

Lattice Animals as Limits of Clusters in Percolation Theory

B. Rockslöf and D. Stauffer

Institut für Theoretische Physik der Universität Köln

Z. Naturforsch. **34a**, 1140–1142 (1979);

received June 1, 1979

We investigate if the limits $p \rightarrow 0$ or $p \rightarrow 1$ for large percolation clusters at concentration p correspond to large lattice animals for fixed size s or fixed perimeter t , respectively. A numerical analysis for the asymptotic number of lattice animals with fixed large perimeter shows that the limit $s \rightarrow \infty$ can be interchanged with the limit $p \rightarrow 0$, but the two limits $t \rightarrow \infty$ and $p \rightarrow 1$ cannot be interchanged.

In the percolation problem each site of an infinite lattice is randomly occupied with probability p ; a cluster is a group of occupied sites connected by nearest-neighbor distances. Its size s is the number of occupied sites, and its perimeter t is the number of empty sites which are nearest neighbors to cluster sites. If g_{st} counts the number of possible configurations (also called "lattice animals") with size s and perimeter t , then

$$n_{st} = g_{st} p^s q^t, \quad q \equiv 1 - p \quad (1)$$

is the average number of percolation clusters of size s with perimeter t , and

$$n_s \equiv \sum_t n_{st} \quad (2a)$$

is the total number of clusters with s sites each. Duarte [1] also investigated sums over cluster sizes s at fixed perimeter t ; we call

$$n_t' \equiv \sum_s n_{st} \quad (2b)$$

the total number of percolation clusters with perimeter t . Similarly,

$$g_s \equiv \sum_t g_{st} \quad \text{and} \quad g_t' \equiv \sum_s g_{st} \quad (2c)$$

are the corresponding total numbers of lattice animals at fixed size s or fixed perimeter t , respectively. In Monte Carlo simulations or other numerical studies [2] one likes to treat the animal problem as a special case of the percolation problem by simply setting $p=0$ in a computer program working at fixed size s . To what extent does the

limit $p \rightarrow 0$ correspond to animals at fixed size s , and the limit $p \rightarrow 1$ to animals at fixed perimeter t , as the following Eq. (3) seems to suggest.

Clearly, if $p \rightarrow 0$ at fixed cluster size s , we have $n_{st} p^{-s} = g_{st} q^t \cong g_{st}$ from Eq. (1) or [2] after summation over all t :

$$n_s(p \rightarrow 0) p^{-s} = g_s. \quad (3a)$$

Similarly, summing up over all s for p close to unity we get

$$n_t'(p \rightarrow 1) q^{-t} = g_t' \quad (3b)$$

for fixed t . It is less clear that this correspondence of percolation cluster numbers n_s and n_t' to animal numbers g_s and g_t' , as shown in Eq. (3), is also valid asymptotically for very large clusters, when we are interested in the limit of s (or t) going to infinity at small but fixed p (or q respectively). Equation (3), instead, is valid only for the opposite ordering of limiting processes, i.e. for p or q going to zero at large but fixed cluster size s or t . We now investigate by a cumulant expansion if these two limits are interchangeable.

The general cumulant expansion for any average denoted by $\langle \dots \rangle$ is [3]

$$\begin{aligned} \ln \langle e^x \rangle &= \langle x \rangle + \frac{1}{2} \langle (x - \langle x \rangle)^2 \rangle + \frac{1}{6} \langle (x - \langle x \rangle)^3 \rangle \\ &+ \frac{1}{24} \langle (x - \langle x \rangle)^4 \rangle - 3 \langle (x - \langle x \rangle)^3 \rangle + \dots \end{aligned}$$

Let us now look at any animal property A_{st} depending on s and t . For our purposes at $p \rightarrow 0$ we define an average by $\langle A_s \rangle = \sum_t A_{st} g_{st} / \sum_t g_{st}$, and at $p \rightarrow 1$ another average by $\langle A_t \rangle' = \sum_s A_{st} g_{st} / \sum_s g_{st}$. Then we have from (1) and (2) with $x = \ln(q^t)$ or $x = \ln(p^s)$, respectively, in the cumulant expansion:

$$\begin{aligned} \ln(n_s p^{-s}) &= \ln[\langle e^{t \ln q} \rangle g_s] \\ &= \ln(g_s) + \langle t_s \rangle \ln(q) \\ &+ \frac{1}{2} \langle (t_s - \langle t_s \rangle)^2 \rangle \ln^2(q) + \dots, \end{aligned} \quad (4a)$$

$$\begin{aligned} \ln(n_t' q^{-t}) &= \ln[\langle e^{s \ln p} \rangle' g_t'] \\ &= \ln(g_t') + \langle s_t \rangle' \ln(p) \\ &+ \frac{1}{2} \langle (s_t - \langle s_t \rangle')^2 \rangle \ln^2(p) + \dots \end{aligned} \quad (4b)$$

