

Corrections to scaling for branched polymers and gels

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We have extended series expansions for both lattice animals and percolation (which model branched polymers and gels, respectively), and also have obtained Monte Carlo simulations of systems 1000 times larger than hitherto studied (17×10^9 sites). We find more precise estimates of the corresponding "correction-to-scaling exponents," and calculate the "correction-to-scaling function" $f_1(z)$ for the first time.

As the critical point is approached, the asymptotic behavior of a critical quantity $Q(x)$ is described by an equation of the form

$$Q(x) = Bx^\mu(1 + B'x^\Omega + \dots), \tag{1}$$

where $x=0$ at the critical point. The "scaling" exponent μ , and the "correction-to-scaling" exponent Ω are believed to be universal, while the amplitudes B and B' are not. Correction-to-scaling phenomena in thermal phase transitions have recently been considerably clarified.¹⁻³ The same cannot be said for the sort of "geometric" phase transitions characterizing aggregation phenomena.⁴ Indeed, measurements of the scaling exponents themselves are notoriously difficult in large part due to the absence of a clear picture of the correction effects.⁵ This work represents a contribution to this end for branched polymers and gels—two important classes of aggregation phenomena modeled by lattice animals and percolation, respectively.

To study this problem, we have used two methods of statistical mechanics—series expansions and Monte Carlo computer simulations—generally reliable in evaluating exponents and subtle correction effects. We have extended the series for both lattice animals and percolation, and have performed Monte Carlo simulations at the percolation threshold for a system of 17×10^9 particles, roughly 1000 times larger than previously published.

Lattice animals. In the lattice animal problem, $Q(x) = A_s$, the number of animals made of s elements (sites or bonds); this quantity is singular in the limit $x = 1/s \rightarrow 0$ and $\mu = \theta$. First, we extended the series for the triangular lattice by one additional term.⁶ Specifically, we calculated A_{st} , the number of clusters with $s = 15$ sites and t perimeter sites. The calculation, with the use of the Martin algorithm,⁷ required 55 h on the IBM 370/168; the next order would require roughly 300 h and was not attempted. We also calculated $A_s = \sum_t A_{st}$, the total number of lattice animals, regardless of perimeter, to order $s = 17$.⁸ The new results are given in Table I.

Directed lattice animals. Suppose that clusters can grow into only one of the 2^d octants of a hypercube. Then we have the directed lattice animal problem, which is related to a large number of natural phenomena ranging from directed polymers to river networks.⁹ It appears that the scaling exponent $\theta_D(d)$ is given in terms of the exponent $\theta(d+1)$ for the isotropic animal problem by the relation $\theta_D(d) = \theta(d+1) - 1$,¹⁰ where $\theta(d=2) = 1$ and $\theta(d=3) = \frac{3}{2}$ are exact.¹¹ This problem is particularly attractive for the present study, since the coefficients A_s^D are known exactly for all s for the square, triangular, and

honeycomb lattices¹² for which only the analytic corrections are present. For this reason, our series analysis methods were first tested on these systems [Fig. 1(a)].¹³

Applying these same methods to the isotropic animal problem, we find [Fig. 1(b)]

$$\Omega_A = 0.86 \pm 0.05. \tag{2}$$

The result is based not only on our extended series for the triangular lattice but also on a recently extended series for the square lattice.¹⁴

Percolation. In the percolation problem,

$$n_s(p) = \sum_t A_{st} p^s (1-p)^t \tag{3a}$$

is the number of clusters with s sites, normalized by the number of lattice sites, and $Q(x) = n_s(p_c)$. From our new A_{st} we extended the series for $n_s(p)$ for the triangular lattice, but even the extended series do not provide highly accurate estimates of Ω_p . Therefore, we carried out Monte Carlo simulations of an $L \times L$ triangular lattice for a range of L from 1000 to 130 000. This is much larger than previously published $n_s(p)$ percolation calculations ($L \leq 4000$).¹⁵ It is customary to calculate the partial sums,

$$N_s(p_c) = \sum_{s' \geq s} n_{s'}(p_c). \tag{3b}$$

Since $x = 1/s$, Eq. (1) predicts that $N_s(p_c) \sim s^{1-\tau}$, where $\mu = \tau = 2 + 1/\delta$. Hence the data plotted in Fig. 2 would be expected to display a plateau for large s corresponding to the expected asymptotic behavior. Previous data for L up to 4000 do not display a clear plateau,¹⁶ while we find a plateau

