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Variation of cluster properties in lattice percolation problem: A prototype of phase transition

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Abstract. Properties of clusters appearing in the site percolation problem on square and cubic lattices are expressed in a way that emphasizes the thermodynamic analogy. It is shown that the analog of the specific heat exhibits expected critical behaviour as a function of the analog of the temperature. The results support the notion that the partition of the specific heat of Ising systems (Borštnik and Lukman, Phys. Rev. E **60**, 2595 (1999)) into the structural and populational component is a meaningful one. Another cluster property which is taken under the scrutiny is the fractal dimensionality of clusters which also indicates the presence of phase transition.

PACS. 05.45.Df Fractals – 36.40.Ei Phase transitions in clusters – 64.60.Ak Fractal and percolation studies of phase transitions

1 Introduction

Percolation phenomena on regular lattices [1] are mainly governed by cluster number dependence upon the density of occupied points. The divergence of the correlation length which is the most characteristic feature of the percolation transition and also of second order phase transitions in thermal problems is due to the appearance of ever larger clusters until the infinite percolation cluster is formed. It was demonstrated by Fortuin and Kasteleyn [2] that the percolation problem is analogous to second order phase transitions. Kunz and Souillard [3] have shown that there exists the essential singularity in cluster numbers at the percolation threshold. Leath and Reich [4] and Stauffer [5,6] addressed also the properties of individual clusters with fixed mass and pointed out the changes in cluster properties below and above the percolation threshold density. The present authors [7] have shown that in the case of two and three-dimensional Ising model the thermodynamic properties can be interpreted in terms of cluster structure and populations. However, in the case of correlated systems cluster structure can not be treated independently of cluster populations, while in the case of noncorrelated percolation problem one can study individual clusters pertaining to an arbitrary state of the system.

In this paper we exploit the thermodynamics analogy of percolation problem and demonstrate how bulk properties can be reproduced as a limit of cluster properties when cluster size tends to infinity. In particular, the analog of specific heat of individual clusters is evaluated and it is shown that it conforms to two and three-dimensional universality classes of the lattice percolation problem. This finding can be exploited in the studies of that component of the specific heat of Ising systems which is due to the rearrangements of cluster structure.

By random occupation of sites on square lattice with probability (= density) p one generates clusters (lattice animals) which can be characterized according to their mass n (number of connected lattice sites), perimeter t (the number of adjacent lattice sites at the outside or inside cluster boundaries) and the overall appearance of the cluster. Let $g(n,t)$ denote the number of distinct n,t clusters. If one is interested in an arbitrary cluster property f one can define its average value as follows [5,6]

$$\langle f_n(\beta)\rangle = \frac{\displaystyle\sum_{t=t_{\min}}^{2(D-1)n+2} f(n,t)g(n,t)\exp(-\beta t)}{\displaystyle\sum_{t=t_{\min}}^{2(D-1)n+2} g(n,t)\exp(-\beta t)}\cdot \qquad (1)$$

In order to promote the thermodynamic analogy we write $(1-p)^t$ in the form of Boltzmann factor $\exp(-\beta t)$ with $\beta = -\ln(1-p)$ figuring as the inverse temperature and the perimeter t playing the role of the energy. The sums run over all possible perimeter values. Lower limit $t_{\min} \propto n^{(D-1)/D}$ is the perimeter of the most compact form of a cluster with n sites, and $t_{\max} = 2(D-1)n + 2$ is the perimeter of the most extended cluster – a linear array of n sites. Exploiting further the thermodynamic analogy one can ask about the existence of phase transition of clusters

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which may occur at some value of β where the "energy" ($\langle t \rangle$) and the "specific heat" ($-\beta^2 \partial \langle t \rangle / \partial \beta$) would exhibit expected critical behaviour as the functions of the "inverse temperature" β. We shall also calculate average radius of gyration $\langle r_n \rangle$ and determine on its basis the fractal dimension of clusters as a function of p or β values.

2 Numerical methods

Our approaches have predominantly numerical character. In the literature one can find several numerical methodologies for generating and evaluating cluster properties. Some approaches [8,9] are limited to the interval close to the percolation threshold density, but in addition, because of thermodynamic analogy of equation (1) one can also apply various Monte Carlo type methodologies either in the classical form [5,6,10] or more modern ones [11,12].

