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Collapse of Percolation Clusters—A Transfer Matrix Study

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Exact calculations using transfer matrices on finite strips are performed to study the two-dimensional problem of site percolation clusters with an attractive nearest neighbor interaction. Thermodynamic quantities such as free energy per site and specific heat are calculated. Finite-size scaling with two strips of different widths yields very accurate approximations of the critical line and the correlation length exponent. The result shows clearly a site percolation fixed point at very high temperatures, a random animal fixed point at intermediate temperatures, a Θ point for the collapse of lattice animals at lower temperatures, and a compact-cluster fixed point at the lowest temperatures.

KEY WORDS: Percolation; lattice animals; Θ point; tricritical point; transfer matrix.

1. INTRODUCTION

Recently there has been interest in the collapse of branched and linear polymers.[1-5] Due to attractive forces induced by interactions with the solvents, polymers can undergo a collapse transition at low temperatures. The corresponding tricritical point Θ had been studied for a long time. For further references, see ref. 1. Derrida and Herrmann[1] calculated the collapse of branched polymers in two dimensions using the transfer matrix on finite strips. They found the thermal correlation length exponent $\nu_1 \approx 0.5095$ and the crossover exponent $\phi = 0.657$. Coniglio[6] formulated the problem of branched polymers in a solvent into a Q-state Potts model. Using the Migdal–Kadanoff renormalization group, he found for $Q = 1$, which should correspond to percolation, the following four fixed points: a

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percolation fixed point, a random animal fixed point, a tricritical Θ point, and a compact-cluster fixed point. At the Θ point he found $\nu_1 \approx 0.51$, in agreement with ref. 1, but a much smaller value for ϕ.

The calculation presented here is an independent check of Coniglio's calculation. The method is a straightforward generalization of the transfer matrix calculation of ref. 1 and therefore the exposition also follows closely that reference.

Rather than introducing attractive interactions into lattice animals as was done in ref. 1, I introduce it into the percolation clusters by the following generating function:

$$G(p, T) \equiv \sum_{N,t,B} A_{N,t}(B)\, p^N q^t [y(T)]^B \tag{1}$$

where $A_{N,t}(B)$ is the number of animals with N sites, t perimeter sites, and B bonds, $y(T)$ is related to the temperature T by

$$y(T) = \exp(1/T) \tag{2}$$

p is the occupation probability for a site, and $q = 1 - p$. Here we consider a bond to exist between any two nearest-neighbor occupied sites of the animal.

If we define the partition function Z_N of a percolation cluster by

$$Z_N \equiv \sum_{t,B} A_{N,t}(B)\, q^t [y(T)]^B \tag{3}$$

then (1) can be rewritten as

$$G(p, T) = \sum_N Z_N p^N \tag{4}$$

From (4) we see that the critical line $\tilde{p}(T)$ is given by

$$\lim_{N \to \infty} \tilde{p}(T)(Z_N)^{1/N} = 1 \tag{5}$$

From (5) it follows that the free energy per site $f(T)$ defined as $Z_N = e^{-Nf(T)/T}$ is given by

$$f(T) = -TN^{-1} \log Z_N = T \log[\tilde{p}(T)] \tag{6}$$

A simple quantity wich contains the geometrical information is the correlation function $g_{0,R}(p, T)$ defined by

$$g_{0,R}(p, T) \equiv \sum_{N,t,B} p^N q^t [y(T)]^B\, \omega_{0,R}(N, t, B) \tag{7}$$

where $\omega_{0,R}(N, t, B)$ is the number of different configurations of an animal of N sites, t perimeter sites, and B bonds which connects the points 0 and R of the lattice. The additional condition of connectivity is the only difference between definitions (1) and (7). As in the case of usual percolation,[7] one can show that if $p < \tilde{p}(T)$, $g_{0,R}$ decreases with R exponentially. This defines a correlation length $\xi(p, T)$,

$$g_{0,R}(p, T) \sim \exp[-|R|/\xi(p, T)] \qquad \text{for large } R \tag{8}$$

One can show that $\xi(p, T)$ diverges when $p \to \tilde{p}(T)$ in the manner

$$\xi^{-1}(p, T) \sim |\tilde{p}(T) - p|^{\nu} \tag{9}$$

with an exponent ν.

