

## **Bond Percolation on a Finite Lattice: The One-State Potts Model Reconsidered**

**Joseph Rudnick<sup>1</sup> and George Gaspari<sup>1,2</sup>**

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Bond percolation on a finite lattice is studied by looking at the Kac mean field model. The investigation utilizes the one-state Potts model connection established by Kasteleyn and Fortuin. To deal with special problems associated with the finite extent of the system we re-cast the partition function, which allows us to investigate the percolation transition in detail. This fundamental new formulation clears up certain ambiguities present in previous treatments and indicates a possible new direction in the study of other replica-type models.

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**KEY WORDS:** Potts model; percolation; mean field theory; finite systems.

### **1. INTRODUCTION**

The problem of percolation has commanded the attention of physicists and applied mathematicians for decades.<sup>(1,2)</sup> This is for several reasons. First, percolation processes play an important role in a variety of physical phenomena, especially those relating to the behavior of random systems.<sup>(3)</sup> Further, it represents a problem in applied mathematics of some interest because of the intrinsic challenge it presents for the mathematician as well as its importance in the theory of graphs and statistics. A major advance in the theory of percolation occurred when Fortuin and Kasteleyn<sup>(4)</sup> pointed out a fundamental mathematical connection between a particular example of a percolating system called bond percolation and a set of statistical mechanical models known as The Potts models.<sup>(5)</sup> This identification strengthened the notion that a transition ought to occur in an infinite per-

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<sup>1</sup> Physics Department, University of California at Los Angeles, Los Angeles, California 90024.

<sup>2</sup> Permanent address: Physics Department, University of California at Santa Cruz, Santa Cruz, California 95064.

colating system in analogy with the phase transition that occurs in systems at finite temperatures.

In the case of the percolating system, the transition is from a system filled with finitely extended clusters of points, or sites, connected by "good" or "active" bonds to a system in which one of the clusters, the "spanning cluster," contains a finite fraction (in an infinite system) of all sites in it. This transition is sharp and nonanalytic. Furthermore, it has many of the hallmarks of a continuous, or critical, point transition in a thermodynamic system at finite temperature. Notably, one can identify critical exponents that describe the singular way in which quantities disappear or go to infinity as the transition is approached.

As in the case of phase transitions, the renormalization group<sup>(6)</sup> has proved to be a tool of considerable power in the analysis of non-analyticities in percolating systems. Real space methods have yielded useful approximations to percolation critical exponents whose reliability is, however, difficult to assess as a result of the uncontrolled approximations that such methods involve. Nevertheless, these methods retain considerable utility. Another approach, possessing the virtue of rigor, in principle at least, is the field theoretically based method that characteristically yields predictions in the form of interdimensional  $\varepsilon$  expansions,<sup>(7-9)</sup> the quantity  $\varepsilon$  being the difference between the spatial dimension of the system of interest and a special lower mean field dimension. The lower mean field dimension for the percolation transition is six, so that  $\varepsilon = 3$  in three dimensions and the value of the low-order expansions that are generated in this approach as the basis of quantitative predictions for critical exponents seems, at first sight, small. This renormalization group approach relies on The Potts model analogy.

The question of the quantitative validity of the  $\varepsilon$  expansion as applied to the percolation transition was addressed by Kirkpatrick in 1976,<sup>(10)</sup> when he performed a numerical experiment to obtain the properties of the percolation transition on large but finite lattices of various spatial dimensionalities. In particular, he looked at the transition in six, five, three, and two dimensions. What he found was intriguing. The  $\varepsilon$  expansion seemed to converge at a disappointingly slow rate close to six dimensionality, but it remained a remarkably good approximation in lower dimensionality. For example, the exponent  $\gamma$  as predicted by the  $\varepsilon$  expansion stayed within 20% of the value obtained numerically by Kirkpatrick.

Thus percolation is a pervasively occurring phenomenon presenting nontrivial theoretical challenges for which a rigorous and useful statistical mechanical analogy exists. The results of calculations based on this analogy which can and have been compared with the results of computer simulations are remarkably accurate.

In this paper, we report the results of the first steps in a project to extend the field theoretical approach to the study of finite percolating systems. This is with an eye to making a more nearly complete connection between the results of the  $\varepsilon$  expansion and those of numerical simulations. Our long-term goal is to develop a theory that allows for the use of finite-size scaling in the analysis of the computer-generated data. Ultimately, we hope to be able to produce curves for the behavior of finite percolating systems that incorporate both the power law behavior that one expects to see in a large but finite system near, but not too close to, a phase transition, and also accurately depict the rounding that occurs asymptotically close to the transition. In other words, we are working toward the production of full crossover curves for the properties of finite percolating systems.

What we report here is the exact results of a finite-size model calculation which are significant first steps toward understanding finite size percolating systems. We have obtained results for the behavior near the percolation transition of key quantities in the mean field, or Kac model of percolation.<sup>(11)</sup> The infinite lattice problem has been investigated in considerable detail by Erdős and Rényi<sup>(12)</sup> and Wu.<sup>(13)</sup> We supplement their results by considering the behavior of this system asymptotically close to the transition, exploiting the Potts model analogy. In the process, we resolve some long-standing puzzles concerning certain mathematical quirks and apparent pathologies of the one-state Potts model, shown by Kasteleyn and Fortuin to have the same properties as the bond percolating system. Thus, our results are of intrinsic interest quite aside from their ultimate utility in a more physically motivated finite-size calculation.

Moreover, our results and methods may well possess virtues that transcend their application to the study of finite percolating systems, as interesting as that subject is. The one-state Potts model belongs to a class of statistical mechanical models that are used in the study of random systems and are known generically as “replica” models. They are themselves only meaningful, in that they yield physically meaningful results, after certain limits have been taken. The connection between the results obtained through this limiting process and the physics of random systems can commonly be rigorously established, but there are often no clear guidelines for the implementation of the limiting procedure in actual calculations. Thus, one has to take a limit of the form  $n \rightarrow 1$ , where  $n$  is the number of states in the Potts model, continuously while, during some of the stages of a calculation at least, the quantity in question can only be allowed to take on integer values. The question as to whether one has lost certain crucial pieces of information regarding the behavior of the system when  $n$  is noninteger lingers, casting doubt on the validity of the calculation, even when no pathology emerges. Another difficulty that arises

with distressing frequency in calculations on replicated systems is that it is unclear how the limit  $n \rightarrow 1$  is to be taken. Often one is faced with more than one way of doing it and has to make a choice based on arguments of dubious physical merit. Thus, while replica methods provide theoreticians with a potentially powerful tool for the study of random systems, these models are commonly fraught with mathematical ambiguities that cast doubt on the validity of even the most apparently benign results.

What we do in the work reported here that sets it apart from previously published investigations on the one-state Potts model is take the limit  $n \rightarrow 1$  almost immediately in our calculations.<sup>(13,14)</sup> The limit is, in fact taken sufficiently early on that there are no ambiguities concerning how it is done and allows the correctness of other limiting procedures to be critically examined. This stratagem also facilitates our study of the model when  $N$ , the number of sites, is large, but *not infinite*. We are able to make precise predictions concerning the behavior of the large, finite Potts model in the mean field limit, while all previous calculations have only been able to accomplish this for infinite systems.

