig.7. Let’s note that, while the exponent $\zeta = 1$ above $T_p(L)$ is good for a wide range of $s$ ($s = 2000 \div 8000$ for $L = 100$), the exponent $\zeta = 1/2$ below $T_p(L)$ is good for a smaller $s$ range ($s = 2000 \div 4400$ for $L = 100$) since finite-size effect become more important below $T_p(L)$. The smaller $T$, the smaller $s$ range is.

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

$$s \sim R^D$$

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 eq.(6) is valid within the connectivity
length $\xi$ for all temperatures, but $\xi$ goes to zero away from $T_p$. Unfortunately data about
this relation are difficult to analyze. Indeed near $T_p(L)$ for every finite system with $L \leq 120$
it seems that $D$ is almost $7/4 = 1.75$ (the fractal dimension of a SAW at $\theta$ point), but for
larger $L$ (see Fig.8 and Tab.1) the fractal dimension $D$ grows slowly to the asymptotic value
2.

IV. CONCLUSIONS

We have numerically investigated the KBD-cluster percolation problem in 2d 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 $\alpha = 0$, $\beta = 0$, $\gamma = 2$, $\nu = 1$,
$\tau = 2$, $\sigma = 1/2$, $\zeta(T > T_p(L)) = 1$, $\zeta(T < T_p(L)) = 1/2$. Moreover at $T_p$ clusters are
compact (fractal dimension $D = 2$). Therefore now we can correct the conclusion of Ref.
[5] and say that, since $T_p = T_c$ and $\nu$ is equal to spin correlation exponent [10], the site
connectivity length $\xi$ goes like the spin correlation length diverging at zero temperature.
Although the exponent $\gamma$ is different the coincidence between $\xi$ and correlation length is
enough to give an efficient Monte Carlo cluster dynamics. [11]

ACKNOWLEDGMENTS

The author is indebted to Antonio Coniglio and to Vittorio Cataudella for many illumin-
ating discussions and a careful reading of the manuscript.

The computation have been done on DECstation 3000/500 with Alpha processor and
DECsystem 5000/200 with RISC processor.
REFERENCES

[1] J.Villain, J. Phys. C 10, 1717 (1977);
G.Forgacs, Phys. Rev. B 22, 4473 (1980).

[2] D.Kandel, R.Ben-Av and E.Domany, Phys. Rev. Lett. 65, 941 (1990);
D.Kandel and E.Domany, Phys. Rev. B 43, 8539 (1991).

[3] A.Coniglio, H.E.Stanley and W.Klein, Phys. Rev. Lett. 42, 518 (1979).

[4] W.Kerler and P.Rehberg, Phys. Rev. B 49, 9688 (1994);
P.D.Coddington and L. Han, Phys. Rev. B 50, 3058 (1994);

[5] V.Cataudella, G.Franzese, M.Nicodemi, A.Scala and A.Coniglio, Phys. Rev. Lett. 47, 381 (1994) and Il Nuovo Cimento 16D N.8, 1259 (1994).

[6] A.Coniglio and W.Klein, J. Phys. A 13, 2775 (1980).

[7] A.Coniglio, N.Jan,I.Maijd and H.E.Stanley, Phys. Rev. B 35, 3617 (1987);
B.Duplantier and H.Saleur, Phys. Rev. Lett. 59, 538 (1987).

[8] D.Stauffer, Introduction to Percolation Theory (Taylor & Francis, London, 1985).

[9] M.D’Onorio De Meo, D.W.Heermann and K.Binder, J. Stat. Phys., 60, 585 (1990).

[10] as for clusters of parallel spin in 2d Ising model (Ref. [6]).

[11] V.Cataudella, G.Franzese, M.Nicodemi, A.Scala and A.Coniglio, in print on Phys. Rev. E (cond-mat/9604169)
TABLES

TABLE I. Numerical estimates of $T_p(L)$ and $D(L)$ for $L = 60 \div 400$. The way used to evaluate $T_p(L)$ and $D(L)$ give us confidence only on digit 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) |
FIG. 1. 1) Example of 2d FF lattice: the spin are on the vertices; solid lines represent ferromagnetic interactions (+$J$) and dashed lines antiferromagnetic interactions ($-J$). 2) Plaquette bond configurations: a) zero bond; b) two parallel vertical bonds; c) two parallel horizontal bonds.
FIG. 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).
FIG. 3. Mean cluster size $S$, percolation probability $P$, number of cluster $N_c$, number of bonds per lattice site $N_b$, mean size of largest cluster $S_I$ and mean size of second largest cluster $S_{II}$ vs. temperature $T$ for lattice sizes $L = 100, 200, 300, 400$. The error bars (often included in symbols) are the statistical errors.
FIG. 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 collapse roughly well.
FIG. 5. Cluster distribution $n_s$ vs. 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 $T_p(L = 100) \approx 0.46$ then for all $T \geq 0.47$, even if the highest bin is not empty, there are only no percolating clusters. Let’s note that for all $T$ above $T_p(L)$ it is $n_s \sim e^{-s}$ and that the distribution become symmetric for $T \to 0$. 
FIG. 6. a) Scaling for $n_s$ following assumption [1] 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 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 part a) but for $(e^{-2/T} - e^{-2/T_p})L^{1/\nu} = 0.823$ (below $T_p(L)$). c) As in part a) but for $(e^{-2/T} - e^{-2/T_p})L^{1/\nu} = 3.567$ (above $T_p(L)$).
FIG. 7. Fit of \( \log(-\log n_s L^2) \) vs. \( \log(s/400) \) for a system with \( L = 100 \) and \( T_p(L) \approx 0.46 \): a) at \( T \approx 0.47 > T_p(L) \) the slope is \( \zeta \approx 1 \); b) at \( T \approx 0.45 < T_p(L) \) the slope is \( \zeta \approx 1/2 \).
FIG. 8. Estimate of $D$ from definition $\text{(3)}$ vs. $1/L$ (see Tab.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 $D$. 