I shall use strip geometries to do the calculation. For such geometries, the lattice is infinite in only one direction. In the next section I shall explain the transfer matrix technique for this problem.

2. TRANSFER MATRIX FOR PERCOLATION CLUSTERS

We calculate exactly the correlation length $\xi_n(p, T)$ defined in (8) on an $n \times \infty$ strip by means of the transfer matrix. Following closely ref. 1, we have that the transfer matrix M gives the recurson relation between the $g_{0,R}(C)$, where C is a connectivity configuration of the sites of column R:

$$g_{0,R+1}(C) = \sum_{C'} M(C, C')\, g_{0,R}(C') \tag{10}$$

The size of the matrix can be strongly reduced by the use of symmetry operations. An example is given in the Appendix. As M does not depend on R, one can, once one has constructed M, calculate $g_{0,R}$ by iterating (10). If λ is the largest eigenvalues of M (λ is positive), each $g_{0,R}$ has the following behavior:

$$g_{0,R} \sim \lambda^{R} \qquad \text{for large } R \tag{11}$$

This means that for strips of width n, the correlation length $\xi_n(p, T)$ is given by

$$\xi_n(p, T) = -(\log \lambda)^{-1} \tag{12}$$

In this paper I will only consider normal strips on the square lattice, i.e., strips in the (1, 0) direction.

3. CALCULATION OF THERMODYNAMIC PROPERTIES ON STRIPS

From (6) we see that the free energy per site $f_n(T)$ of the cluster in the limit $N \to \infty$ is given by

$$f_n(T) = T \log[\tilde{p}_n(T)] \tag{13}$$

where $\tilde{p}_n(T)$ is the smallest positive value p for which

$$\lambda[\tilde{p}_n(T), T] = 1 \tag{14}$$

Therefore the energy e_n and the specific heat c_n are given by

$$\begin{aligned} e_n &= N^{-1} d \log Z_N / d(1/T) = d[f_n(T)/T]/d(1/T) \\ &= -T^2 d \log \tilde{p}_n(T)/dT = -T^2 \tilde{p}_n(T)^{-1} \, d\tilde{p}_n(T)/dT \end{aligned} \tag{15}$$

$$c_n = de_n/dT = -2T\tilde{p}_n^{-1} d\tilde{p}_n/dT + T^2 \tilde{p}_n^{-2} (d\tilde{p}_n/dT)^2 - T^2 \tilde{p}_n^{-1} d^2\tilde{p}_n/dT^2 \tag{16}$$

Equations (15) and (16) differ from Eq. (17) and (18) of ref. 1, which presumably are misprints. Figure 1 represents c_n as a function of temperature for several strip widths. The specific heat has a peak, which, as n increases, gets sharper and also increases in height. The position of the peak decreases monotonically with n and seems to approach a transition

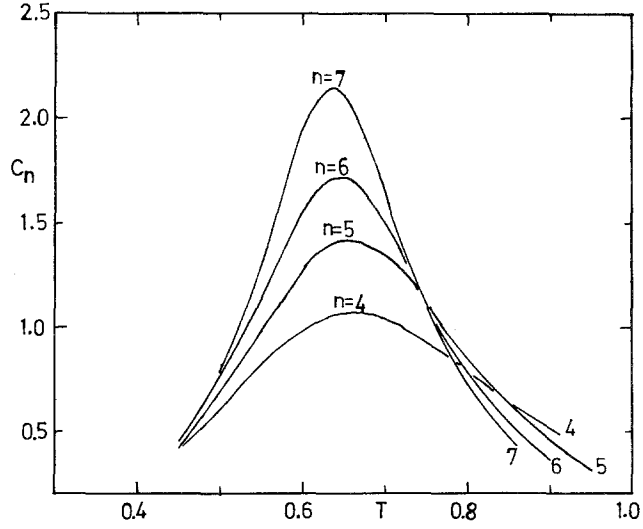

Fig. 1. Specific heat c_n against temperatire for different strip widths n.

temperature between 0.6 and 0.5. Comparing this figure with the corresponding Fig. 2 of ref. 1, one sees that for the same n, the height of the peak is lower here for percolation clusters, but the positions of the peaks are close to each other in the two cases.