In Section 2 the model is presented and formal exact expressions are derived for the partition function of the one-state Potts model for a system of finite size. Correspondence with the generating function for the appropriate bond percolation problem is also established. The general results are developed in this section. The effects of finite size are given in Section 3. Conclusions are drawn in Section 4. Some of the more intricate mathematical detail is developed in the appendixes.

## 2. THEORY OF THE ONE-STATE POTTS MODEL FOR A FINITE SIZE SYSTEM

The effective Hamiltonian for the mean field Potts system is of the form

$$\beta H = -\frac{J}{2N} \sum_{\substack{jk \\ j \neq k}} \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_k + \sum_j \mathbf{h} \cdot \boldsymbol{\sigma}_j \quad (1)$$

where  $\beta$  is the inverse temperature,  $1/kT$ , and the quantity  $\boldsymbol{\sigma}_j$  is an  $n$ -dimensional vector occupying the  $j$ th site of a lattice; this degree of freedom is constrained to point along one of the principal directions of the  $n$ -dimensional vector space in which it is embedded. Notice that every  $\boldsymbol{\sigma}_j$  is coupled to every other  $\boldsymbol{\sigma}_j$ . The factor of  $1/N$  that multiplies the bilinear term keeps the energy properly extensive, i.e., the interaction energy scales linearly with  $N$ . The second term on the right-hand side of (1) represents a linear coupling of  $\boldsymbol{\sigma}$  with a uniform external symmetry-breaking field,  $\mathbf{h}$ . The

characteristic of the system under study that allows exact calculations is the long range of the interaction between the degrees of freedom. Because the interaction couples every  $\sigma_j$  with every other  $\sigma_j$ , one can imagine each degree of freedom seeing an average  $\sigma$  that contributes to a site-independent effective field,  $h_{\text{eff}}$ . In the infinite system, one characteristically replaces

$$\sum_j \sigma_j$$

by

$$N\langle \sigma \rangle$$

where the brackets denote the thermal average. However, in the finite system one must keep careful track of the differences between the two expressions. It is just this difference that gives rise to finite-size effects.

As in all problems in equilibrium statistical mechanics, the central goal here is the evaluation of the partition function,

$$Z_n = \sum_{\{\sigma\}} e^{-\beta H} \tag{2}$$

where the summation is over all configurations of the  $\sigma_j$ 's. Simple counting tells us that in a lattice with  $N$  sites there are  $n^N$  such configurations. The limit  $n \rightarrow 1$  is thus trivial, for in that limit there is only *one* configuration for the system to take. However, one interesting and nontrivial limit is

$$F = \frac{1}{Z_1} \lim_{n \rightarrow 1} \left( \frac{Z_n - Z_1}{n - 1} \right) = \left( \frac{\partial}{\partial n} \ln Z_n \right)_{n=1} \tag{3}$$

where

$$Z_1 = e^{NJ/2 - Nh} \tag{4}$$

is the partition function corresponding to a single-state system which has all the  $\sigma_j$ 's aligned in the direction of  $h$ , which in turn points along one of the principal axes of the embedding space of the  $\sigma_j$ 's.

Fortuin and Kasteleyn<sup>(4)</sup> have established the following relation for the quantity  $F$ , and the generating function for the percolation problem:

$$F = \left( \sum n_m^c e^{+mh} \right) \tag{5}$$

where  $n_m^c$  is the average number of clusters containing  $m$  sites. Taking derivatives of  $F$  with respect to  $h$ , the magnitude of  $h$ , we obtain successive

moments of the cluster size distribution. These quantities are among those that behave in a singular manner at the percolation transition.<sup>(13,15)</sup>

The evaluation of the partition function is achieved by first noting that the first term on the right of (1) can be written as follows:

$$-\frac{J}{2N} \left| \sum_j \sigma_j \right|^2 + \frac{J}{2N} \sum_j |\sigma_j|^2 \quad (6)$$

so that the contribution of the bilinear term in the effective Hamiltonian to  $e^{-\beta H}$  can be rewritten

$$e^{-J/2} \left( \frac{N}{2\pi J} \right)^{n/2} \int \cdots \int e^{(\mathbf{y} - \mathbf{h}) \cdot \boldsymbol{\sigma} - (N/2J) \mathbf{y} \cdot \mathbf{y}} d\mathbf{y} \quad (7)$$

where the  $n$ -dimensional vector  $\mathbf{y}$  is integrated over all space. The term  $\boldsymbol{\sigma}$  in the exponent is shorthand for  $\sum_j \sigma_j$ . This representation of the bilinear term in the Boltzmann factor is the first step in the Hubbard–Stratonovitch transformation.<sup>(16)</sup> It has the immediate effect of decoupling the degrees of freedom from each other. They couple *indirectly* through the intermediate “field”  $\mathbf{y}$ . The constant term  $e^{-J/2}$  will henceforth be dropped since it plays no role in the subsequent development.

The next step in evaluating the partition function,  $Z_n$ , is to sum eq. (7) over the configurations of the  $\sigma_j$ 's. Because the  $\sigma$ 's are now decoupled those sums can be performed independently. The term to be summed over the configuration of a single  $\sigma_j$  is

$$\exp(\boldsymbol{\sigma}_j \cdot \mathbf{y} - \sigma_j \cdot \mathbf{h}) \quad (8)$$

Summing (8) over the  $n$  possibilities for the direction of each of the unit vectors  $\boldsymbol{\sigma}_j$  we obtain for our partition function

$$Z_n = \left( \frac{N}{2\pi J} \right)^{n/2} \int \cdots \int \left[ \exp \left( -\frac{N}{2J} \mathbf{y} \cdot \mathbf{y} \right) \right] (e^{(\mathbf{y}_1 - \mathbf{h}_1)} + \cdots + e^{(\mathbf{y}_n - \mathbf{h}_n)})^N d\mathbf{y} \quad (9)$$

Now, the term  $(e^{(\mathbf{y}_1 - \mathbf{h}_1)} + \cdots)^N$  in (9) is the coefficient of  $c^N/N!$  in the power series expansion in  $c$  of

$$\exp[c(e^{(\mathbf{y}_1 - \mathbf{h}_1)} + \cdots + e^{(\mathbf{y}_n - \mathbf{h}_n)})] \quad (10)$$

Thus the partition function is just the coefficient of  $c^N/N!$  in

$$\left( \frac{N}{2\pi J} \right)^{n/2} \int \cdots \int \exp \left[ -\frac{N}{2J} \mathbf{y} \cdot \mathbf{y} + c(e^{(\mathbf{y}_1 - \mathbf{h}_1)} + \cdots + e^{(\mathbf{y}_n - \mathbf{h}_n)}) \right] d\mathbf{y} \quad (11)$$

