Pis'ma v ZhETF, vol. 75, iss. 3, pp. 191 – 195

Two-dimensional site-bond percolation as an example of self-averaging system

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Submitted 27 December 2001

The Harris-Aharony for statical model criteria predicts, that if specific heat exponent $\alpha \geq 0$, then this model does not exhibit self-averaging. In two-dimensional percolation model the index $\alpha = -\frac{1}{2}$. It means, that in accordance with Harris-Aharony criteria, this model can exhibit self-averaging properties. We study numerically the relative variance R_M and R_χ of the probability of site to belong the "infinite" (maximum) cluster M and the mean finite cluster sizes χ. It was shown, that two-dimensional site-bound percolation on the square lattice, where the bonds play role of impurity and sites play role of statistical ensemble, over which the averaging performed, exhibit self-averaging properties.

PACS: 64.60.Cn, 75.10.Hk

1. Introduction. The influence of disorder onto phase transition is one of important questions of the phase transition theory. In experimental measurements the thermodynamical properties of one (or several) samples of large (with respect to molecule number) sizes usually studies. So its important to know, can one sample of large size with quenched realization of impurities represents the properties of model? The self-averaging properties of the system give the answer on this question. If some quantity is self-averaging, the measurement for one large sample give the reasonable value for all samples of such size. If the quantity is not self-averaging, the increasing of the system size does not make the measurement for a single sample representative.

Lets consider some statistical model with impurities on the d-dimensional lattice of linear size L, in which we average some quantity $X(\omega)$ for certain sample ω – impurity realization over some impurity ensemble Ω. Here we assume, that $X(\omega)$ is exact thermal average for impurity realization ω. Lets denote $[X]$ the average over all impurity realizations ensample Ω: $[X] = \sum_{\omega\in\Omega} P(\omega)X(\omega)$, where $P(\omega)$ is the probability of impurity realization ω. Then variance $V_X = \sum_{\omega\in\Omega} P(\omega)X^2(\omega) - [X]^2$. Lets define the relative variance of X: $R_X = V(x)/[X]^2$. This quantity characterize the size depending properties of model. If $R_X(L) \sim L^x$, $x = -d$ the quantity X is said to be strongly self-averaging, If $x < 0$ the X said to be weak self-averaging, and if $\lim_{L\to\infty} R_X(L) \to \text{const}$, than X is nonselfaveraging. Now we talk about self-averaging of disordered system, so we study the averaging over all impurity realization, instead of self-averaging of a pure system, when we study the averaging over all statistical ensemble (for example, over all possible spin configuration for a spin models).

The Harris criteria stands [1], that the weak randomness don't change the critical behavior of the d-dimensional second-order phase-transition model, if specific heat index $\alpha < 0$ which corresponds that the pure correlation length index $\nu > 2/d$. As was first mentioned by Brout [2], far for critiality where the system size is much greater than correlation length $L \gg \xi$, all additive thermodynamical quantities are strongly self-averaging. The self-averaging properties of a disordered system near the critiality obeys Harris-Aharony (HA) criteria see [3] and [4]. This criteria states, that if randomness is irrelevant the system is governed by a pure fixed point and the relative variance $R_X \sim L^{\frac{\alpha_p}{\nu_p}}$, where α_p and ν_p is the critical exponents of a pure system. But if the system is governed by a random fixed point, than $\lim_{L\to\infty} R_X = \text{const}$. This criteria explain numerical results of many works [5 – 7]. Shai Wiseman and Eytan Domany in [7] show, that Ashkin-Teller model with $\alpha < 0$ is weakly self-averaging.

Two-dimensional percolation, which can be treated as a q-state Potts model with $q \to 1$, is one of the most popular two-dimensional statistical models with the second-order phase transition. Two-dimensional percolation critical index $\alpha = -\frac{1}{2} < 0$ and in accordance with HA criteria we can expect, that this model exhibit weak self-averaging properties. We study numerically the relative variance R_M and R_χ of the probability of a site to belong the maximum cluster size M (the analog of magnetization) and the mean finite cluster size χ (the

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analog of the magnetic susceptibility). It was shown, that two-dimensional site-bound percolation, where the bonds play role of impurities and sites play role of statistical ensemble, over which the averaging performed, exhibit self-averaging properties. The article is arranged as follows. In the Section 2 we describe site-bond percolation model and two type of impurities distribution, in the Section 3 we discuss the self-averaging criteria and its phenomenological derivation, in the Section 4 we presents the numerical results and Section 5 is conclusion.