4. TWO STRIP RENORMALIZATION, CRITICAL LINE

Let us make the usual assumption of the phenomenological renormalization that[8]

$$\xi_n(\tilde{p}(T), T)/n = \xi_m(\tilde{p}(T), T)/m \tag{17}$$

Applying (17) to two strips of width n and $n-1$ and fixed T, one obtains for each n the estimate for the critical line $\tilde{p}_c(T)$ shown in Fig. 2 and 3.

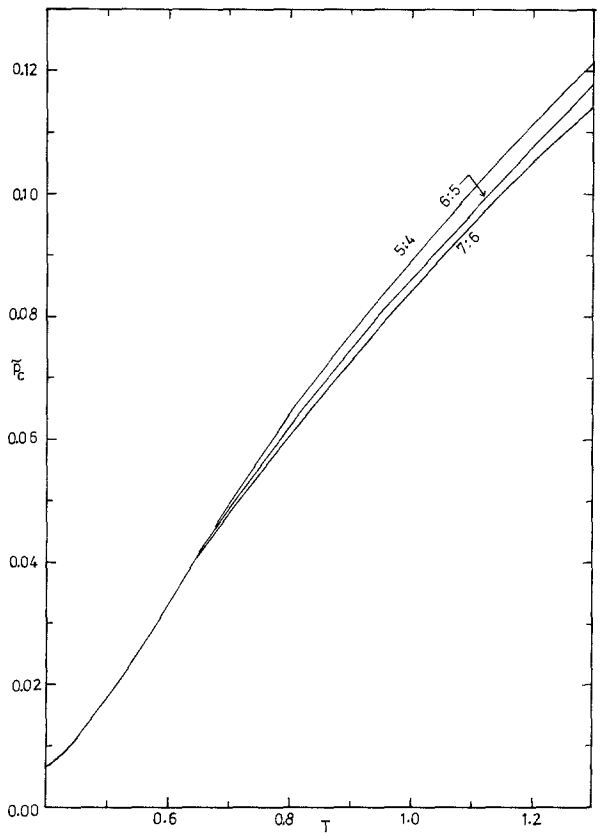

Fig. 2. Value of $\tilde{p}_c(T)$ at which the correlation length diverges against temperature obtained for an n to $n-1$ renormalization for different pairs of values n, $n-1$.

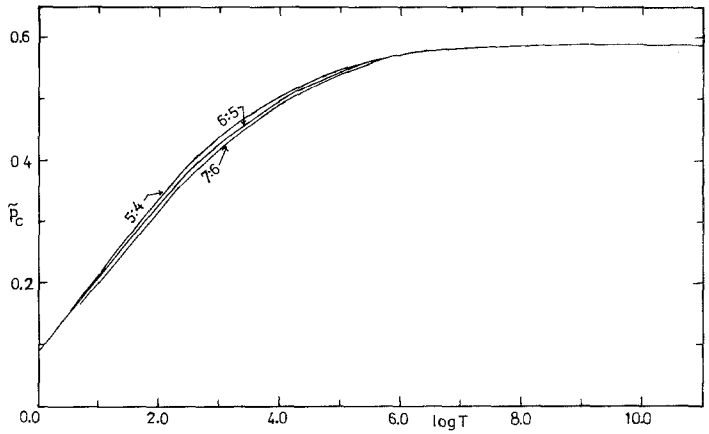

Fig. 3. Same as Fig. 2, but against log T, for large values of the temperature T.

