Scaling properties of the perimeter distribution for lattice animals, percolation and compact

clusters

LETTER TO THE EDITOR

Scaling properties of the perimeter distribution for lattice animals, percolation and compact clusters

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Abstract. Scaling properties of the cluster distribution function and mean cluster size in the ensemble of clusters with fixed perimeter are analysed. The relevant scaling exponents are determined in all three regions of interest: lattice animals ($p < p_c$), percolation ($p = p_c$) and compact clusters ($p > p_c$). Also, a form of the lattice animal distribution function in the statistical ensemble of clusters with fixed perimeter is presented. In particular, we compare the exponents α and β, defined through $\langle t \rangle_s \sim s^\alpha$ and $\langle s \rangle_t \sim t^\beta$, where $\langle t \rangle_s$ is the mean perimeter t of s-site clusters (the s-ensemble) and $\langle s \rangle_t$ is the corresponding quantity in the t-ensemble.

The percolation model has been extensively analysed during the last decade (Stauffer 1979, 1985, Essam 1980 and references therein), both because of its formal appeal and its practical importance. This model and its variants form a basis for the description of geometric aspects in a number of phenomena such as polymerisation and gelation, catalysis, hydrodynamics and cloud processes. One is typically interested in statistics of clusters formed by the process of random occupation of elements (sites or bonds) on a lattice. A cluster is a group of connected occupied elements, characterised by the number s of elements it contains (cluster elements) and the number t of its unoccupied nearest neighbours (perimeter elements). Each element is occupied with probability p and the two parameters s and t determine the statistical probability $p^s(1-p)^t$ for the occurrence of the cluster.

For most of the work done on percolation theory and related topics one focuses on a single parameter function $n_s(p)$, the distribution of clusters of mass s, which sums over all the information about the perimeter t of the clusters. On the other hand, there are some applications (e.g. colloidal catalysis) where the cluster mass is irrelevant. Catalytic activity is proportional to the number of empty sites neighbouring the cluster ('catalytic surface' of the cluster), which is identical to the cluster perimeter. In this case the appropriate statistical distribution should be the one which specifies the fraction of clusters having a given perimeter t, regardless of their mass s. Starting with this 'perimeter distribution' function one can calculate various statistical averages, which we will refer to as the t-ensemble averages, in contrast to the s-ensemble averages commonly studied. In what follows, we will show that the cluster perimeter distribution and the related averages have some interesting scaling features which have not been apparent from the analysis based on the usual s-ensemble approach. The scaling behaviour of these quantities will be analysed in all three regions of interest: (i) percolation ($p = p_c$), (ii) lattice animals ($p < p_c$) and (iii) compact clusters ($p > p_c$).

(a) The s-ensemble. The average number of s-element clusters per lattice site $n_s(p)$ is defined as

$$n_s(p) = \sum_t p^s(1-p)^t g_{st} \tag{1}$$

where g_{st} represents the number of geometrically distinct clusters with s occupied elements and t perimeter elements. In the case of the s-ensemble averages, the mean cluster perimeter as a function of $q = 1 - p$ is defined as

$$y_s(q) \equiv \langle t \rangle_s = \frac{\sum_t t g_{st} q^t}{\sum_t g_{st} q^t} = \frac{\mathrm{d} \ln Z_s}{\mathrm{d} \ln q} = (q/Z_s)(\mathrm{d}Z_s/\mathrm{d}q). \tag{2a}$$

Here

$$Z_s \equiv \sum_t g_{st} q^t = p^{-s} n_s(p) \tag{2b}$$

plays the role of the partition function for an ensemble of clusters of fixed size s. The asymptotic behaviour of $\langle t \rangle_s$ is known:

$$\langle t \rangle_s = \begin{cases} A(p)s & p < p_c \\ [(1-p)/p]s + Bs^{(d-1)/d} & p \geq p_c. \end{cases} \tag{3}$$

Here $A(p)$ and B are scaling amplitudes, d is the lattice dimension and p_c is the critical probability. If we write $\langle t \rangle_s \sim s^\alpha$, the above expressions tell us that in the limit $s \to \infty$ and at any $p \neq 1$, $\langle t \rangle_s \sim s$, and therefore $\alpha = 1$. Note that in the limit $p \to 1$ the correction to scaling term $s^{(d-1)/d}$ becomes dominant and replaces the $[(1-p)/p]s$ term.