Expression (11) contains integrals that when taken over real  $y_i$ 's diverge for any finite  $N$  as long as  $\text{Re}(c) > 0$ . These integrals are to be understood formally as generating functions for a power series expansion in  $c$ , which can be extracted in principle from the *convergent* integrals over real  $y_i$  for  $\text{Re}(c) < 0$ . Alternatively, one can make the integrals converge when  $\text{Re}(c) > 0$  by deforming the integration contours as described in Appendixes A and B. These deformations do not affect the power series expansions, but do result in branch cuts terminating at the origin in the complex  $c$  plane. This analytic structure is discussed in the first two Appendixes. The discontinuity across a cut vanishes as  $c \rightarrow 0$  more rapidly than any positive power of  $c$ . The integrations over the various components of the vector  $y$  can now be carried out independently, resulting in the following expression for the partition function:

$$\left(\frac{N}{2\pi J}\right)^{n/2} \prod_{j=1}^n \left[ \int \exp\left(-\frac{N}{2J} y_j^2 + ce^{(y_j - h_j)}\right) dy_j \right] \tag{12}$$

If we imagine that  $h_1$  is nonzero and equal to  $h$ , while  $h_{j>1} = 0$ , the expression in (12) becomes

$$\begin{aligned} &\left(\frac{N}{2\pi J}\right)^{n/2} \left[ \int \exp\left(-\frac{N}{2J} y_1^2 + ce^{(y_1 - h)}\right) dy_1 \right] \\ &\times \left[ \int \exp\left(-\frac{N}{2J} y^2 + ce^y\right) dy \right]^{n-1} \end{aligned} \tag{13}$$

To obtain the proper limit for the connection with percolation, set  $n = 1 + \Delta$  in (13) and expand to first order in  $\Delta$ :

$$\left(\frac{N}{2\pi J}\right)^{1/2} \left[ 1 + \frac{\Delta}{2} \ln\left(\frac{N}{2\pi J}\right) + O(\Delta^2) \right] \sum (ce^{-h}) \left\{ 1 + \Delta \ln\left[\sum(c)\right] + O(\Delta^2) \right\} \tag{14}$$

where

$$\sum(c) = \int_{-\infty}^{\infty} \exp\left(-\frac{N}{2J} y^2 + ce^y\right) dy \tag{15}$$

The generating function for percolation (5) is the coefficient of  $c^N/N!$  in the contribution to (14) that is of first order in  $\Delta$ , except for the factor  $Z_i^{-1}$ , which need not concern us for now. The desired result is the coefficient of  $c^N/N!$  in

$$\left(\frac{N}{2\pi J}\right)^{1/2} \sum (ce^{-h}) \left\{ \frac{1}{2} \ln\left(\frac{N}{2\pi J}\right) + \ln\left(\sum(c)\right) \right\} \tag{16}$$

The task remaining is to extract the coefficient of  $c^N/N!$  in the power series expansion of  $\sum(ce^{-h}) \ln[\sum(c)]$ .

The coefficient of  $c^N/N!$  in  $\sum(ce^{-h})$  is just

$$\int_{-\infty}^{\infty} \exp\left[-\frac{N}{2J}y^2 + N(y-h)\right] dy = \left(\frac{N}{2\pi J}\right)^{1/2} \exp\left(\frac{NJ}{2} - Nh\right) \quad (17)$$

The more difficult task of obtaining the corresponding coefficient in  $\sum(ce^{-h}) \ln \sum(c)$  will be accomplished formally by multiplying  $\sum(ce^{-h}) \ln \sum(c)$  by  $N!/(2\pi ic^{N+1})$  and then performing an integral over complex  $c$  around a contour that encircles the origin. Since  $c=0$  is a branch point of  $\sum(c)$  we choose a contour with asymptotically small radius that starts just above the branch cut on the real  $c$  axis and ends, after encircling the origin counterclockwise, just below the branch cut. This contribution to the generating function then becomes

$$\frac{1}{2\pi i} \left(\frac{N}{2\pi J}\right)^{1/2} \int_C \frac{N!}{c^{N+1}} \left[ \int \exp\left(-\frac{N}{2J}y^2 + ce^{y-h}\right) dy \right] \ln \left[ \sum(c) \right] dc \quad (18)$$

where  $C$  denotes the contour described above. Combining this with equation (17) allows us to write a formal expression, which is exact, for the generating function of mean field percolation problem for  $N$  sites

$$F = \left(\frac{N}{2\pi J}\right)^{1/2} \left[ \exp\left(\frac{NJ}{2} - Nh\right) + \frac{N!}{2\pi i} \int_C \frac{1}{c^{N+1}} \sum(ce^{-h}) \ln \sum(c) dc \right] \quad (19)$$

Equation (16) and (19) contain important new results for the one-state Potts model which we now discuss. In order to proceed further, the contour integral must be evaluated. We begin by noting that the factor  $Ny^2/2J$  in the exponential in the integrand in (15) varies, for large  $N$ , very rapidly with  $y$ . This allows us to use the method of steepest descents under general circumstances in the evaluation of  $\sum(ce^{-h})$ . It is straightforward to verify that the use of this method yields essentially the same result for the coefficient of  $c^N/N!$  as was obtained in equation (17). Since  $\ln[\sum(c)]$  varies qualitatively less rapidly with  $c$  than  $\sum(ce^h)$ , we can write the integral (18) as a double integral over

$$\exp\left[-\frac{N}{2J}y^2 + ce^{y-h} - (N+1)\ln(c)\right] \ln \left[ \sum(c) \right] \quad (20)$$

Under the assumption that  $\ln[\sum(c)]$  varies relatively slowly with  $c$ , we



evaluate the double integral by looking for extrema in the exponential as a function of both  $y$  and  $c$ . The extremum equation for  $y$  is

$$\frac{N}{J} y + ce^{y-h} = 0 \quad (21)$$

and for  $c$ :

$$e^{y-h} - \frac{N+1}{c} = 0 \quad (22)$$

The solutions of these two equations are

$$y = J \quad (23)$$

and

$$c = (N+1) e^{-J+h} \quad (24)$$

Now we insert these solutions in the exponential. The exponent becomes

$$\begin{aligned} & -\frac{N}{2J} \cdot J^2 + (N+1) e^{-J+h} \cdot e^{J-h} - (N+1) \ln[(N+1) e^{-J+h}] \\ & = J \left( \frac{N}{2} + 1 \right) - (N+1) h - (N+1) \ln \left[ \frac{N+1}{e} \right] \end{aligned} \quad (25)$$

When exponentiated, this yields, at leading order in  $N$ ,  $1/N! \exp(-Nh + JN/2)$ . Our result for the contour integral is thus

$$\begin{aligned} & \exp \left( \frac{JN}{2} - Nh \right) \cdot \ln \sum [(N+1) e^{-J+h}] \\ & \simeq \exp \left( \frac{JN}{2} - Nh \right) \cdot \ln \sum [N e^{-J+h}] \end{aligned} \quad (26)$$

This result for the one-state Potts model partition function will be called the *replacement* result, because it follows from the replacement of  $c$  by  $Ne^{-J+h}$  in  $\ln[\sum(c)]$ . Proceeding with the evaluation, we are left with the integral

$$\ln \left[ \int \exp \left( -\frac{N}{2J} y^2 + Ne^{y-J+h} \right) dy \right] \quad (27)$$

With  $y = z + J$ , the integral becomes

$$\begin{aligned} & \ln \left\{ \int \exp \left[ -\frac{N}{2J} (z + J)^2 + Ne^{z+h} \right] dy \right\} \\ &= \ln \left\{ \int \exp \left[ -\frac{N}{2J} (z^2 + J^2) + N(e^{z+h} - z) \right] dy \right\} \end{aligned} \quad (28)$$

Using the method of steepest descent again, we arrive at the extremum equation

$$-\frac{z}{J} + (e^{z+h} - 1) = 0 \quad (29)$$

This, in the limit  $h = 0$ , is just the percolation equation for the  $N = \infty$  limit of the model we are investigating. The quantity  $J$  takes the role of the probability of a bond's being "good," or "active." Actually, for the case at hand that probability is  $J/N$ . The quantity  $z/J$  is the fraction of the sites contained in the spanning cluster. Note that when  $h = 0$  equation (29) has the positive solution  $z = 0$  when  $J < 1$  and a positive nonzero solution when  $J > 1$ . The appearance of this nonzero solution heralds the onset of percolation. The mean field theory of percolation on an infinite lattice has been treated at length elsewhere,<sup>(13)</sup> and we will not discuss it any further here. However, the steepest descent evaluation of the replacement formula for the generating function, equation (28), will be developed further in Appendix A in order to clarify and resolve certain ambiguities encountered in mean field infinite-lattice percolation theory.