TABLE I. The cluster numbers A_{st} calculated for the triangular lattice, where s is the number of cluster sites ($s=15$) and t is the number of perimeter sites ($17 \leq t \leq 34$). We also confirmed $A_{16} = 4474080844$ and found the new result $A_{17} = 21866153748$ (Ref. 8).

t	A_{st}	t	A_{st}	t	A_{st}
17	42	23	1936836	29	140848650
18	759	24	5521212	30	170827614
19	5774	25	13878262	31	170852124
20	34164	26	30469044	32	133777587
21	153406	27	58629684	33	72798008
22	589094	28	98009115	34	20478999

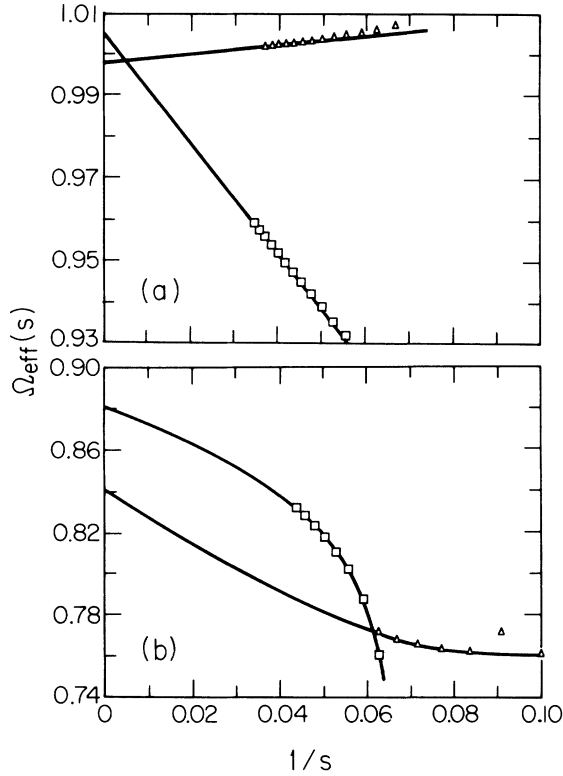


FIG. 1. Successive estimates for the correction-to-scaling exponent Ω_A for (a) directed site lattice animals on square and triangular lattices, and (b) isotropic lattice animals on the same two lattices. We see that the method predicts the correct value, $\Omega_A = 1$, for (a). Plotted is the function $\Omega_{\text{eff}}(s) = -2 + \ln Y / \ln X$, where $Y = (R_s - 1) / (R_{s-1} - 1)$ and $X = (s - 1) / s$. Here $R_s = W_{s+1} W_{s-1} / W_s^2$ and $W_s = s^\theta A_s$. We found results consistent with (2) using other extrapolation methods, and also using the exponential form of correction to scaling (Ref. 14).

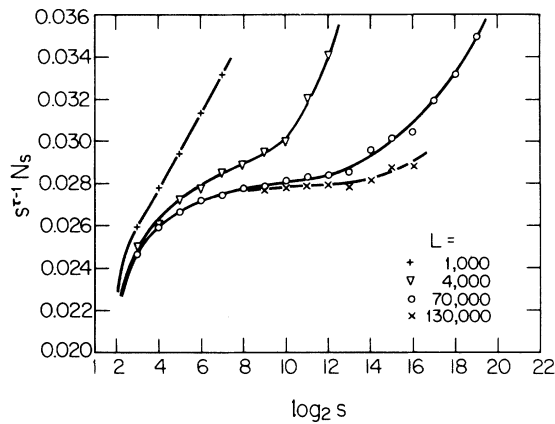


FIG. 2. Dependence of $\log_2 s$ of $s^{\tau-1} N_s(p_c)$, obtained by Monte Carlo simulations for an $L \times L$ triangular lattice, for a sequence of increasing values of L . Approximately 26 h of central processing unit time on a CDC 7600 were required for the case $L = 130\,000$. The points for $L = 4\,000$ are from Ref. 16.

for our systems with $L = 35\,000, 70\,000, 95\,000,$ and $130\,000$ (Fig. 2). The deviations from the plateau for smaller sizes s can be fitted to an $s^{-\Omega_p}$ law, and from the data we find a result somewhat lower than previous calculations^{4,16,17} (but see Ref. 18),

$$\Omega_p = 0.64 \pm 0.08 \quad (4)$$

The actual statistical errors were much smaller.