2. Two-dimensional site-bond percolation model and canonical and grand-canonical impurity distribution.

Site-bond percolation is a combination of pure site percolation and pure bond percolation. In pure site percolation one investigate clusters of occupied sites. In pure bond percolation one investigate clusters of sites, connected by occupied bonds. In site-bond percolation one investigate clusters of occupied sites connected by occupied bonds. Each site is occupied with probability p_s, each bond is occupied with probability p_b. In critical point (p_s^*, p_b^*) the correlation length becomes infinite. Yanuka and Engelman [8] proposed approximate formula for a critical curve in (p_s, p_b) plane

$$\log(p_s)/\log(p_s^*) + \log(p_b)/\log(p_b^*) = 1.$$

The two-dimensional site-bond percolation belongs the same universality class, as the two-dimensional pure site percolation. Lets define n_C the mean number of clusters of size C per lattice site. Then the probability of a site to belong to the maximum cluster is

$$M = n_{C_{\max}} C_{\max} \tag{1}$$

and the mean finite cluster size

$$\chi = \sum_{C, C \neq C_{\max}} n_C C^2 / \sum_{C, C \neq C_{\max}} n_C C. \tag{2}$$

Near the critical point (p_s^*, p_b^*) this quantities scales as follows

$$M(p_s, p_b = p_b^*) \sim (p_s - p_s^*)^{+\beta}, \;\; p_s > p_s^*, \;\; \beta = 1/18 \tag{3}$$

and

$$\chi(p_s, p_b = p_b^*) \sim (p_s - p_s^*)^{-\gamma}, \;\; \gamma = 43/18 \tag{4}$$

The correlation length scaling index $\xi(p_s, p_b = p_b^*) \sim (p_s - p_s^*)^{-\nu}$ is $\nu = \frac{4}{3}$.

As we write above, each bond is occupied with probability p_b and empty with probability $1 - p_b$. So the total number of occupied bonds on the lattice fluctuates. This method to generate the impurity configuration is known as Grand Canonical (GC) by analogy with Grand Canonical statistical ensemble with fluctuating number of particles. But we can fix the number of occupied bonds N_b and then distribute they randomly on the lattice. This method to generate the impurity configuration is known as Canonical (C) by analogy with Canonical statistical ensemble with fixing number of particles.

3. Self-Averaging criteria. Lets explain the HA criteria via simple phenomenological reasons [6]. In this section we use the T temperature as a parameter of model but lets remind, that in the case of percolation the role of this parameter play the site concentration p_s.

We characterized every sample (impurity realization) ω of size L by a pseudo-critical temperature $T^*(\omega, L)$. $T^*(\omega, L)$ fluctuates around its mean value, averaging over all impurity configurations $T^* = [T^*(\omega, L)]$. Introduce the reduced temperature of each sample

$$\dot{t}_\omega = \frac{T - T^*(\omega, L)}{T^*}. \tag{5}$$

In the vicinity of critical point the quantity X scales as

$$X_\omega(T, L) = L^\rho \tilde{Q}_\omega(\dot{t}_\omega L^{y_t}). \tag{6}$$

Here ρ – the exponent, characterizing the behavior of $[X]$ at T^* and thermal scaling index $y_t = 1/\nu$ are assumed to be universal for all samples. The form of function $\tilde{Q}_\omega$ was assumed to be sample dependent. We assume (this relation is numerically checked in the next section)

$$(\delta T^*)^2 \sim \left(\delta \dot{t}_\omega\right)^2 \sim L^{-d}. \tag{7}$$