### 3. FINITE-SIZE EFFECTS

The percolation transition on the infinite lattice is sharp and non-analytic, while on a finite lattice it will be rounded and without singularities. To look more closely at the latter transition, we have to improve on the replacement approximation. To that end, we look more closely at the problem of extracting the coefficient of  $c^N/N!$  in  $\sum (ce^{-h}) \ln[\sum(c)]$ .

For the moment, consider the problem for the function

$$\sum (ce^{-h}) \frac{P_i}{(c_i - c)} \quad (30)$$

The relevance of the following calculation to the problem at hand is easily demonstrated using the analytic properties of  $\sum(c)$ . Indeed, in Appendix B

it will be seen that  $\ln[\Sigma(c)]$  can be written as an appropriate integral of a function of the form

$$\int \frac{P(c')}{c' - c} dc'$$

where  $P(c') =$  discontinuity of  $\ln \Sigma(c')$  across the real axis. Knowing this, we proceed with the calculation. The sought after coefficient is just  $e^{-Nh}$  times the corresponding coefficient in

$$\Sigma(c) \frac{P_i}{(c_i - ce^h)} \tag{31}$$

We proceed as follows. First, note that the simple pole  $P_i/(c_i - ce^h)$  can be written

$$P_i \int_0^\infty e^{-(c_i - ce^h)t} dt \tag{32}$$

Thus, what is needed is the coefficient of  $c^N/N!$  in

$$P_i \iint \exp \left[ -\frac{N}{2J} y^2 + c(e^{y-h} + t) - c_i t \right] dy dt \tag{33}$$

which is

$$P_i \iint [e^{y-h} + t]^N \exp \left( -\frac{N}{2J} y^2 - c_i t \right) dy dt \tag{34}$$

The factor  $[e^{y-h} + t]^N$  can be expanded binomially. The double integral (34) becomes

$$P_i \iint \left( \sum_{j=0}^N \frac{N!}{j!(N-j)!} e^{j(y-h)} t^{(N-j)} \right) \cdot \exp \left( -\frac{N}{2J} y^2 - c_i t \right) dy dt \tag{35}$$

There are three cases to be distinguished: (1) the first few terms in the series dominate ( $j \ll N$ ), (2) the last few terms dominate  $J \approx N$ , and (3) terms in the middle of the expansion are the most important. It is straightforward to show that we are justified in neglecting all but the first few terms in (35) when  $c_i e^{y-h}$  is smaller than  $N$  or more precisely

$$\frac{N - c_i e^{(y-h)}}{\sqrt{N}} \ll 1 \tag{36}$$

The last few terms dominate when the inequality above is reversed. The third case applies when

$$\frac{N - c_i e^{(y-h)}}{\sqrt{N}} = O(1) \tag{37}$$

This latter case, when the middle terms are important, will be the case when we are near the phase transition and this is the case we now consider.

### 3.1. Importance of the Middle Terms

Set

$$c_i e^{(y-h)} = N + aN^{1/2} \tag{38}$$

Then the sum in (35) becomes

$$\begin{aligned} & \sum_{l=0}^N \frac{N!}{c_i^{N+1}} \cdot \frac{(N + aN^{1/2})^l}{l!} \\ &= \sum_{l=0}^N \frac{N!}{c_i^{N+1}} \cdot \frac{(N + aN^{1/2})^{-l}}{(N-l)!} \cdot [c_i e^{y-h}]^N \\ &\cong \sum_{l=0}^N \frac{1}{c_i} \cdot \exp[N(y-h) + N \ln N - N - (N-l) \ln(N-l) \\ &\quad + N - l - l \ln(N + aN^{1/2})] \\ &= \sum_{l=0}^N \frac{1}{c_i} \cdot \exp \left[ N(y-h) - \frac{l^2}{2N} - laN^{-1/2} + O\left(\frac{l^2}{N^3}\right) \right] \\ &\cong \frac{1}{c_i} \cdot \int_0^\infty \exp \left[ N(y-h) - \frac{l^2}{2N} - laN^{-1/2} - \frac{l^3}{6N^2} + l \frac{a^2}{2N} \right] dl \tag{39} \end{aligned}$$

Where Stirling’s formula was used to obtain the first approximate equality above. The result for (35) is thus the following double integral:

$$\begin{aligned} & \int_{\mathcal{R}} \left( \frac{P_i}{c_i} \cdot \int_0^\infty \exp \left( -\frac{l^2}{2N} - laN^{-1/2} - \frac{l^3}{6N^2} + l \frac{a^2}{2N} \right) dl \right. \\ & \quad \left. \times \exp \left[ N(y-h) - \frac{N}{2J} y^2 \right] \right) dy \tag{40} \end{aligned}$$

where the subscript  $\mathcal{R}$  on the  $y$  integration is to indicate that it is to be restricted to a region to be described in more detail later. Restrictions on the  $y$  integration also apply in cases (1) and (2).

It is a straightforward exercise to verify that in the limit  $|a| \gg 1$  the integral over 1 in (40) yields an expression appropriate to case (1) or (2).

We are almost in a position to extract the desired result. Our next task is to determine the singularity structure of  $\ln[\Sigma(c)]$ .

**3.2. Analytic Properties of  $\ln[\Sigma(c)]$**

In Appendix B, we saw that the function  $\Sigma(c)$  is analytic in the complex  $c$  plane except for a cut that starts at  $c=0$  and extends to  $c = \infty$  along the real  $c$  axis. The discontinuity across this cut is pure imaginary. In the limit of large  $N$  we may distinguish between two regions.

**3.2.1.**  $c < (N/J) e^{-1}$ . Here

$$\Sigma(c) \cong K_1 \exp\left(-\frac{N}{2J} y_1^2 + ce^{(y_1-h)}\right) \pm i \cdot K_2 \exp\left(-\frac{N}{2J} y_2^2 + ce^{(y_2-h)}\right) \quad (41)$$

where  $K_1$  and  $K_2$  are multiplicative constants associated with Gaussian integrations about the extremum points  $y_1$  and  $y_2$ . These two points are, respectively, the maximizing and minimizing solutions of the extremum equation (21) the plus sign applies above the cut and the minus sign below. The discontinuity in the log is thus  $e^{-O(N)}$ .