(b) The t-ensemble. Definition (1) focuses interest on the s-dependent properties. However, on the level of the g_{st} function, the variable s has little precedence over the variable t and one can define two types of averages. In the t-ensemble, one defines basic averages through the summation over index s. For example, the mean cluster size $\langle s \rangle_t$ at a fixed perimeter t is defined as

$$y_t(K) \equiv \langle s \rangle_t = \frac{\sum_s s g_{st} K^s}{\sum_s g_{st} K^s} = \frac{\mathrm{d} \ln Z_t}{\mathrm{d} \ln K} = (K/Z_t)(\mathrm{d}Z_t/\mathrm{d}K). \tag{4a}$$

Here K is a generalised statistical weight, analogous to $q = 1 - p$ of (2) and

$$Z_t = \sum_s g_{st} K^s \tag{4b}$$

is the t-ensemble partition function. When we speak about the probabilistic properties, we usually use probability p for the statistical weight K. The above weight K is meant to apply to more general behaviour (Family and Coniglio 1980, Harris and Lubensky 1981).

The t-ensemble average, $\langle s \rangle_t$ of (4a), was analysed by Duarte (1978), who considered $\langle s \rangle_t$ defined only with the statistical weight $K = 1$. However, he associated the observed scaling behaviour with the lattice animal (LA) problem. If we write $\langle s \rangle_t \sim t^\beta$, his work suggests the value $\beta \simeq 1.5$. This is somewhat surprising, since from experience with thermodynamic variables, one expects the exponents α and β to be related as $\beta = 1/\alpha$ and therefore the last value does not agree with $\alpha = 1$ obtained from (3).

Our aim here is to examine in more detail the t-ensemble averages through the analysis of the partition function Z_t and the mean cluster size $\langle s \rangle_t \sim t^\beta$ in all three asymptotic regions of interest: percolation, lattice animals and compact clusters, and to connect the value of β with the value of the s-ensemble exponent α. We also give

arguments showing that definition (4) of $\langle s \rangle_t$ for LA problems should be defined with the value of K equal to the LA fixed point value $K = K_A$ (Family and Coniglio 1980, Harris and Lubensky 1981).

(i) *Percolation region.* We start from the percolation free energy G (Kasteleyn and Fortuin 1969, Essam and Gwylim 1971). In the s-ensemble

$$G(p, h) = \sum_s e^{-sh} n_s(p) = \sum_s e^{-sh} p^s \sum_t g_{st} q^t. \tag{5a}$$

Equivalently

$$G(p, h) = \sum_s K^s Z_s(q) \tag{5b}$$

where $K = p\,e^{-h}$ and h is the ghost field. In the t-ensemble notation, the free energy of (5a) can be expressed as

$$G(p, K) = \sum_t q^t Z_t(K) \tag{6a}$$

with $Z_t(K)$ defined through (4b). From the s-ensemble analysis we know (Nakanishi and Stanley 1980) that, in the vicinity of the percolation critical point, $n_s(p)$ scales as

$$n_s(p) \sim s^{-\tau} f(s^\sigma (p - p_c)) \tag{6b}$$

(Stauffer 1979, Essam 1980), where σ and τ are the two independent percolation exponents. Combining (5) and (6b), we see that in the vicinity of p_c the free energy scales as

$$G = \begin{cases} (p - p_c)^{(\tau-1)/\sigma} & [h = 0,\ K = 0] \\ (K/K_c - 1)^{\tau-1} = h^{\tau-1} & [p = p_c,\ K = p_c\,e^{-h}]. \end{cases} \tag{7}$$