So the variance of the argument of the function $\tilde{Q}_\omega$ scales as

$$\left(\delta \dot{t}_\omega L^{y_t}\right)^2 \sim L^{-d+2/\nu}. \tag{8}$$

Lets remind the scaling relation [9] $\alpha = 2 - \nu d$. So the variance V_x of quantity X at the critical point scales as

$$V_X \sim L^{2\rho} \left(\delta \dot{t}_\omega L^{y_t}\right)^2 \sim \\ \sim L^{2\rho - d + 2/\nu} = L^{2\rho + (2 - d\nu)/\nu} = L^{2\rho + \alpha/\nu}. \tag{9}$$

and the relative variance ($[X] \sim L^\rho$)

$$R_X = \frac{V_X}{[X]^2} = L^{2\rho + \frac{\alpha}{\nu} - 2\rho} = L^{\alpha/\nu}. \tag{10}$$

So we obtain the Harris-Aharony criteria: *if scaling index $\alpha = const < 0$, then the model is self-averaging, and for quantity X the relative variance* $R_X \sim L^{\alpha/\nu}$ from simple scaling relations.

4. Numerical results. In our computation the bond play the role of impurities. So we fix the bond concentration $p_b^* = 0.875$, and consider the site concentration p_s as parameter of our model.

1) generate (by C and GC methods) the bond configuration ω;

2) for this bond configuration generate a set of site configuration (for site we use only GC method). For each site configuration we calculate the probability of a site to belong the maximum cluster and the mean finite cluster size;

3) we average this quantities over site realizations and get mean values $M(p_s, p_b)$ and $\chi(p_s, p_b)$. We split the set of site configurations onto ten series to evaluate the numerical inaccuracy ΔM and $\Delta\chi$;

4) perform steps 1.–3. for another bond configuration.

Dependence of $\chi_\omega(p_s)$ for three different bond realizations $\omega = 1, 2, 3$ is shown on Fig.1. Lets calculate the

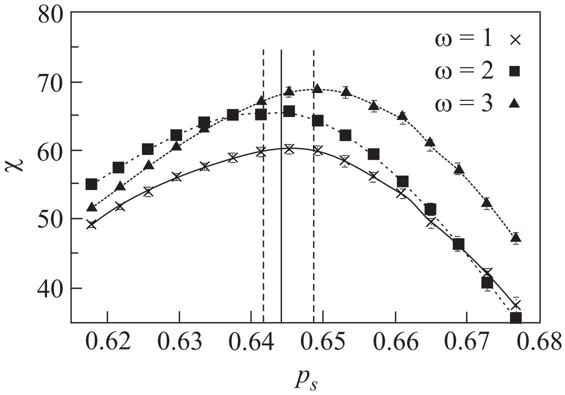

Fig.1. The mean finite cluster size $\chi(p)$ for three realization of impurities. The critical concentration $p_s^*(\omega)$ for each realization ω, is shown by vertical lines

pseudocritical site concentration $p_s^*(\omega)$ for each bond realization ω. We assume, that the mean finite cluster size $\chi_\omega(p_s)$ have maximum in the pseudocritical point $p_s^*(\omega)$. So we approximate the data for χ_ω near the maximum of χ_ω by parabola $\chi_\omega(p_s) \simeq a - b\,(p_s - p_s^*(\omega))^2$ and treat $p_s^*(\omega)$ as pseudocritical concentration for bond realization ω. The location of pseudocritical points for bond realizations $\omega = 1, 2, 3$ is shown on Fig.1 by vertical lines.

Lets find the critical point p_s^*. We calculate $[p_s^*(L)]$ – the mean critical site concentration, averaged over 100 bond realizations, created by GC- and C-methods as a function of lattice size L. This numerical data, and results of approximation:

$$\text{C-method:}[p_s^*(L)]_C \simeq 0.6519(5) - 0.34(10)L^{-0.94(9)}, \tag{11}$$

$$\text{GC-method:}\ [p_s^*(L)]_{GC} \simeq 0.6511(4) - 0.39(15)L^{-1.02(11)} \tag{12}$$

is shown on Fig.2. So we take the concentration $p_s^* = 0.6515$ (averaged over C- and GC-methods) as critical. The variance of pseudocvitical concentration behaves as $(\delta p_s^*)^2 \sim L^{-2}$ – see Fig.3, as we assumed in the previons section.