We have used two computational approaches:

i) A Monte Carlo methodology was designed on the basis of multiple histogram method of Ferrenberg and Swendsen [11,12]. A connected random cluster with n lattice sites was subjected first to thermalization and subsequently to productive modification moves. Each move consisted of a choice of a random site which is then relocated to the perimeter provided that the cluster remains connected and that the standard Metropolis acceptance criterium ($\Delta t < 0$ or $\exp(-\beta' \Delta t) > \xi$ for $\Delta t > 0$ where β' is the current "inverse temperature" and ξ is a random number uniformly distributed over the interval $[0, 1)$) is fulfilled. As a result the histogram $h_n(t) \propto g(n,t) \exp(-\beta' t)$ representing the probability that the cluster is found in the state with the perimeter t, and cluster property $\langle r_n(t) \rangle$ was stored. Subsequently one can determine the average value of the cluster properties for an arbitrary β value. For low enough n values ($n \leq 50$) a few histograms suffice but for $n > 100$ one can hardly perform enough runs throughout the β interval to attain sufficient accuracy at the midpoint of β' values. In this way we succeeded to retrieve cluster properties with good enough statistics up to $n = 300$ in two-dimensional lattice and with $n = 100$ only, in three-dimensional case. For larger n values the space of possible cluster shapes becomes so vast that independent runs which sample 10^7 cluster configurations and consume days of CPU time on high performance workstations, do not produce convergent results.

ii) Close to the percolation threshold density it is worth to generate the clusters directly by means of Leath [8] algorithm which enables one to generate individual clusters with random size and p-dependent bias. The advantage of the algorithm lies in its ability to generate individual isolated clusters, which can be then analysed in terms of their mass, perimeter, radius of gyration, or any other property.

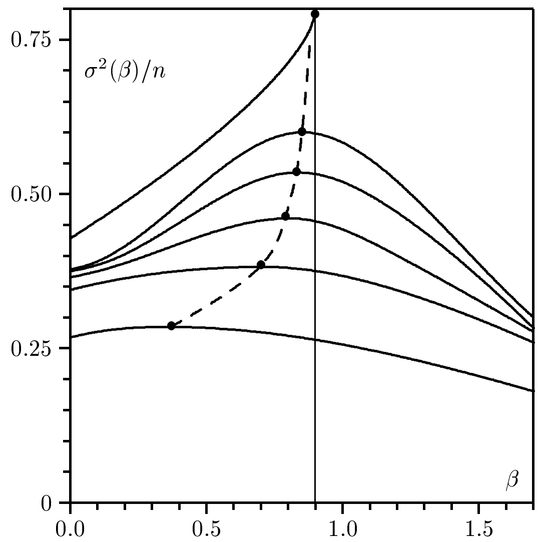

Fig. 1. Plot of $\sigma^2(\beta)/n = c_p(n,\beta)/(n\beta^2)$ for clusters on square lattice for $n = 20$ (bottom curve), 50, 100, 200, 300 and for the $n \to \infty$ limit (top curve) as a function of $\beta = -\ln(1-p)$. The dashed curve connects the maxima, which approach β_c (marked with vertical line) with growing n values.

3 "Specific heat" and critical exponents of individual clusters

Let us now focus our attention on the "specific heat" (c_p) of clusters with the emphasis on the size dependence and critical properties. There are two possibilities to calculate c_p. Either as a temperature derivative of the "energy", $c_p/\beta^2 = -\partial \langle t_n \rangle / \partial \beta$, or through the relation

$$c_p(n,\beta)/\beta^2 = \sigma^2(n,\beta) = \langle t_n^2 \rangle - \langle t_n \rangle^2, \qquad (2)$$