Numerical evidence in two and three dimensions [1, 2, 4, 5] has shown that $\langle t_s \rangle = bs + \dots$ for large s , and presumably also the width $\langle (t_s - \langle t_s \rangle)^2 \rangle$ varies as s . Moreover, for large animals,

$$\ln(g_s) = s \ln(\lambda) - \theta \ln(s) + \dots$$

Reprint requests to Prof. D. Stauffer, Institut für Theoretische Physik, Universität, Zùlpicherstr. 77, 5000 Köln 41, West Germany, since B. Rockslöf is student at the Theodor-Schwann-Gymnasium, 4040 Neuss, West Germany. 0340-4811/79/0900-1140 \$ 01.00/0

Please order a reprint rather than making your own copy.

[6]. Thus for $p \rightarrow 0$ and $s \rightarrow \infty$ (4a) gives (provided the higher terms of the cumulant expansion do not disturb us):

$$\ln(n_s p^{-s}) = s \ln \lambda + b s p(1 + O(p)) + \dots, \quad (5)$$

or $(n_s p^{-s})^{1/s} \cong \lambda e^{bp}$,

where the neglected terms $(+\dots)$ vary less than s with increasing cluster size. Thus the two limits can be interchanged for the leading terms:

$$\lim_{s \rightarrow \infty} \lim_{p \rightarrow 0} (n_s p^{-s})^{1/s} = \lim_{p \rightarrow 0} \lim_{s \rightarrow \infty} (n_s p^{-s})^{1/s} = \lambda. \quad (6)$$

In short, we have $n_s \sim (\lambda p)^s$ near $p=0$ for large clusters, connecting the animal λ with the percolation n_s for small concentration, as desired.

In the other case, for p close to unity, the situation is not so nice. Duarte [1] found $\langle s_t \rangle' \propto t^y + \dots$ for large t , with y about $3/2$ significantly larger than unity, in striking contrast to the $\langle t_s \rangle \propto s$ relation mentioned above. Furthermore we analyzed the polynomials of [7] to find the numbers g_t' of animals at fixed perimeter. Assuming

$$g_t' \propto \lambda' t^{-\theta'} \quad (t \rightarrow \infty) \quad (7a)$$

we found a ratio analysis in the triangular lattice:

$$\lambda' \cong 4.6 \pm 0.3; \quad \theta' \cong 5.5 \pm 1. \quad (7b)$$

Our error bars may be regarded as rather optimistic in view of the rather strong scattering shown in Fig. 1 for the ratios g_t'/g_{t-1}' plotted versus $1/t$. Equation (7a) predicts these data to follow a straight line with intercept λ' and slope $-\theta'\lambda'$, and we see that only the last few points are approximated well by (7a). More accurately, Table 1 gives the consecutive estimates for λ' and θ' , if in the ratio plot we fit a straight line through two consecutive data points. A few more points in the series of [7] would help to get more accurate extrapolations; but we feel our data show reliably that θ' is nearly one order-of-magnitude larger than the $\theta \cong 1$ exponent describing g_s . We have no explanation for this surprisingly large value of θ' .

Equation (4b) now takes for $p=1-q$ close to unity the form

$$\begin{aligned} \ln(n_t' q^{-t}) &= \ln g_t' - \langle s_t \rangle' \cdot q + \dots \\ &= t \ln \lambda' - \text{const } t^y q + \dots \end{aligned} \quad (8a)$$

for large clusters, and now the two limits $t \rightarrow \infty$ and $q \rightarrow 0$ cannot be interchanged:

$$\begin{aligned} \lim_{p \rightarrow 1} \lim_{t \rightarrow \infty} (n_t' q^{-t})^{1/t} &= \infty; \\ \lim_{t \rightarrow \infty} \lim_{p \rightarrow 1} (n_t' q^{-t})^{1/t} &= \lambda'. \end{aligned} \quad (8b)$$