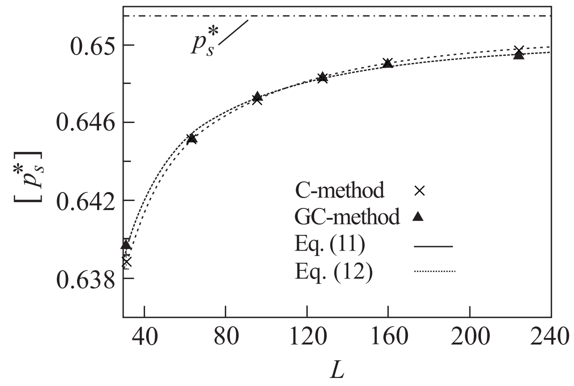

Fig.2. The mean pseudocritical site concentration $[p_s^*]$ as a function of lattice size L for a bond realization, created by C and GC methods, results of approximation by power function of L, and extrapolated critical concentration $p_s^* = 0.6515$

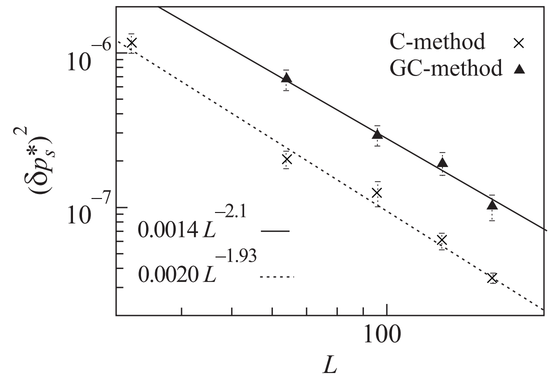

Fig.3. The variance $(\delta p_s^*)^2$ of critical concentration as a function of lattice size L for microcanonical (crosses) and canonical (triangles) distributions, and results of approximation by function aL^{-b}

Lets investigate the self-averaging properties of M and χ in the critical point ($p_b^* = 0.875, p_s^* = 0.6515$).

Now we describe computational procedure, that we use to calculate the relative variance. Here we follow the way [5, 6]. First we can mention, that for each impurity realization ω instead of exact value of quantity X_ω we get some averaged over site configuration value $\bar{X}_\omega$ with numerical error

$$\left(\delta \bar{X}_\omega\right)^2 = \frac{\sigma_{p_b,\omega}}{N_s/\tau_\omega}. \quad (13)$$

Here N_s is the number of site configurations (the length of Monte-Carlo (MC) run) and τ_ω is autocorrelation time. To calculate $\left(\delta \bar{X}_\omega\right)^2$ we split the MC sequence of site configurations of lenth N_s onto 10 subsequences and treat each subsequence as independent. We define by $[\dots]$ averaging over impurity – bond configurations. So the error of $[\bar{X}_\omega]$ averaged over N_b bond configurations is

$$\left(\delta[\bar{X}_\omega]\right)^2 = \frac{1}{N_b - 1} \sum_{\omega \in \Omega} \left([\bar{X}^2_\omega] - [\bar{X}_\omega]^2\right). \quad (14)$$

Total total error $\left(\delta[\bar{X}_\omega]\right)^2$ have two contribution terms the sample to sample fluctuation of exact X_ω around $[X_\omega]$ and the fluctuations of $\bar{X}_\omega$, averaged over a finite number of spin configurations, around X_ω for each bond realization ω:

$$\left(\delta[\bar{X}_\omega]\right)^2 = \frac{V_X}{N_b} + \left[\frac{\sigma_{p_b,\omega}}{N_b N_s/\tau_\omega}\right]. \quad (15)$$