where $\sigma(n,\beta)$ means the width of the probability distribution of perimeter values for the clusters with mass n generated at the "inverse temperature" β. Numerically, the first approach is an indirect one since one should first determine $\langle t_n \rangle$ and then take the derivative. The latter approach is a direct one and it was used in connection with the Monte Carlo methodology specified above under i). The results which were obtained are shown in Figures 1 and 2 for $n = 20$, 50, 100 and in $D = 2$ case also for $n = 200$ and 300. At first glance it becomes apparent that for each n value $c_p(n,\beta)/\beta^2$ exhibits a peak whose position approaches with growing n the percolation threshold "inverse temperature" ($\beta_c = 0.8983$ which corresponds to $p = p_c = 0.5927$ in two dimensions and $\beta_c = 0.37338$ which corresponds to $p = p_c = 0.3116$ in three dimensions). For $D = 2$ the approach towards β_c of the location of the peak with growing n is consistent with the scaling behaviour in the form $\Delta\beta(n) \propto n^{-1/\nu}$ with $\nu = 1.33$ being the correlation length critical exponent. The weak point of the above mentioned results is the inability to study big enough clusters. We tried to overcome this problem by means of the results generated on the basis of Leath's algorithm which enabled us to study the cluster properties close to β_c on much wider interval of cluster

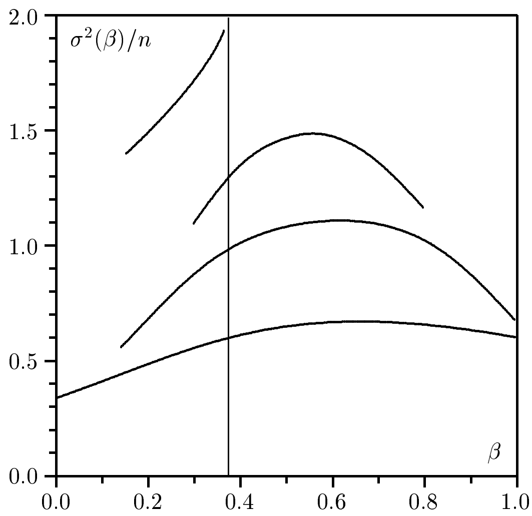

Fig. 2. Plot of $\sigma^2(\beta)/n$ for $n = 20$ (bottom curve), 50, and 100 and $n \to \infty$ limit (top curve). See also the caption of Figure 1.

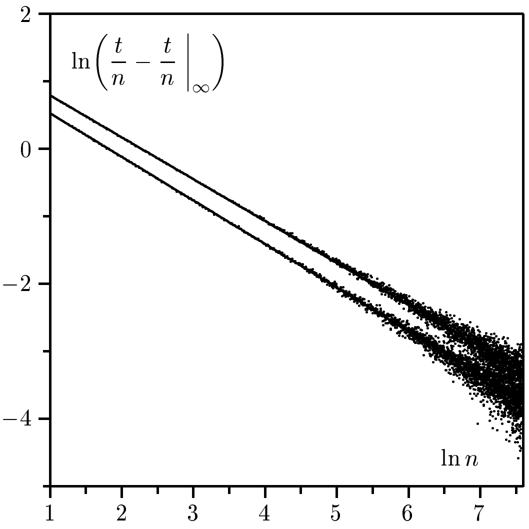

Fig. 3. The two sets of data-points calculated at $\beta = \beta_c$ give evidence that average cluster perimeter in two (lower set of data-points) and three dimensions (upper set of data-points) behaves as predicted by equation (3). The slope and the vertical position of the lines which are drawn through the points, determine the $k(\Delta\beta)$ and $b(\Delta\beta)$ parameters whose $\Delta\beta$ dependence is shown in the next figure. The value of the parameter $t/n|_\infty$, which is of crucial importance for the evaluation of the uppermost line in Figures 1 and 2 is determined as that value at which the set of datapoints lies on a straight line.

masses – up to $n = 2\,000$. The advantageous feature of this latter approach is that it leads to limiting behaviour ($n \to \infty$) of cluster properties as one can see in Figure 3 where it is shown that the cluster perimeters obey the relation

$$\langle t(n,\beta)\rangle = \frac{t}{n}\Big|_\infty(\beta)n + k(\beta)n^{b(\beta)}. \qquad (3)$$

This assumption is based upon the scale invariance property, which should be fulfilled at least at the percolation threshold, but numerical evidence suggests that the relation is valid on a wide β interval (linear relationship between $\langle t_n\rangle$ and n was demonstrated for the lattice animal limit by several authors [4–6]). By extensive and careful analysing of numerical results we were able to unravel the β dependence of the parameters $\frac{t}{n}|_\infty(\beta)$, $k(\beta)$ and $b(\beta)$. The β dependence of $k(\beta)$ and $b(\beta)$ is plotted in Figure 4. No dramatic temperature dependence can be observed. The quantity $\frac{t}{n}|_\infty(\beta)$ leads us to the "specific heat" of infinite clusters after the (numerical) derivative is taken. If the critical behaviour of the "specific heat" is supposed to behave as $c_p(n,\beta)/(n\beta^2) = \text{const}_1 - \text{const}_2(1-\alpha)|\Delta\beta|^{-\alpha}$, then the "energy" should behave as

$$\frac{t}{n}\Big|_\infty(\beta) = \text{const}_3 - \text{const}_1\Delta\beta + \text{const}_2|\Delta\beta|^{1-\alpha}. \qquad (4)$$