The situation for p slightly different from p_c is more complex than for $p = p_c$.¹⁹ If we assume a constant effective Ω_p throughout the critical region, then the one-variable scaling law in (1) is replaced by the two-variable ansatz¹⁶

$$n_s(p) = s^{-\tau} [f_0(z) + s^{-\Omega_p} f_1(z)] \quad (5)$$

Here $z = (p - p_c) s^\sigma$ is the scaled variable, $f_0(z)$ the ‘‘scaling function,’’ and $f_1(z)$ the overall effective correction-to-scaling function. While $f_0(z)$ has been calculated previously,^{16,20} $f_1(z)$ has not been calculated for any critical point. We calculated both $f_0(z)$ and $f_1(z)$ from the intercept and slope, respectively, of plots of $s^\tau n_s(p_c)$ vs $s^{-\Omega_p}$ (Fig. 3).

In summary, we have extended the series expansions for lattice animals and percolation on the triangular lattice, and obtained Monte Carlo cluster counts on the triangular lattice for much larger system sizes than hitherto studied. Analysis of our new results (and other recent enumeration data) reveals more precise estimates of the correction-to-scaling exponents for lattice animals and percolation. Moreover, the correction-to-scaling function $f_1(z)$ has been calculated for the first time for any second-order phase transition.

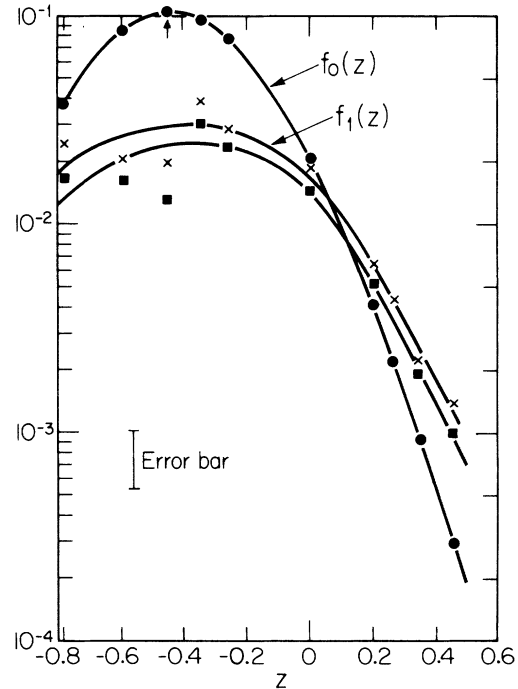


FIG. 3. Scaling function $f_0(z)$ and correction-to-scaling function $-f_1(z)$ obtained by Monte Carlo simulation on the triangular lattice normalized by 1.4. Two different trial values of Ω_p were used in calculating $f_1(z)$, $\Omega_p = 0.6$ (\times), and $\Omega_p = 0.7$ ($+$); the function $f_0(z)$ was not visibly different for the two cases. Note that $f_1(z)$ is not monotonic and hence is not proportional to $f_0'(z)$.

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$$A_s^D = s^{-\theta} \lambda^s (1 + C_1 s^{-\Omega_A} + C_2 s^{-2\Omega_A} + C_3 s^{-3\Omega_A}) ,$$

which can be written in the compact form [see A. J. Guttmann, J.

Phys. A 15, 1987 (1982), and references therein]

$$A_s^D = s^{-\theta} \lambda^s \exp(D_1 s^{-\Omega_A} + D_2 s^{-2\Omega_A} + D_3 s^{-3\Omega_A}) .$$

We found $D_1 = -\frac{1}{8}$ and $D_3 = \frac{1}{200}$, while $D_2 = 0$. Our series analysis correctly predicts these exact results.

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¹⁸It is possible that (4) is not the true Ω_p , corresponding to an irrelevant operator, but rather the Aharony-Fisher correction proposed in Ref. 1. Applied to percolation, this suggests that one should already in the leading term replace $\epsilon = p_c - p$ by $(\epsilon + \epsilon^2 + 1/s + \dots)$, and replace $1/s$ by $(1/s + 1/s^2 + \epsilon/s + \dots)$. At $p = p_c$, one would have in (4) a correction $s^{\sigma-1}$ where $\sigma = 1/\beta\delta$ and $1 - \sigma = \frac{55}{91} = 0.604$, a number compatible with the Monte Carlo estimate (4). This would explain why all numerical estimates (Refs. 4, 16, and 17) are lower than the conjecture $\Omega_p = \frac{96}{91}$ [B. Nienhuis, J. Phys. A 15, 199 (1982)].

¹⁹For fixed cluster size s , the function $n_s(p)$ has a maximum at some $p_{\max}(s)$ which occurs within the scaling region $|p_c - p| \sim s^{-\sigma}$. Our Monte Carlo analysis for $L = 35\,000$ and $70\,000$ gives $\Omega_p \approx 0.8$, slightly higher than at p_c .

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