Here N_b is the number of bond configurations. We can calculate

$$\left[\frac{\sigma_{p_b,\omega}}{N_b N_s/\tau_\omega}\right] = \frac{1}{N_b}\left[\left(\delta \bar{X}_\omega\right)^2\right]$$

by averaging error $\left(\delta \bar{X}_\omega\right)^2$ over bond configuration ω. So we can express the relative variance via $\left(\delta[\bar{X}_\omega]\right)^2$ and $\left[(\delta \bar{X}_\omega)^2\right]$:

$$R_X = \frac{V_X}{[\bar{X}_\omega]^2} = \frac{1}{[\bar{X}_\omega]^2}\left(N_b \left(\delta[\bar{X}_\omega]\right)^2 - \left[(\delta \bar{X}_\omega)^2\right]\right). \quad (16)$$

The numerical data for relative variance R_M and R_χ for C and GC methods, computing in accordance (16), are shown on Fig.4 and Fig.5 respectively. We can see, that points lies on the straight lines in double-logarithmic scale. So we approximate the data by power function aL^b on the interval $L \in [48, 128]$. The results of approximation are plotted on Fig.5 and Fig.4 and placed below. As we can expect, for GC method the relative variance is greater, than for C-method, because of fluctuation of bond number.

$$\mathrm{C}: R_M \simeq 0.0041(3) L^{-0.504(19)},$$

$$\mathrm{GC}: R_M \simeq 0.0147(15) L^{-0.50(2)},$$

$$\mathrm{C}: R_\chi \simeq 0.0243(2) L^{-0.53(2)},$$

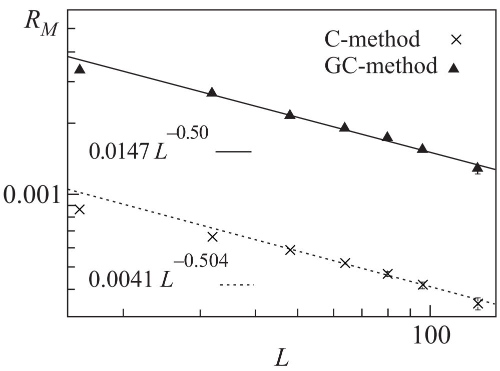

Fig.4. The relative variance R_M of probability of a site to belong to maximum cluster M as a function of lattice size L for GC (crosses) and C (triangles) distributions, and results of approximation by function aL^{-b}

$$\mathrm{GC}: R_\chi \simeq 0.0259(5) L^{-0.51(5)}.$$

We see, that with excellent agreement with HA criteria, relative variance of measured quantities is proportional $R \sim L^{-1/2} = L^{\alpha/\nu}$. So we can state, that this model is self-averaging.

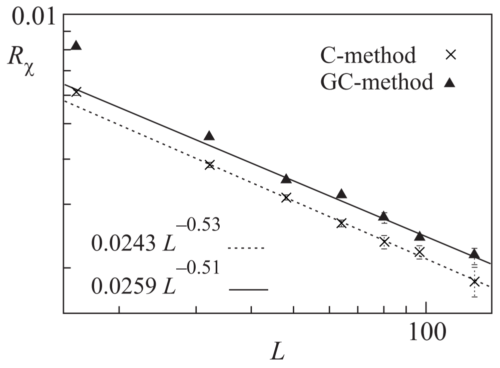

Fig.5. The relative variance R_χ of the mean finite cluster size χ as a function of lattice size L C (crosses) and GC (triangles) distributions, and results of approximation by function aL^{-b}

5. Conclusion. We show numerically, that two-dimensional site-bond percolation exhibit self-averaging. In our numerical experiments bonds play role of quenched disorder, and sites play role of statistical ensemble. We find, that relative variance scales $R_M \sim L^{-1/2}$, $R_\chi \sim L^{1/2}$, where $-1/2 = \alpha/\nu$. We think, that we can consider the sites as quenched disorder and bonds, as statistical ensemble, and results be the same.

We can also expect for site percolation, that if we "froze" the state of some sites and average over other sites, we get the same weakly self-averaging behavior with respect this "frozen" sites, which play role of quenched disorder. Of cause, the same is valid for bond percolation too.

The author is grateful Joint SuperComputer Center (www.jscc.ru) for disposed computational resources.

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