The same results should be valid if G is represented by the t-ensemble expression (6a) and we can therefore rewrite (7) as

$$G = \sum_t q^t Z_t = \begin{cases} (q - q_c)^{(\tau-1)/\sigma} & [h = 0,\ K = 1 - q] \\ (K/p_c - 1)^{\tau-1} & [q = q_c,\ K = p_c\,e^{-h}]. \end{cases} \tag{8}$$

Equation (8) implies that Z_t scales as

$$Z_t = t^{-\tau} \lambda^t f(t^\sigma (q - q_c)) \tag{9}$$

with $\lambda = 1/q$. One can prove (9) by the substitution of (9) in (8) and subsequent integration over the variable t. The scaling form (9) implies that at the percolation fixed point $[p = p_c,\ h = 0]$, Z_t scales as

$$Z_t = t^{-\tau} (1/q_c)^t \tag{10}$$

which is quite analogous to the behaviour of the s-ensemble partition function Z_s at $p = p_c$:

$$Z_s = p_c^{-s} n_s(p_c) = s^{-\tau} (1/p_c)^s. \tag{11}$$

The result (10) can also be derived from the definition of Z_t by approximating the sum over s by an integral which is then calculated by the saddle point method. Thus, in the vicinity of p_c (Stauffer 1985) we can write $g_{st} = [\Lambda(x)]^s n_s(p) s^{-1/2}$, with $\Lambda(x) = (1+x)^{1+x}/x^x$ and $x = s/t$. Then

$$Z_t = \int dx\, t s^{-\tau-1/2} \exp[t(x \ln p + (1+x) \ln(1+x) - x \ln x)]. \tag{12}$$

Maximising the exponent with respect to x, one obtains the most dominant value of x, $x = p/q$, and, after calculating the integral, recovers expression (10).

The scaling form (10) agrees rather well with the exact numerical values for $Z_t(p_c)$. In figure 1(a) we present for the triangular site (TS) and square site (SS) problems the exact values of the ratio Z_{t+1}/Z_t, which should, according to (10), scale as $\lambda(1 - \tau/t)$. The extrapolation to $t \to \infty$ gives the estimates $\lambda = 1/q_c = 1.9 \pm 0.1$ for the TS problem (which should correspond to the percolation threshold $p_c = 0.474 \pm 0.05$) and the value $\lambda = 2.4 \pm 0.1$ for the SS problem (corresponding to $p_c = 0.585 \pm 0.05$). The p_c values obtained in this fashion are somewhat lower than the true values $p_c = 0.5$ (TS) and $p_c = 0.593$ (SS). Apparently, the scaling region of the data in the t-ensemble is *smaller* than in the s-ensemble that results in the above errors in the estimates of λ and p_c.

(ii) LA region. In order to find the t-ensemble function Z_t which describes the properties of lattice animals, we must choose the proper value of the generalised statistical weight K appearing in Z_t. This issue has not been treated correctly in the past.
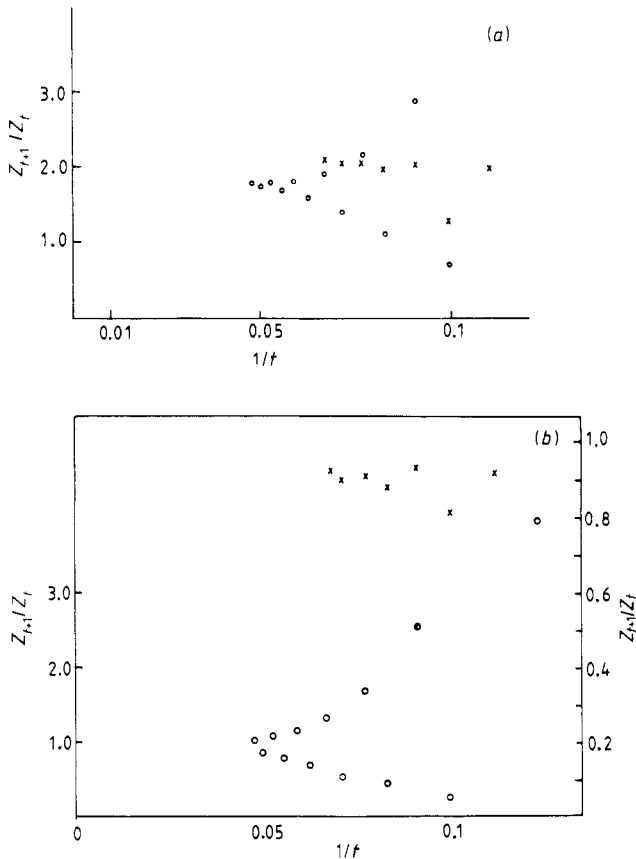

