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Cluster Shape and Critical Exponents near Percolation Threshold*

P. L. Leath

Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, and Physics Department, Rutgers University, New Brunswick, New Jersey 08903†

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The shape of the large, random clusters, occurring near percolation threshold c_0, is shown to be such that the mean cluster boundary-to-bulk ratio $\langle b\rangle/\langle n\rangle$ gives c_0. A Monte Carlo calculation yields that the cluster size distribution is proportional to a Gaussian in b/n which is independent of concentration and narrows to a δ function as $n\to\infty$; the asymptotic behavior gives c_0 and the critical exponents.

In recent years, we have seen an evolution in the understanding of a remarkable new regularity of nature in the universality of critical indices.[1] The renormalization group has been developed to calculate these universal exponents.[2] But, surely the underlying source of this universal behavior is a limit theorem on the probability distribution of the fluctuations that occur near critical points. In the results presented here, I report a new form for the probability $P(n,b)$ of finding, for large n, a fluctuation extending over n lattice sites and bounded by b sites. This probability distribution is indicative of a new kind of limiting behavior. For simplicity, we consider here the site-percolation problem on a simple square lattice, where each site is randomly occupied (or not) with a probability c (or $1-c$) which is independent of the occupation of other sites. The common characteristic of the so-called "percolation problems" in nature is the direct relation between the various physical properties and the moments of the cluster size distribution, a relation which allows one to calculate the singular behavior of those physical properties by studying the cluster size distribution.[3]

An exact, general expression for the probability $P(n,b)$ of a nonnull cluster of n occupied sites isolated from the rest of the lattice by a boundary of b vacant sites was given by Fisher and Essam[4] in 1961, namely,

$$P(n,b)=M(n,b)c^{n-1}(1-c)^b, \tag{1}$$

where $M(n,b)$ is the number of distinct clusters of size n and boundary b that can be drawn from a single origin. For $c<c_0$, where no infinite cluster exists, this probability is normalized, i.e., $-\sum_{n,b}P(n,b)=1$. Thus multiplying Eq. (1) by c, summing over all n and b, and then differentiating with respect to c, we obtain the identity

$$1=\langle n\rangle-[c/(1-c)]\langle b\rangle \text{ for } c<c_0. \tag{2}$$

As the concentration c approaches the critical concentration c_0, the mean cluster size $\langle n\rangle =\sum_{n,b}nP(n,b)\sim A(c_0-c)^{-\gamma}$ diverges with critical exponent γ. When $\langle n\rangle$ diverges, we see from Eq. (2) that the mean boundary size $\langle b\rangle$ must also diverge with the same exponent γ. Thus, we find that the shape of the large clusters is governed by

$$\langle b\rangle\to\alpha_0\langle n\rangle \tag{3}$$

as c approaches c_0, where α_0 is related to the critical concentration by

$$c_0=(1+\alpha_0)^{-1}. \tag{4}$$

Thus, the critical concentration may simply be obtained from the limiting behavior of the mean boundary-to-bulk ratio $\langle b\rangle/\langle n\rangle$. These results are true on any lattice.

In order to study the behavior of the cluster size distribution for large n, I performed a Monte Carlo calculation of $P(n,b)$ by assigning random occupation to sites on a square lattice and keeping the statistics on the number of sites n and the number of boundary sites b in each randomly generated cluster. Instead of studying all the clusters in a finite segment of the lattice, I generated and studied only one cluster at a time. By this means I obtained statistics on about 100 000 clusters at $c=0.50$ and about 24 000 clusters at $c=0.55$. More details of this calculation will be presented in a forthcoming publication.[5] The results of the Monte Carlo calculation satisfy Eqs. (1) and (2) and, for large n, are fitted by the following empirical formula quite well:

$$P(n,\alpha)=Kn^{-\chi}(c/c_\alpha)^{n-1}\times[(1-c)/(1-c_\alpha)]^{\alpha n}m(n,\alpha), \tag{5}$$

where $\alpha=b/n$, $c_\alpha=(1+\alpha)^{-1}$, K and χ are constants, and $m(n,\alpha)$ is the normalized Gaussian

$$m(n,\alpha)=(2\pi)^{-1/2}\sigma(n)^{-1}\times\exp\{-[\alpha-\mu(n)]^2/2\sigma^2(n)\}, \tag{6}$$

with the mean $\mu(n)$ and standard deviation $\sigma(n)$ of $m(n,\alpha)$ given by