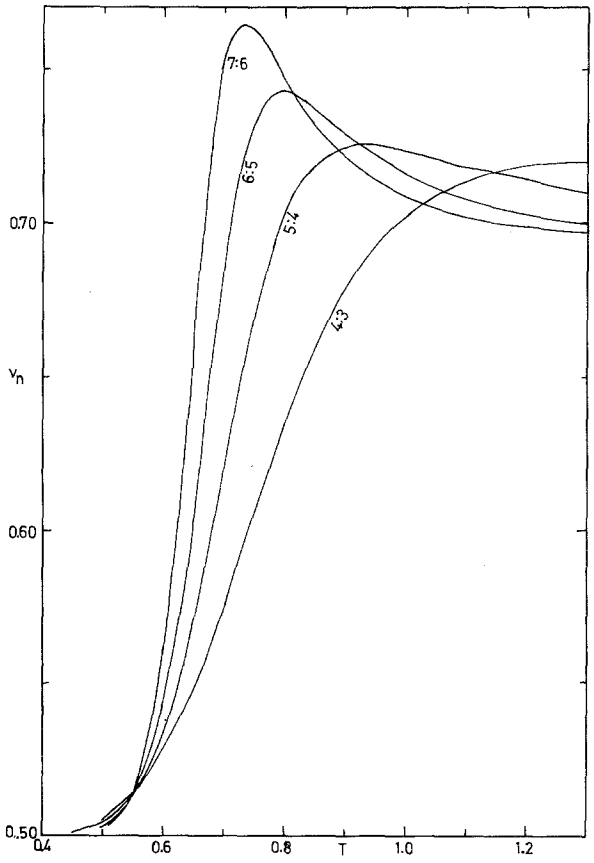

Fig. 4. Exponent ν of the correlation length against temperature obtained from an n to $n-1$ renormalization for different pairs of values n, $n-1$.

Figure 2 plots $\tilde{p}_c(T)$ vs. T for small T. Comparing this figure with the corresponding Fig. 6 of ref. 1, one sees that for small values of T our $\tilde{p}_c(T)$ is very close to the lattice animal critical line $\tilde{x}_c(T)$. But for very large values of T, $\tilde{p}_c(T)$ shown in Fig. 3 approaches the percolation value $\tilde{p}_c(\infty) = 0.59274$.[7]

With the two-strip renormalization one can also calculate the exponent ν by looking at the derivative λ' of the eigenvalue with respect to p,[7]

$$\nu_n^{-1} = 1 + \log[(\lambda_n'/\lambda_n)/(\lambda_{n-1}'/\lambda_{n-1})]/\log[n/(n-1)] \tag{18}$$

This ν is presented in Fig. 4 and 5. From Fig. 4 we see that at low temperatures one clearly obtains the exponent $1/d$, where d is the spatial dimension. From Fig. 5 we see that at very high temperatures, the percolation exponent $\nu \approx 0.135$[7] is asymptotically approached for large n. At about $T = 0.550$ there seems to be a point where all curves cross with a value of the exponent of about $\nu \approx 0.513$. These values are very close to the ones found for the collapse of branched polymers in ref. 1: $T \approx 0.535$ and $\nu \approx 0.512$. For T a little above this point the exponent increases sharply to a value which for $n = 7$ is about 0.77 and the tendency is toward even higher values for larger n. The strong change of ν around $T \approx 0.550$ indicates that this is the theta region. The estimate for the exponent ν_1 is taken to be the point where all curves cross, i.e., $\nu_1 \approx 0.513$. The estimate for ν_2 is taken to

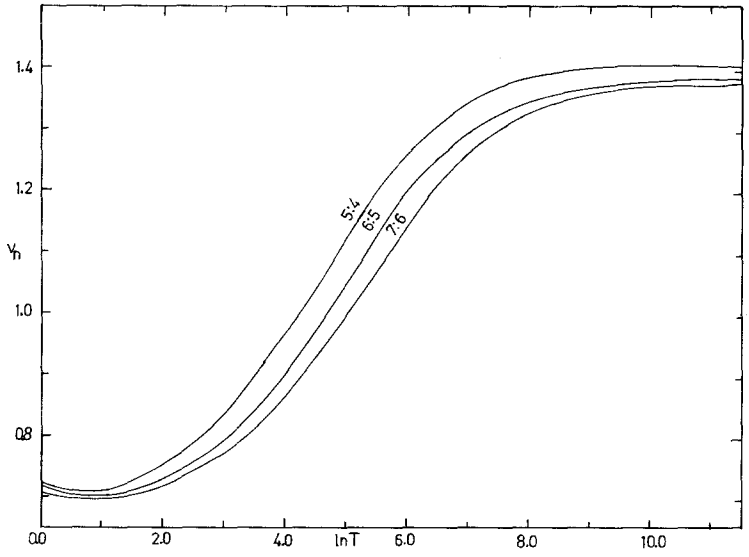

Fig. 5. Same as Fig. 4, but against log T, for large values of the temperature T.