**3.2.2.**  $c > (N/J) e^{-1}$ . In this case the extremum equation has no real solutions. The real and imaginary parts of  $\Sigma(c)$  are of the same order of magnitude. When  $c - (N/J) e^{-1} = \delta$  we have, neglecting overall multiplicative factors,

$$\Sigma(c) \cong K \exp\left(-\frac{N}{2J} y_{\pm}^2 + ce^{(y_{\pm}^2-h)}\right) \quad (42)$$

where, as before,  $K$  is associated with the Gaussian integration about one of the *complex* extremum point  $y_{\pm}$ . The plus subscript refers to the extremum point with positive imaginary part and applies just above the cut. The minus subscript refers to its complex conjugate and applies just below. Here the discontinuity in the logarithm is  $O(1)$ .

We know that, given this analytic structure, we can reconstruct the function  $\ln[\Sigma(c)]$  by multiplying the discontinuity in the function at  $c'$  on the branch cut by  $1/(c - c')$  and integrating along the cut out to a contour that encloses the point  $c$ , and then around that contour, as discussed in Appendix B.

Our desired result is thus obtainable in the form of an integral over the real variable  $c_1$  in which  $P_i$  is the discontinuity of  $\log[\Sigma(c_1)]$ . To this, of course, we add the integral around the closing contour. In this paper, we

concentrate on the region in which the percolating transition takes place, and here the third case above holds [ $c \cong (N/J) e^{-1}$ ].

Thus, the generating function for the percolation problem is proportional to the integral

$$\int_0^{C_m} \int_R dy \operatorname{Im} \ln \sum(c) \left[ \int_0^\infty \exp \left( -\frac{l^2}{2N} - laN^{-1/2} - \frac{l^3}{6N^2} + l \frac{a^2}{2N} \right) dl \right] \times \exp \left[ N(y-h) - \frac{N}{2J} y^2 \right] \tag{43}$$

Expression (43) is a key element in our analysis of the one-state Potts model phase transition. In order to facilitate the analysis, it proves useful to reparametrize it in terms of variables that scale with the proper power of  $N$ , the number of lattice sites. To do this we write

$$\begin{aligned} c &= (N/J + N^{1/3} \Delta) e^{-1+h} \\ \frac{1}{J} &= (1 + N^{-1/3} t) \\ l &= LN^{2/3} \\ y &= [1 + N^{-1/3}(-t - L + w)] \\ h &= HN^{-2/3} \end{aligned} \tag{44}$$

With the above substitutions, and after some tedious but straightforward manipulations, the exponent in (43) reduces to

$$\begin{aligned} &\left( \frac{N}{2} - \frac{N^{2/3}t}{2} + \frac{N^{1/3}t^2}{2} - \frac{t^3}{2} \right) - \frac{N^{1/3}w^2}{2} - \frac{(L+t)^3}{6} + \frac{t^3}{6} - \Delta L \\ &+ w \left( t^2 + tL - \frac{tw}{2} \right) - Nh + O(N^{-1/3}) \end{aligned} \tag{45}$$

The term  $-N^{1/3}w^2/2$  in (45) represents a strong Gaussian-type damping,  $w$  will be characteristically  $O(N^{-1/6})$  and therefore the last term in (45) can be neglected. After integrating over  $y$ , which is  $w$ , in (45) we are left with

$$\exp \left( \frac{NJ}{2} - Nh \right) \int d\Delta \operatorname{Im} \left[ \ln \sum(c) \right] \int_0^\infty \exp \left[ \frac{-(L+t)^3}{6} + \frac{t^3}{6} - \Delta L \right] dL \tag{46}$$

where  $c = (N/J + N^{1/3}\Delta) e^{-1+h}$ . In order to proceed further, we need to perform a similar reduction for  $\Sigma(c)$ .  $\Sigma$  is defined by the integral

$$\Sigma(c) = \int \exp\left(-\frac{N}{2J}y^2 + ce^y\right) \tag{47}$$

By setting  $y = 1 + N^{-1/3}x$  and proceeding as before, we obtain

$$\begin{aligned} \Sigma(c) = \Sigma(\Delta) \simeq \int_c \exp\left[\frac{N}{2J} + N^{1/3}\left(\Delta + \frac{H}{J}\right) \right. \\ \left. + (\Delta + H)x + \frac{x^3}{6} + O(N^{-1/3})\right] \end{aligned} \tag{48}$$

However, since only the  $\text{Im} \ln \Sigma$  is required the terms in the exponent proportional to  $N$  and  $N^{1/3}$  can be omitted. They contribute to the real part of  $\Sigma$  only. Putting the two results just obtained together we end up with the following expression for percolation generating function in the vicinity of its phase transition ( $1/J = 1 + N^{-1/3}t$ ):

$$\begin{aligned} \int d\Delta \left( \left\{ \int_0^\infty \exp\left[\frac{-(L+t)^3}{6} + \frac{t^3}{6} - \Delta L\right] dL \right\} \right. \\ \left. \times \text{Im} \ln \left\{ \int_c \exp\left[(\Delta + H)x + \frac{x^3}{6}\right] dx \right\} \right) + K_c \end{aligned} \tag{49}$$

The term  $K_c$  in (49) represents the contribution to the generating function that comes from the integration along the center contour  $\Gamma$  as discussed in Appendix B. This term provides a smooth background to the much more

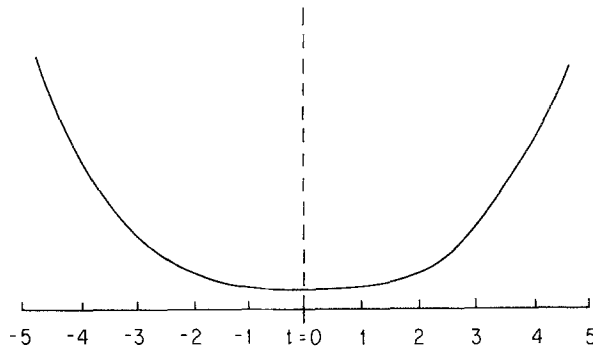


Fig. 1. The percolation generating function plotted versus the variable  $t$ , defined in (44). Smoothly varying background contributions have been eliminated.

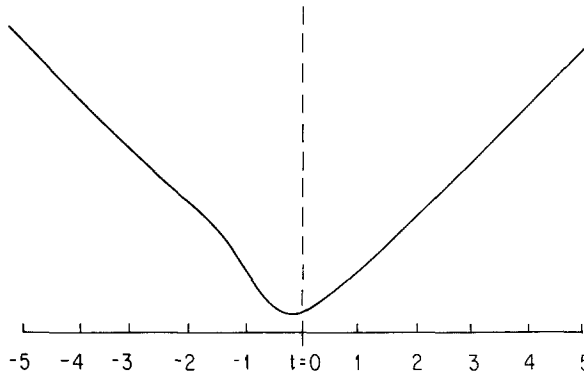


Fig. 2. The second derivative of the percolation generating function plotted versus the variable  $t$ , defined in (44). A background contribution with constant slope has been eliminated.

rapidly varying contribution from the first term in (49). The contour  $C$  is described in Appendix B where an asymptotic expression is developed for  $\Sigma(c)$ .