We succeeded to determine all the parameters which appear in equation (4). The results are presented as the uppermost curve in Figures 1 and 2. The results are encouraging, although not very accurate. In the limit $n \to \infty$ our estimate for the range of α values is the interval $0.5 < -\alpha < 0.8$, the same for two as well as for three-dimensional case.

In the percolation problem the critical exponents α, $\tilde\beta$ and γ are usually defined by the moments of cluster numbers – what reflects the properties of cluster populations. The critical exponent α is supposed to have

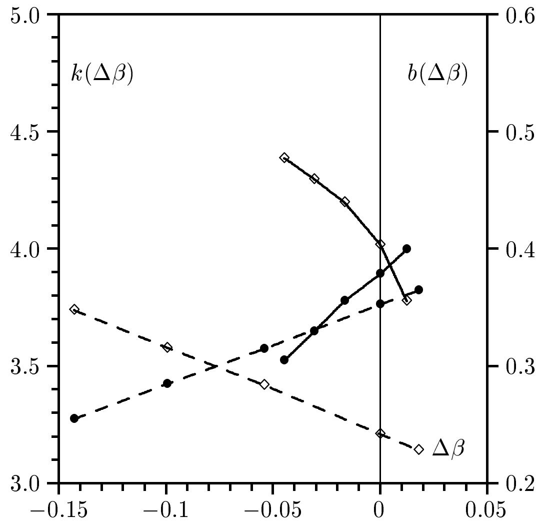

Fig. 4. "Inverse temperature" dependence of the parameters $k(\beta)$ and $b(\beta)$ for square ($D = 2$) and cubic ($D = 3$) lattice. Dashed lines: $D = 2$; solid lines: $D = 3$; $\diamond$ symbols: $k(\Delta\beta)$ (see the vertical scale at left); $\bullet$ symbols: $b(\Delta\beta)$ (see the vertical scale at right).

the value $\alpha = -2/3$ in two dimensions and $\alpha = -0.64$ in three dimensions [13]. In thermodynamic systems the critical exponents are usually interpreted as structural determinants, but the two categories are connected, as we have shown earlier [7]. In the case of Ising models the specific heat, for instance, can be split into two contributions emerging from changes in cluster structure and cluster populations. We showed that the structural component of the specific heat is the dominant one, but we had severe troubles to characterize its temperature behaviour in the vicinity of the critical point. The study of percolation prototype of the structural component of the specific heat is more simple because the clusters do not interact and one can obtain the results by treating individual clusters. It is worth to exploit this opportunity which can also improve our understanding of the correlated lattice systems.

As a matter of curiosity it is worth pointing out that in two-dimensional case the peaks of $c_p(\beta)/\beta^2$ approach β_c from left, while in three dimensions the peaks approach from the opposite side. Let us also point out the fact that it would be possible to deduce from Figures 1 and 2 the n dependence of critical exponent α. We can see on the basis of the shape of the curves that for finite n values $-\alpha$ exceeds unity, and only in the limit of infinite clusters it falls below one.