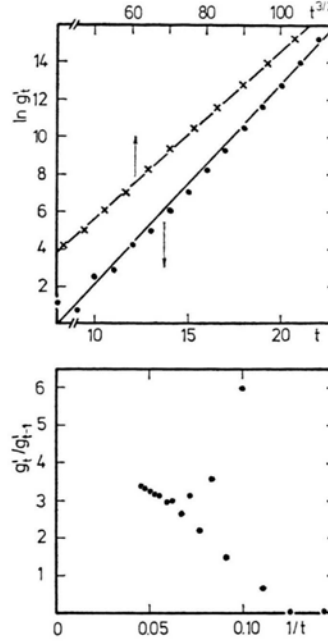


Fig. 1. Numerical test of Equation (7). The upper part shows g_t' plotted logarithmically versus t and versus t^y with $y = 3/2$. The lower part is a ratio analysis for the parameters λ' and θ' , with the solid line corresponding to Equation (7b).

In this sense, while near $p=0$ we may identify as in (3a) the percolation clusters at fixed s with the animals, $n_s \sim g_s p^s$ at least for the leading terms, this identification would be wrong near $p=1$ at fixed t : The approximation $n_t' \sim g_t' q^t$ of (3b) does not work in the limit of t going to infinity at fixed small q . This asymmetry in the relation between large percolation clusters and large lattice animals is traced back to the large exponent y observed [1] in the size-versus-perimeter relation of animals.

[One might speculate that instead of (7a) a different asymptotic form like $g_t' \propto t^{-\theta''} \lambda'' (t^y)$ is valid. Indeed Fig. 1 shows this form to fit our data

Table 1. Consecutive estimates of parameters λ' and θ' found from two consecutive ratios g_t'/g_{t-1}' of Figure 1. ($\lambda' = q_t + (t-1)^2(q_t - q_{t-1})/t$ and $\theta' = (q_t - q_{t-1})(t-1)^2/\lambda'$ with $q_t = g_t'/g_{t-1}'$.) Only the last points, giving the best extrapolation, are shown.

t	q_t	λ_t'	θ_t'
18	3.16	5.85	8.28
19	3.18	3.60	2.19
20	3.28	4.95	6.76
21	3.33	4.40	5.08
22	3.40	4.78	6.35

quite well. But then Eq. (8a) would be replaced by $\ln(n_t' q^{-t}) = t^y \ln(\lambda'') - \text{const } t^y q + \dots$, making the limits $q \rightarrow 0$, $t \rightarrow \infty$ interchangeable now. Then we would have for $q \rightarrow 0$ and $t \rightarrow \infty$: $n_t' \sim q^t \lambda''(t^y)$, with both $y \cong 3/2$ and λ'' larger than unity. Thus for $t \rightarrow \infty$ at fixed small q the cluster numbers n_t' would go to infinity. But the sum $\sum_t t n_t'$ is the probability that an arbitrary lattice site belongs to the perimeter of some finite cluster; this probability cannot be larger than unity, and thus n_t' must go to zero, not to infinity, for $t \rightarrow \infty$. This contradiction shows that $\log(g_t')$ cannot vary more quickly than t

with increasing t , and in particular cannot vary as $t^{3/2}$. Therefore (7a) presumably is correct.]

In conclusion we found that the asymptotic behavior of large clusters is more complicated for $p \rightarrow 1$ than for $p \rightarrow 0$. Thus, for example, nucleation theory [8], which needs cluster numbers for $p \rightarrow 1$, presumably cannot use for these cluster numbers the exponent θ' determined in (7), since that exponent refers to a limiting process ($p = 1$) different from the one needed in nucleation theory ($p \rightarrow 1$).

We thank P. Hei for encouraging discussions.

- [1] J. A. M. S. Duarte, Z. Naturforsch. **33a**, 1404 (1978) and Z. Physik B **33**, 97 (1979).
- [2] D. Stauffer, Physics Reports, in press.
- [3] B. R. Martin, Statistics for Physicists, Academic Press, London 1971, page 18.
- [4] J. A. M. S. Duarte, Nuovo Cim. Letters **22**, 707 (1978) and J. Physique (Paris), to be published.
- [5] H. P. Peters, D. Stauffer, H. P. Hlters, and K. Loewenich, Z. Physik B, to be published.
- [6] M. F. Sykes and M. Glen, J. Phys. A **9**, 87 (1976).
- [7] M. F. Sykes, D. S. Gaunt, and M. Glen, J. Phys. A **9**, 715 (1976).
- [8] K. R. Bauchspiess and D. Stauffer, J. Aerosol Sci. **9**, 567 (1978), with further literature on nucleation problems.