At this point, to obtain exact results in the region of the phase transition, numerical integration of (49) is required. As an illustration Fig. 1 and 2 are the numerical results for the generating function itself and its second derivative. The latter quantity being the analog of the specific heat. For this model, the mean field percolation model in the infinite site limit, the specific heat has a discontinuous slope. However, as Fig. 2 demonstrates the discontinuity is rounded off for system with a finite number of sites, as we expected.

#### 4. CONCLUSIONS

Our studies of the one-state Potts model on a finite lattice have led to a reformulation of the partition function and, ultimately, to numerical algorithms for the calculation of thermodynamic quantities in the immediate vicinity of the percolation transition. In particular, we are able to assess in quantitative detail the rounding effects of finite size. In this section, we comment on some aspects of our calculational method on the results we have obtained and on some possible extensions.

First, it is interesting to compare our approach with those previously employed. All other treatments of the one-state Potts model have the vector  $\sigma$  returning to an integer dimensionality until later on in the



calculation. In the case of the Kac model treated, for example (see the paper by Wu), the Hamiltonian after some processing takes on the form

$$\frac{N}{2J} \mathbf{S}^2 - N \ln \left( \sum_{i=1}^n e^{S_i} \right) \tag{50}$$

where the  $n$ -dimensional vector,  $\mathbf{S}$  is subject to the requirement

$$\sum_{i=1}^n S_i = 0 \tag{51}$$

Assuming that the ordering is along the “ $i$ ” axis we make the replacement

$$\begin{aligned} S_1 &\rightarrow -(n-1) S \\ S_i &= \dots = S_n = +S \end{aligned} \tag{52}$$

so that (50) becomes

$$\begin{aligned} N \left[ \frac{(n-1)^2 S^2 + (n-1) S^2}{2J} - \ln (e^{-(n-1)S} + (n-1) e^S) \right] \\ \rightarrow N(n-1) \left( \frac{S^2}{2J} + e^S - S \right) + O(N(n-1)^2) \end{aligned} \tag{53}$$

Thus the  $n$ -state partition function is

$$\exp N(n-1) \left[ \frac{-S^2}{2J} + (e^S - S) \right] + O(N(n-1)^2) \tag{54}$$

Note that the leading term in  $(n-1)$  in the exponential corresponds to the replacement approximation Eq. (28) in Section 2. In the case of a standard thermodynamic system, one proceeds by looking for a maximum in the exponent, reasoning that in the limit of large  $N$  this contribution to the partition function dominates all others. In this way, one is led to the extremum equation,

$$\begin{aligned} 0 &= \frac{d}{dS} \left[ \frac{-S^2}{2J} + (e^S - S) \right] \\ &= -\frac{S}{J} + e^S - 1 \end{aligned} \tag{55}$$

which is just the equation of state (29) with  $y$  replaced by  $S$ .

There are, however, two difficulties associated with this approach. First, the argument for the asymptotic dominance of the configuration that

maximizes the exponent in (54) does not survive the limiting procedure required to obtain the proper correspondence between the one-state Potts model and percolation. To achieve that correspondence one *first* takes the limit  $n \rightarrow 1$  and *then* the limit  $N \rightarrow \infty$ . Proceeding as described in Section 2, one is left with Eq. (28) for the percolation generating function.

Assuming, for the time being, that we *are* justified in taking the limit  $N \rightarrow \infty$  before allowing  $n$  to be infinitesimally close to one we see an even worse problem emerging when we examine the exponent in (56). While the expression  $(S^2/2J) - (e^S - S)$  has local minima at and around  $S=0$  (for  $J \approx 1$ ) the true minimum of the expression above, and hence the true maximum of lies at  $S = -\infty$ , where the expression diverges to  $-\infty$ . This free energy minimum, which obviously dominates all other contributions to the partition function, is commonly ruled out by *fiat*. It is simply noted that the quantity  $S$  corresponds to a probability in percolation, and that a negative probability has no meaning. Such an argument, unfortunately, does nothing to elucidate the mathematical structure leading to this pathological and apparently fictitious minimum. It simply rescues the model, and in the process casts doubt on the utility of the Potts model connection. The one consolation is that the correct equation of state can be obtained by directly considering graph statistics, and *without* recourse to the Potts model connection.

An additional problem with previous calculational approaches is worthy of note. The one-state Potts model free energy, in the presence of an ordering field,  $h$ ,

$$N \left[ -\frac{S^2}{2J} - (e^{S+h} - S) \right] \quad (56)$$

subject to the equation of state,

$$\frac{S}{J} = e^{S+h} - 1 \quad (57)$$

is equal to the generating function

$$F = \sum_j n_j^c e^{jh} \quad (58)$$

This means that in our mean field model

$$\sum_j j n_j^c e^{jh} = \frac{\partial F}{\partial h} = N e^{S+h} \quad (59)$$

Setting  $h = 0$  we have

$$\sum j n_j^c = N e^S$$

We know that the left-hand side is just equal to the total number of sites on the lattice. This sum rule holds whether the percolation transition has occurred or not. The right-hand side, however, departs from that number below the percolation transition, when there is a positive solution to (56). What has happened is that the contribution of the percolating cluster to the sum

$$\sum_j j n_j^c$$

has disappeared. This will occur when the quantity  $h$  is nonzero and negative, no matter how small, as long as when the limit  $N \rightarrow \infty$  has been taken. One cannot apparently take the limit  $h = 0$  before going to the thermodynamic limit. The ability to take limits in this latter order is crucial to the investigation of percolation on a finite lattice. As indicated in Appendix C the method we use here allows us to take limits in the proper order, and the sum rule is covered, even at the percolation transition.

The resolution of the above paradoxes is an important result. It indicates that our approach, or one like it, may prove useful in the investigation of other replicated models, including spin glasses, that suffer from a more serious problem. One might hope for a mathematically unambiguous resolution to the de Almeida–Thouless instability.<sup>(17)</sup> Such work, however, lies in the future.

As for results relevant to percolation, we are able to present useful algorithms for the calculation of key thermodynamics quantities in the immediate vicinity of the percolation transition.<sup>3</sup> The curve displayed in Fig. 2 is the result of the implementation of one such algorithm. This curve displays both the rounding effects of finite size on the specific heat analog and some unremarkable structure that goes beyond a simple rounding off of the cusp one would see in an infinite system. Whether this structure would be visible in a Monte Carlo study of mean field percolation in a small lattice is not at all obvious. Nevertheless, at sufficient resolution and for a large enough sample it ought to show up.

<sup>3</sup> We note that finite-size scaling has been applied to percolation by Derrida and De Seze,<sup>(18)</sup> who utilize transfer matrices and Nightingale's<sup>(18)</sup> phenomenological renormalization group approach. A finite-size scaling analysis of nonrandom mean-field-type spin systems has been carried out by Botet *et al.*<sup>(18)</sup> We are grateful to the referee, who brought these works to our attention.

The next stage in our study of percolation on a finite lattice is to consider the more physically reasonable short-ranged bond problem. Preliminary studies indicate that the method developed here can be carried over to this much more relevant problem. Calculations are now in progress.

## ACKNOWLEDGMENTS

The bulk of this work reported here was completed while both authors were at the University of California, Santa Cruz. One author (J.R.) wishes to thank the NSF for partial support. Discussions with Professor Harold Widom led to the elucidation of key points in the analysis presented in this paper. His contributions are gratefully acknowledged.