Figure 1. (a) Ratio of the subsequent values of the t-ensemble partition function Z_{t+1}/Z_t at the percolation threshold as a function of $1/t$ for the TS ($\bigcirc$) and SS ($\times$) problems. Values of the ratio extrapolated to $1/t \to 0$ give the value of parameter $\lambda = 1/q_c = 1/(1 - p_c)$. ($b$) Ratio of the subsequent values of the t-ensemble partition functions Z_{t+1}/Z_t at the value K equal to the lattice animal fixed point value K_A for the TS ($\bigcirc$) and SS ($\times$) problems. The left-hand scale is for the TS and the right-hand scale for the SS problems.

We start from the result of the s-ensemble analysis which gives the following scaling behaviour for the free energy in the lattice animal region (Sykes and Glen 1976):

$$G = \sum_s K^s n_s^A = (K - K_A)^{\theta - 1}. \tag{13a}$$

In this equation, $n_s^A = s^{-\theta} \lambda_A^s$ is the number of lattice animals of size s, λ_A is the lattice animal growth parameter and $K_A = 1/\lambda_A$ is the LA critical value of the field K. The scaling fields $(K - K_A)$ and $(q - 1)$ are equivalent in the LA region (Family 1982, Djordjevic 1985). Therefore the free energy must also scale as

$$G \sim (q - 1)^{\theta - 1}. \tag{13b}$$

If the function G of (6) must obey (13b), then the t-ensemble partition function Z_t defined in (4b) must, in the LA region, scale as

$$Z_t \sim \Lambda^t t^{-\theta} \tag{14}$$

with the t-ensemble LA growth parameter Λ equal to 1 and the normal LA value of the exponent $\theta(\theta = 1$ if $d = 2)$. We can use the fact that $\Lambda = 1$ to determine the value of the field K which, in the LA region, gives Z_t of the form (14). With this in mind we present in figure 1(b) the ratio Z_{t+1}/Z_t as a function of $1/t$ for the TS and SS problems. The intercepts of these functions with the $1/t = 0$ axis, must be equal to $\Lambda = 1$. This is indeed the case if the K used in the calculations of Z_t takes the LA fixed point value $K_A = 0.192$ for the TS and $K_A = 0.246$ for the SS problems.

Since the t-ensemble growth parameter Λ is equal to 1, $\ln Z_t$ should behave as $\ln Z_t \sim t \ln \Lambda + \theta \ln t = \theta \ln t$. This can be used as another test for the value of the field K corresponding to the LA partition function Z_t. In figure 2 we present function $\ln Z_t$ plotted against t for $K = 0.2, 0.246, 0.3$ for the SS problem. It is obvious that the curve for $K = K_A = 0.246$ is closest to the expected logarithmic behaviour. Thus, the above analysis indicates that the t-ensemble partition function for the LA problem should be defined as $Z_t = \sum_s K_A^s g_{st}$.
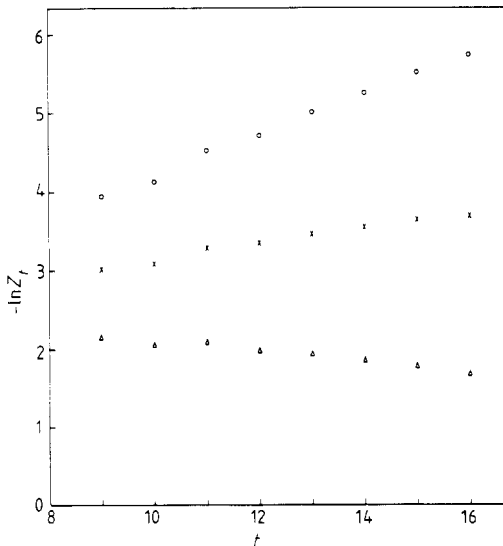

Figure 2. Dependence of $-\ln(Z_t)$ on the value of perimeter t for $K = 0.2$ (○), $K = K_A = 0.246$ (×) and $K = 0.3$ (△) for the SS problem.