$$\mu(n)=\alpha_0+A/n^\psi \tag{7a}$$

and

$$\sigma(n)=B/n^\varphi, \tag{7b}$$

where α_0, A, ψ, B, and φ are constants. This result was obtained as follows. First, the factor $Kn^{-\chi}(c/c_\alpha)^{n-1}[(1-c)/(1-c_\alpha)]^{\alpha n}$ was guessed from the exact solution for the Bethe lattice (or Cayley tree) which can easily be obtained from Eq. (1) and the results in Ref. 1. Then I used Eq. (5) as a definition of the then unknown, but normalized $m(n,\alpha)$. As a first check of this guess, I numerically evaluated $I(n)=\sum_{b/n}Kn^{-\chi}m(n,b/n)=Kn^{-\chi}$ to see whether it was indeed independent of the concentration c. This was accomplished by weighting the contribution of each cluster to $I(n)$ by the factor $\{(c/c_\alpha)^{n-1}[(1-c)/(1-c_\alpha)]^{\alpha n}\}^{-1}$. The histogram (of bin width $\Delta n=10$) of the numerical results obtained for $I(n)$ is shown in Fig. 1 for independent runs at the two concentrations $c=0.50$ and $c=0.55$. The best least-squares fit of $I(n)$ by the form $Kn^{-\chi}$, for n in the range $75<n<905$, gives $\chi=0.97\pm0.007$ and $K=0.257\pm0.01$,

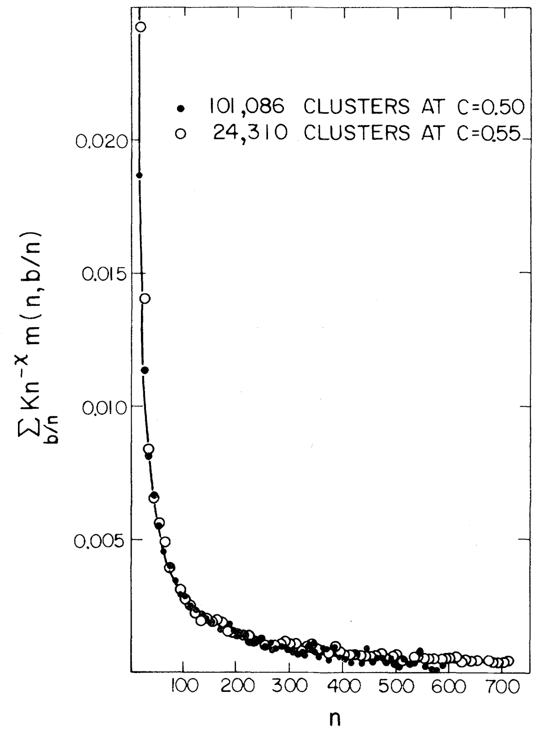

FIG. 1. The integrated, weighted probability $\sum_b P(n,b)\times\{(c_\alpha/c)\,[(1-c_\alpha)/(1-c)]^\alpha\}^n$ versus n.

where the errors are statistical. That this result is independent of concentration (as long as there are reasonable statistics in each histogram bin) is a check on the validity of Eq. (1).

I then explicitly calculated m with the results shown in Fig. 2, where $m(n,b/n)$ is plotted versus b/n for clusters of size $n=105$ and 205, respectively. The histograms of the data shown in Fig. 2 are of bin widths $\Delta n=10$, and $\Delta(b/n)=0.01$; the statistical errors in the data are indicated at a few selected points. The smooth curves are the results of a least-squares fit of the data by Gaussian forms with variable standard deviations and means. That the data is indeed Gaussian can be seen in Fig. 3 where the integral $\int_{-\infty}^{b/n}m(n,\alpha)\,d\alpha$ of the data in Fig. 2 is replotted versus b/n for $n=105$, on an arithmetic probability (or "Gaussian") scale. The straightness of the data plot indicates the degree of Gaussian character. Thus, Eq. (6) is verified. The n dependence of the mean $\mu(n)$ and standard deviation $\sigma(n)$ are then easily deduced by fitting $\mu(n)$ and $\sigma(n)$ by the forms given in Eq. (7), either by a logarithmic plot or by a least-squares fit by Eq. (7). The results are as follows: For the mean position $\alpha_0=0.704\pm0.04$, $A=2.53\pm0.5$, and $\psi=0.512\pm0.09$, and for