## APPENDIX A

In this appendix, we investigate the analytic structure of the integral

$$I(c) = \int_C \exp \left[ -\frac{N}{2J} z^2 + c(e^z - z) \right] dz$$

and develop an asymptotic expansion  $I(c)$  when  $c = N \gg 1$ .

For  $c > 0$ , there are two choices for the contour  $C$  which keeps the integral finite, and when  $c < 0$ , the entire real axis suffices. The appropriate contours are shown in Figure 3. It is easy to show that  $c = 0$  is a branch

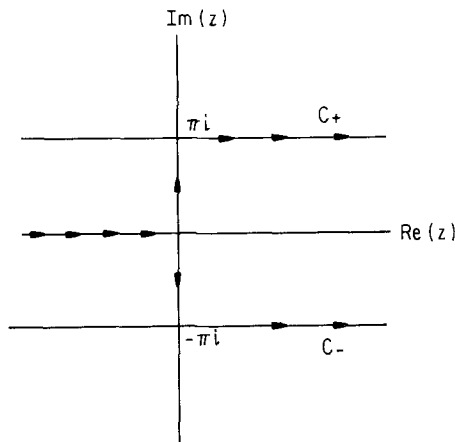


Fig. 3. The two contours which are used to defined the integrals  $I(N)$  and  $I(c)$ .

point of  $I(c)$  and the positive real axis can be chosen as a branch cut. Just above the cut, if  $C_+$  path is chosen then  $C_-$  must be chosen just below the cut. The integrals  $I_+$  and  $I_-$  are conjugates of one another, so the discontinuity across the cut

$$I_+(c) - I_-(c) = 2 \operatorname{Im} I_+(c) \tag{A1}$$

These results will be used in Appendix B and here we are interested in developing an asymptotic expansion for  $I$  when  $c = N$  which will lead to explicit results for the generating function in the replacement approximation.

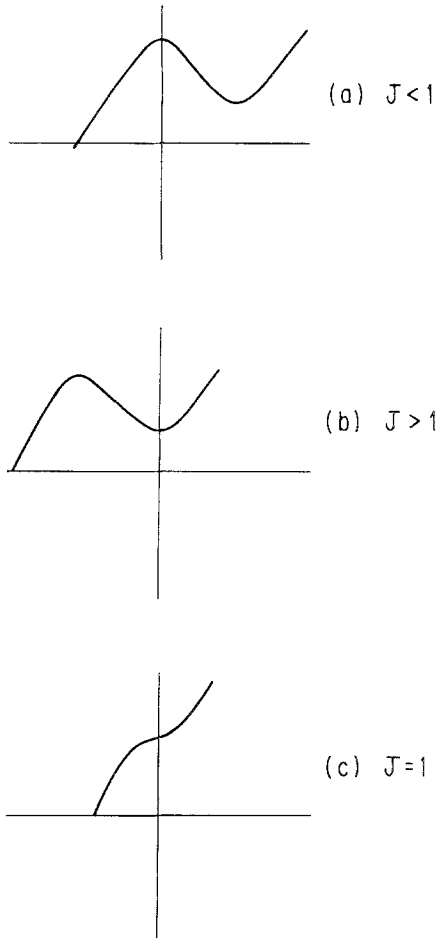


Fig. 4. The behavior of the exponent,  $g(z) = -z^2/2J + (e^z - z)$ , near its extrema points for (a)  $J < 1$ , (b)  $J > 1$ , and (c)  $J = 1$ .

We have

$$I(N) = \int e^{Ng(z)} dz \quad (\text{A2})$$

where  $g = -z^2/2J + (e^z - z)$ . The contours  $C_+$  (or  $C_-$ ) can be deformed so that  $g(z)$  is always real and, for large  $N$ , most of the contribution to the integral will come from the region near the maximum of  $g(z)$ . The extrema points are determined by the equation  $g' = 0$ , which leads to

$$\frac{z}{J} = (e^z - 1) \quad (\text{A3})$$

A simple graph of (A3) shows that there are always two real roots, one at  $z_1 = 0$ , and the second root is  $> 0$  for  $J < 1$  and  $< 0$  for  $J > 1$ . For  $J \approx 1$  it is given approximately by  $z_2 = 2[(1/J) - 1]$ . From the second derivative of  $g$  it is also clear that for (a)  $J < 1$ , extremum at  $z_1 = 0$  is a max and  $z_2 = 2[(1/J) - 1] > 0$  is a minimum along the real axis; (b)  $J > 1$  extremum at  $z_2 = 2[(1/J) - 1] < 0$  is a max and  $z_1 = 0$  is minimum along the real axis. In both cases, the maximum occurs for the smallest  $z$ . The function  $g$  is schematically shown in Fig. 4. It is clear from Fig. 4 that the steepest-descent method leads to the correct description of the mean field percolation phase transition and avoids arbitrariness in selecting the proper roots present in the infinite lattice result. Presumably the latter ambiguity is

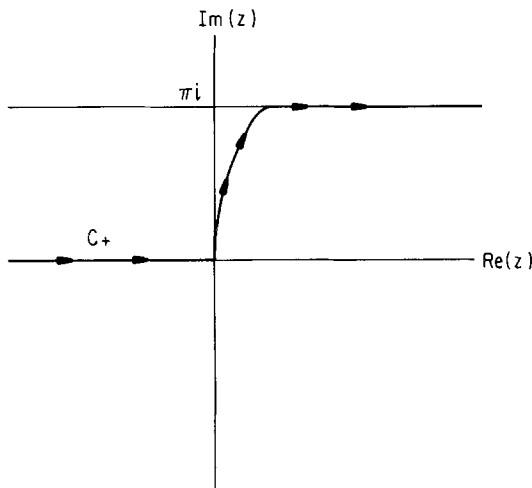


Fig. 5. Steepest-descent path used to evaluate the integral,  $I(c)$  for the case  $J < 1$ .

introduced by taking the thermodynamic limit too early in the calculation of the replica system.

The steepest-descent evaluation of  $I(N)$  is straightforward, with the only complication arising when results near the transition  $J = 1$  are needed. For this case, cubic terms must be retained in the calculation because the second derivative  $g''(z) = (-1/J) + e^z \rightarrow 0$  as  $J \rightarrow 1$ . However, even for this case, the path  $C_+$  (or  $C_-$ ) can be deformed so that  $g(z)$  is real yet pass through the maximum of  $g(z)$ . It is determined analytically by requiring  $\text{Im } g(z)$  to be zero. The contour leaves the real axis at the minimum point, i.e., at  $z = 0$  for  $J < 1$  or  $z = 2[(1/J) - 1]$  for  $J > 1$  and then follows a curve given by the equation  $y = \sqrt{3} [x^2 + (2r/s)x]^{1/2}$  where  $r = |g''|$  and  $s = g'''$  out to  $z = \pi i + \infty$ . The path, for the case  $J < 1$ , is drawn in Figure 5.