be the peak value of ν, i.e., $\nu_2 \approx 0.77$ for $n = 7$. The crossover exponent is then given by $\phi = \nu_1/\nu_2 \approx 0.66$. Comparison of Fig. 4 with Fig. 7 of ref. 1, shows that they are very similar. We therefore conclude that the collapse of branched polymers and the collapse of percolation clusters are indeed the same.

From Fig. 5 we see that ν_n has a minimum at values of $\log T$ between 1.0 and 2.0. The value of ν_n at this minimum is about 0.7. With increasing n, this minimum tends to approach the lattice animal value $\nu \approx 0.64$[7] with $\log T \approx 1.5$. From Fig. 3 we see that at this value of T, $\tilde{p}_c(T) \approx 0.25$, which is the critical fugacity for lattice animals on the square lattice.[7] This value of ν corresponds to the exponent for random lattice animals. The present calculation therefore confirms the conclusions of Coniglio.[6]

5. CONCLUSION

The present transfer matrix calculation of site percolation clusters with attractive nearest neighbor interaction confirms the conclusions of a tricritical Potts model at $Q = 1$ using the Migdal–Kadanoff renormalization group. This shows that the tricritical Potts model at $Q = 1$ is in the same universality class as the collapse of branched polymers at the Θ point. For the tricritical Potts model at $Q = 1$, Nienhuis[9] had conjectures, based on the Coulomb gas method, $\nu_1 = \phi = 8/15 = 0.533...$. This means that both the present calculation and that of ref. 1, which gives $\nu_1 \approx 0.5095$ and $\nu_2 \approx 0.657$, are significantly different from Nienhuis' conjecture.

APPENDIX

In this appendix I give as an example the transfer matrix for site percolation with attractive nearest neighbor interaction on a strip of width 4

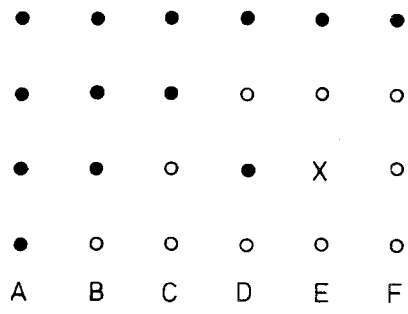

Fig. 6. The six different configurations that can occur in a strip of width $n = 4$. (●) Occupied and connected sites; (×) occupied and not connected sites; (○) empty sites.

with periodic boundary conditions. I follow the same method as in ref. 1. First I list all the possible configurations at column R (see Fig. 6). Due to the periodic boundary conditions, only six configurations remain. Then one relates the probabilities A_R, B_R, C_R, D_R, E_R, and F_R of these configurations at column R to their probabilities at column $R+1$:

$$A_{R+1} = p^4q^5[(y^3A_R + y^2B_R + yC_R + yD_R + yE_R + F_R)]$$

$$B_{R+1} = p^3qy^3[4y^2A_R + (y^2+3y)\,B_R + 2(y+1) \times C_R + 2(y+1)\,D_R + (2y+1)\,E_R + 3F_R]$$

$$C_{R+1} = p^2q^2y^2[4yA_R + 2(y+1)\,B_R + (y+2)\,C_R + 4D_R + 2E_R + 2F_R]$$

$$D_{R+1} = p^2q^2y^2(2A_R + B_R + D_R)$$

$$E_{R+1} = p^2q^2y(B_R + 2C_R + yE_R + F_R)$$

$$F_{R+1} = pq^3y(4A_R + 3B_R + 2C_R + 2D_R + E_R + F_R)$$

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