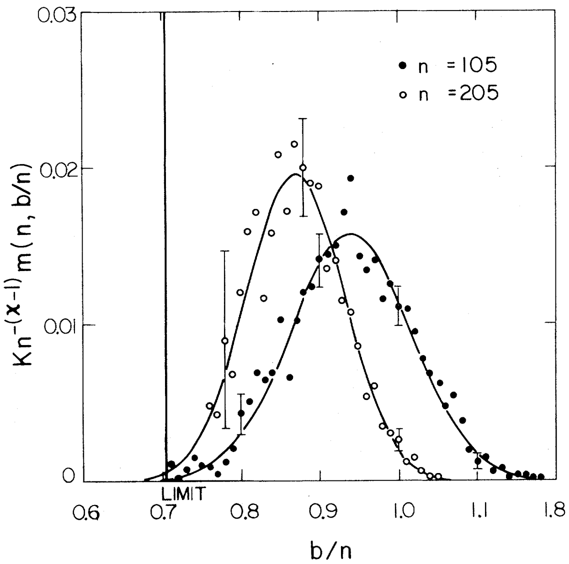

FIG. 2. The form of $m(n, b/n)$ versus b/n. The data points are the results of the Monte Carlo calculations at $c=0.50$ for histogram bins centered at $n=105$ and 205. The vertical line at $b/n=0.704$ represents the limiting δ function, extrapolated from the data as $n\to\infty$, and the smooth curves are Gaussians fitted to the data.

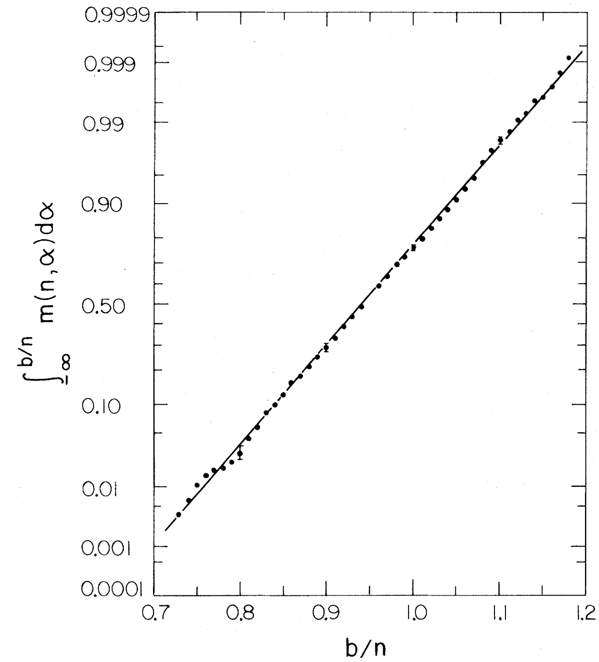

FIG. 3. An arithmetic probability plot of $\int_{-\infty}^{b/n} m(n,\alpha) \times d\alpha$ versus α, for the $n=105$ data of Fig. 2. If this function were $\mathrm{erf}(b/n)$, the plot would be a straight line.

the standard deviation $B=0.250\pm0.096$ and $\varphi=0.40\pm0.04$. Details of this fit to the data will be presented in a forthcoming publication.[5]

In order to understand the predictions of this empirical formula for the values of the critical exponents,[3] we find the most singular part of the Lth moment $\langle n^L\rangle$ of the cluster size distribution, namely $\int_0^\infty dn\, n^L \int_{-\infty}^{\infty} d\alpha\, P(n,\alpha)$. Using Eqs. (5)–(7), the α integral can be evaluated by the method of steepest descents to obtain the asymptotic form for large n. In this integral we keep only the largest powers of n (assuming $\varphi<\frac{1}{2}$ so that terms in $n^{2\varphi}$ are neglected when added to terms linear in n), and finally, we keep only the lowest-order terms in $x=c_0-c$. The resulting n integral can be done analytically, with the following resulting singular behavior,

$$\langle n^L\rangle \propto x^{-(L+\varphi+1/2-\chi)/\varphi} \text{ for } x\ll 1. \quad (8)$$

Since the $L=0$ moment gives β and the $L=1$ moment gives γ, we set

$$(\chi-\varphi-\tfrac{1}{2})/\varphi=\beta, \quad (9a)$$

and

$$\varphi^{-1}=\beta+\gamma. \quad (9b)$$

Then, since $L=-1$ gives the singular part of the free energy per site which has critical exponent $(2-\alpha)$, we find that the empirical result here yields the scaling law $\alpha+2\beta+\gamma=2$, which is reassuring. The numerical values for γ, β, and α obtained using Eqs. (9) are $\gamma=2.34\pm0.3$, $\beta=0.19\pm0.16$, and $\alpha=-0.72\pm0.4$, which are consistent with the previously obtained values, although the statistical errors are rather large here. The previously obtained values of the critical exponents in two dimensions include, from Harris *et al.*,[6] the series-expansion result $\alpha=-0.7\pm0.2$, $\beta=0.148\pm0.004$, and $\gamma=1.85\pm0.2$, and the Monte Carlo result $\beta=0.14\pm0.02$ and $\gamma=1.9\pm0.2$; the result, obtained from an analysis by Harris *et al.*[6] of a previous Monte Carlo calculation of Dean and Bird,[7] $\beta=0.16\pm0.02$ and $\gamma=2.1\pm0.2$; and the result of two separate series-expansion calculations[8] $\beta=0.14\pm0.03$ and $\gamma=2.1\pm0.2$. The exponent $\varphi^{-1}=\beta+\gamma=\Delta$ interestingly gives some new physical meaning to the gap exponent Δ.