Consistency of this conclusion is also demonstrated in figure 3(a) where we show the effective exponent $\theta(t)$ as a function of $1/t$ which, after the extrapolation to $t \to \infty$, gives $\theta = 1$ for both lattices. The effective exponent $\theta(t)$ is defined as (Riedel and Wegner 1974)

$$\theta(t) = \frac{\ln(Z_{t+1}/Z_t)}{\ln[(t+1)/t]}. \tag{15}$$

(iii) Compact cluster region. Finally, let us derive the relation between Z_t and t for compact clusters. For numbers g_{st} we use the expression (Essam 1980)

$$g_{st} = [\Lambda(x)]^s \exp[-as^{(d-1)/d}] \qquad x = s/t, a = \text{constant}. \tag{16}$$

The RG analysis of the generalised percolation problem shows that the parameter K takes the value one for the compact clusters fixed point and Z_t must be equal to

$$Z_t = \left(\sum_s K^s g_{st}\right)_{K=1} = \int ds\, \Lambda^s \exp(-as^{(d-1)/d}) K^s|_{K=1}$$

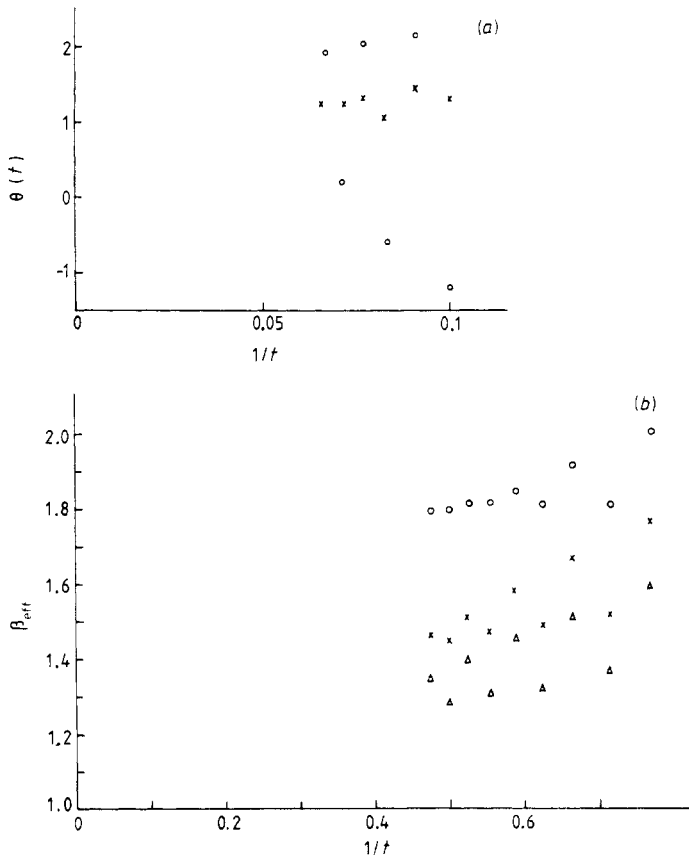$$= \int ds\, K^s \exp[(t+s)\ln(t+s) - s\ln s - t\ln t - as^{(d-1)/d})]. \tag{17}$$

Figure 3. (a) Effective exponent $\theta(t)$ as a function of $1/t$ for the TS ($\bigcirc$) and SS ($\times$) problems. Extrapolation to $t \to \infty$ is consistent with the expected value $\theta = 1$ for lattice animals. (b) Effective exponent $\beta_{\text{eff}}(t)$ as a function of $1/t$ for the TS problem at three values of the weight K: $K = 1$ ($\bigcirc$), $K = 0.5$ ($\times$) and $K = 0.192$ ($\triangle$).