4 Fractal dimensionality of clusters

From the scale invariance principle it follows that at the percolation threshold densities the percolation clusters are fractal objects with fractal dimension $d(p_c) = D - \tilde{\beta}/\nu$ where $\tilde{\beta}$ and ν are the critical exponents, what gives the value $d(p_c) = 1.896$ in two dimensions and $d(p_c) = 2.48$ in three dimensions. Off the percolation threshold density the situation is not clear at all. According to Stauffer [5,6] the p-dependence of fractal dimensionality of clusters appearing in the site percolation problem on square lattice might be in a form of a step function with $d = D - \tilde{\beta}/\nu$ at $\beta = \beta_c$, with $d = d_{LA}$ at $\beta < \beta_c$ and $d = D$ at $\beta > \beta_c$ where $d = d_{LA}$ means the lattice animal (LA) limit which is valid at infinite temperatures ($\beta = 0$ or $p = 0$). The LA limit appears when the Boltzmann factor in equation (1) is of unity value and thus all the clusters (called in this case the lattice animals) are contributing with the same weight. One should also consider the possibility that off the percolation threshold density the fractality concept is not operative for clusters and in this case fractal dimension can be only defined at $\beta = \beta_c$. In what follows we shall present our numerical evidence regarding the fractal properties of clusters on square and cubic lattice for wide range of "temperatures". The results were obtained by combined effort, using the methodologies described earlier under i) and ii).

Close to the percolation threshold large enough clusters were generated by means of Leath's algorithm. The clusters were analysed [5,6,14–16] by counting the number of occupied sites in concentric squares with side L and then the fractal dimension was determined from the relation $\rho(L) \propto L^{D-d}$, where $\rho(L)$ is the density of occupied sites in the square with sides L. Off the percolation threshold large enough clusters were not available and to generate the representative clusters one should use the methodology described above under i) and then the clusters were analysed in the same way as the clusters generated by Leath's algorithm.

Another possibility to determine the fractal dimension of clusters proceeds over the definition which is valid for fractal objects: $n \propto r_n^{d(\beta)}$ where n means again the mass of a cluster and r its size – radius of gyration, for instance. The clusters which were generated by either of two methodologies were analysed in such a way that radii of gyration were calculated and then the fractal dimension was determined from the log – log plot of the size – mass relation.

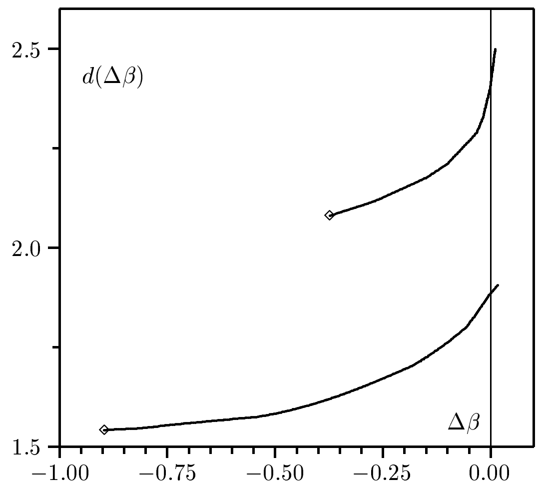

Fig. 5. Dimensionality of an average cluster as a function of $\Delta\beta = \beta - \beta_c$ where β is the "inverse temperature" $\beta = -\ln(1-p)$. Upper curve refers to the clusters generated on cubic lattice and lower curve refers to square lattice clusters. At $\beta = 0$ we speak about "lattice animal limit" (presented in the figure with the $\diamond$ symbols), which means that each cluster (lattice animal) is taken with equal weight. At higher β values the clusters are weighted according to the "Boltzmann factor" $(1-p)^t = \exp(-\beta t)$ what diminishes the contribution of clusters with large perimeter and favours more compact clusters. Therefore $d(\beta)$ approaches the value of D at positive $\Delta\beta$ values.

The results are presented in Figure 5. The dimension of lattice animal limit was determined to be 1.54 ± 0.05 and 2.08 ± 0.1 for square and cubic lattices, respectively. The results for $D = 2$ agree within the error bounds with the early results of Stauffer [5,6] and also with the Grassberger's [17] value of the backbone dimensionality of the percolation cluster. Within the bounds of our result for $D = 3$ case lie also the results for LA limit of Parisi and Sourlas [18] with $d_{LA} = 2$. With growing β values the fractal dimension grows and, as it can be seen in Figure 5 rises rather steeply at $\beta = \beta_c$ where it is close to $d_c = D - \tilde{\beta}/\nu$ value and then continues growing towards $d = D$. The uncertainties of d values are similar to that given above for d_{LA} values. There is no guarantee that the continuous variation of $d(\Delta\beta)$ is a real feature on a wide "temperature" interval, but close to β_c one can consider the $d(\Delta\beta)$ variation as a nice example of a prototype of a phase transition – similar to the c_p variation depicted in Figures 1 and 2.

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