The mean-field exponents $\beta=\gamma=1$ are recovered as $\chi\to\frac{3}{2}$ and $\varphi\to\frac{1}{2}$ in Eqs. (9); just at $\varphi=\frac{1}{2}$, it should be noted, there enter other corrections which were neglected above since terms in $n^{2\varphi}$ were neglected for large n, when compared to terms linear in n. That the standard deviation shrinks as $n^{-1/2}$ is the usual central limit behavior. In this case, the nonclassical exponents arise from this new limiting behavior. Details of these and other properties found for the large clusters near percolation threshold are planned to be published shortly.[5]

Finally, Kasteleyn and Fortuin[9] have derived the analogy between the percolation problem and a particular limit of a system exhibiting a thermodynamic phase transition (the one-component Potts model). Thus, it is possible that a limiting behavior, similar to that reported here, but in the surface-to-volume ratios of fluctuations near thermodynamic critical points may generally be a primary factor in thermodynamic critical behavior.

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†Permanent address.

[1]M. E. Fisher, Rev. Mod. Phys. 46, 597 (1974).

[2]K. G. Wilson and J. Kogut, Phys. Rep. 12C, 75 (1974).

[3]A. G. Dunn, J. W. Essam, and J. M. Loveluck, J. Phys. C 8, 743 (1975).

[4]M. E. Fisher and J. W. Essam, J. Math. Phys. (N.Y.) 2, 609 (1961).

[5]P. L. Leath, to be published.

[6]A. B. Harris, T. C. Lubensky, W. K. Holcomb, and C. Dasgupta, Phys. Rev. Lett. 35, 327 (1975).

[7]P. Dean and N. F. Bird, National Physical Laboratory Report No. Ma 61, 1966 (unpublished), and Proc. Cambridge Philos. Soc. 63, 477 (1967).

[8]M. F. Sykes, J. L. Martin, and J. W. Essam, J. Phys. A 6, 1306 (1973); M. F. Sykes, M. Glen, and D. S. Gaunt, J. Phys. A 7, L105 (1974).

[9]P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn., Suppl. 26, 11 (1969); C. M. Fortuin and P. W. Kasteleyn, Physica (Utrecht) 57, 536 (1972).

New Upper Bound on Total Cross Section at High Energy

Hiroyuki Yokomi
Department of Applied Mathematics, Faculty of Engineering Science, Osaka University, Toyonaka, Osaka 560, Japan
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The Froissart-Martin bound on the total cross section is improved by taking into account the multiplicity distribution of secondary particles, in addition to the unitarity, analyticity, and polynomial boundedness of the scattering amplitude in the Martin ellipse.

Since Froissart[1] found an upper bound on the total cross section (σ_t) at high energies, much effort to improve it has been made.[2,3] At present the Froissart-Martin bound is represented as[4]

$$\sigma_t < (4\pi/t_0)\ln^2(s/s_0), \tag{1}$$

where s is the square of the c.m. energy, t_0 is the square of the mass of the lowest energy state which couples to the t channel, and s_0 is some unknown scale factor. A proof has been made under considerably weaker assumptions than the original ones: the unitarity condition, analyticity, and polynomial boundedness of the scattering amplitude in the Martin ellipse.[5] Conversely, Kinoshita[6] and Martin[3] have shown that it is not possible to improve the energy dependence of the bound under the same assumptions. The possibility of improvement, however, has been discussed by Khuri[7] in terms of the location of zeros of a multiparticle generating function constructed from σ_n, where σ_n is the cross section for n-particle production.

In this note I show that the multiplicity distribution of secondary particles is indeed important for the bound of σ_t. Namely, I improve the Froissart-Martin bound such that

$$\sigma_t < \frac{4\pi}{t_0}\left[1+\left(\frac{\langle n\rangle}{D}\right)^2\left(1-\frac{2}{\langle n\rangle}\right)^2\right]^{-1}\ln^2\left(\frac{s}{s_0}\right), \tag{2}$$

where $\langle n\rangle$ and D^2 are the mean value and dispersion ($D^2=\langle n^2\rangle-\langle n\rangle^2$) of the multiplicity distribution, respectively.

The proof of (2) is as follows: From the defining formulas of σ_t, $\langle n\rangle$, and $\langle n^2\rangle$,

$$\sigma_t-\sigma_2=\sum_{n\geq 3}\sigma_n,$$

$$\langle n\rangle\sigma_t-2\sigma_2=\sum_{n\geq 3}n\sigma_n,$$

$$\langle n^2\rangle\sigma_t-4\sigma_2=\sum_{n\geq 3}n^2\sigma_n,$$