By equating to zero the derivative with respect to s of the function in the exponent we obtain s_m, the most dominant value of s. Thus $s_m \sim t^{d/(d-1)}$ and the saddle point approximation of the above integral is then

$$Z_t = \exp[t^{d/(d-1)} \ln K - tA(K)]_{K=1}. \tag{18}$$

Hence $\ln Z_t$ scales as $t^{d/(d-1)} \ln K - tA(K)$. This result is expected physically, since compact clusters behave as homogeneous clusters and their mass s scales as the geometric volume R^d (R-cluster radius) while perimeter t scales as the cluster surface R^{d-1} which results in the relation $s \sim t^{d/(d-1)}$.

Let us now concentrate on the numerical data for the mean size $\langle s \rangle_t$ at a fixed cluster perimeter t (4). We determine numerically the effective exponent β as a function of field K. As we vary K between 0 and 1 we obtain the result that the exponent β changes between values 1 and 2. The results for the TS problem are presented in figure 3(b) for three values of the parameter K: $K = 1$, $K = p_c$ and $K = K_A$. We performed the same analysis for the ss and honeycomb lattices and obtained similar results. In the lattice animal region ($K = K_A$) we obtain $\beta = 1.1 \pm 0.1$, which includes the expected value $\beta = 1$. In the percolation region ($K = p_c$) we obtain $\beta = 1.2 \pm 0.2$ and in the compact clusters region ($K = 1$), we get $\beta = 1.8 \pm 0.2$, which includes the expected value 2. In this letter we rely on the extended data for $\langle s \rangle_t$ from Sykes *et al* (1976) and Duarte (1981). It should be emphasised that, although for compact clusters $\ln Z_t \sim t^{d/(d-1)} \ln K + tA(K)$ and the amplitude of the $t^{d/(d-1)}$ factor tends to zero when $K \to 1$, the mean cluster size $\langle s \rangle_t$ defined in (4) scales as $t^{d/(d-1)} + t$. The compact cluster and lattice animal influences, $t^{d/(d-1)}$ and t respectively, are clearly present at all values of K. This basically explains the deviations of the effective exponent from both the asymptotic values $\beta = 1$ (LA) and $\beta = 2$ (CC) which we observe even at the K values below the percolation threshold as well as close to $K = 1$. We have also repeated the Duarte (1978) analysis of $\langle s \rangle_t$. After extrapolating the effective exponent $\beta(t)$ to $t \to \infty$, we obtained the value $\beta = 1.75$, significantly higher than the Duarte value of 1.5.

In conclusion, our results for the t-ensemble exponent agree with the relation between s and t in the s-ensemble; i.e. for percolation and lattice animals we obtain a linear dependence and for the compact cluster a volume to surface dependence of the homogeneous clusters. The reason that the observed (effective) t-ensemble exponent β is changing continuously from the value 1 to 2 is the influence of compact clusters for which $\langle s \rangle_t \sim t^{d/(d-1)} + t$. This quadratic dependence on t in $d = 2$ is more important than linear dependence so, although the amplitude of the quadratic term is decreasing with decreasing parameter K, its influence remains important. This is in contrast to the s-ensemble average $\langle t \rangle_s$ where the influence of the compact clusters appears as a correction to the leading linear dependence on s, i.e. as a correction term $s^{(d-1)/d}$. It should also be stressed that the limit $K \to 0$ in the t-ensemble averages do not correspond to the LA problem but rather extract only the terms with $s = s_{min}$ which, for given t, are proportional to $2t$, i.e. it corresponds to the linear clusters. The LA properties are obtained in the limit $K = K_A$. The conclusion that the LA problem corresponds to the $p \to 0$ limit of the percolation problem is correct (Stauffer 1985) when we consider the averages in the s-ensemble because in the definitions like (2) the powers of p^s or K^s cancel out and their presence is irrelevant.

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