### APPENDIX B

The analytic properties of

$$\Sigma = \int \exp[-(N/2J)z^2 + ce^z] dz$$

are very similar to  $I(c)$  discussed in Appendix A. The appropriate contours which define  $\Sigma$  are again  $C_+$  and  $C_-$ . The integral has a branch point at the origin,  $c = 0$ , and the positive real  $c$  axis may be taken as a branch cut to constrain  $\Sigma$  to be a single-valued function of  $c$ . The function is discontinuous across the real  $c$  axis with  $C_+$  being the appropriate contour just above and  $C_-$  being the one below. The discontinuity is given by

$$\lim_{\epsilon \rightarrow 0^+} \Sigma(c + i\epsilon) - \Sigma(c - i\epsilon) = 2 \text{Im } \Sigma(c^+) \tag{B1}$$

Aside from the branch along the positive real axis,  $\Sigma(c)$  has no other singularities in the finite  $c$  plane, nor does it have zeros. This implies that  $\Sigma(c)$ , or for that matter  $\ln \Sigma(c)$ , can be expressed as

$$\Sigma(c) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\Sigma(c')}{c' - c} dc' \tag{B2}$$

where the contour,  $\Gamma$ , for the integration over  $c'$  is drawn in Fig. 6.

$$\Sigma(c) = \frac{1}{2\pi i} \left[ \int_0^{c_m} \frac{\Sigma_{C_+}(c') - \Sigma_{C_-}(c')}{c' - c} + \int_{\Gamma} \frac{\Sigma(c')}{c' - c} dc' \right] \tag{B3}$$

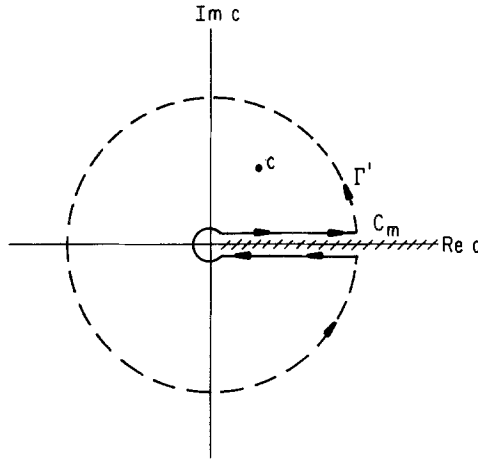


Fig. 6. Contour  $\Gamma$  specified in Eq. (B2), the Cauchy formula for  $\Sigma(c)$ .

Using Eq. (B1) and defining

$$\sigma(c) = \frac{1}{2\pi i} \int_{\Gamma'} \frac{\Sigma(c')}{c' - c} dc'$$

we have

$$\Sigma(c) = \frac{1}{\pi i} \int_0^{c_m} \frac{\text{Im} \Sigma_{c_+}(c')}{c' - c} dc' + \sigma(c) \tag{B4}$$

where  $\sigma(c)$  has no singularities for finite  $c$ . This result also holds for the  $\ln \Sigma(c)$  and was what was used in the text. As we shall see below, when  $c > (N/J) e^{-1}$  the  $\text{Im} \Sigma$  becomes large and the integral along the real axis is dominant whereas when  $c < (N/J) e^{-1}$   $\sigma(c)$  dominates.

Since we will always be in the region of large  $N$ , the  $\text{Im} \Sigma(c)$  can be determined using the method of steepest descents. We write our integral as

$$\Sigma_{c_+}(c) = \int_{c_+} \exp[(-N/2J) z^2 + ce^z] dz = \int_{c_-} e^{g(z)}$$

the extremum points are determined from  $g' = 0$  and are the solutions to the equation

$$c = (N/J) ze^{-z} \tag{B5}$$

A simple graph of the right-hand side of (B5) shows that for  $c < (N/J) e^{-1}$  there are two real roots  $z_1$  and  $z_2$ , which approach 1 ( $z_1$  and



$z_2 \rightarrow 1$ ) as  $c \rightarrow (N/J)e^{-1}$ , but when  $c > (N/J)e^{-1}$  there are no real solutions to B5.

Case 1: when  $c \leq (N/J)e^{-1}$  the two roots will be close to 1. Anticipating this we set

$$\begin{aligned} z &= 1 + N^{-1/3} y, & y \text{ and } \Delta \ll 1 \\ c &= (N/J) - N^{1/3} \Delta, \end{aligned} \tag{B6}$$

Substituting (B6) into (B5) and to lowest order we have

$$\begin{aligned} y^2 &= 2\Delta + O(N^{-1/3}) \\ \text{so} \quad z_1 &= 1 - (2\Delta)^{1/2} N^{-1/3}, & z_2 &= 1 + (2\Delta)^{1/2} N^{-1/3} \end{aligned} \tag{B7}$$

A plot of  $g(z)$  is shown in Fig. 7 in the region of the extrema. As the figure indicates,  $z_1$  corresponds to a maximum along the real axis and  $z_2$  to a minimum. The reverse is true parallel to the imaginary axis.

As long as we are not too close to the transition ( $J = 1$ ) the integral is dominated in region  $z_1$  and the usual Gaussian approximation suffices. Hence for

$$\begin{aligned} c &< (N/J)e^{-1} \\ \sum_+(c) &= K_1 \exp[(-N/2J)z_1^2 + ce^{z_1}] + iK_2 \exp[(-N/2J)z_2^2 + ce^{z_2}] \end{aligned} \tag{B8}$$

and for  $N \gg 1$

$$\text{Im } \sum_+ \ll \text{Re } \sum_+$$

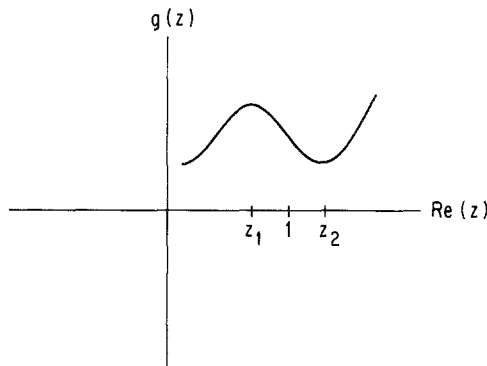


Fig. 7. A plot of  $g(z) = -(N/2J)z^2 + ce^z$  for the case,  $c < (N/J)e^{-1}$ .

Case 2:  $c > (N/J) e^{-1}$ . Now the extremum points are complex. Following the same analysis, but defining  $c = [(N/J) + N^{1/3} \Delta] e^{-1}$ , the roots are given by

$$\begin{aligned}
 y_1 &= i(2\Delta)^{1/2} \left[ 1 + \frac{i}{3} N^{-1/3} (2\Delta)^{1/2} \dots \right] \\
 y_2 &= -i(2\Delta)^{1/2} \left[ 1 - \frac{i}{3} N^{-1/3} (2\Delta)^{1/2} \dots \right]
 \end{aligned}
 \tag{B9}$$

$\Sigma_+$  will be proportional to  $e^{g(z_1)}$ , except very close to the transition point, resulting in a phase function  $e^{i(1/3)(2\Delta)^{3/2}}$  to lowest order. Hence we have

$$\text{Im} \ln \Sigma_+ = \frac{1}{3} (2\Delta)^{3/2}
 \tag{B10}$$

However as the transition region is approached,  $\Delta \rightarrow 0$ , the Gaussian approximation is no longer valid and cubic terms contribute to the leading term in the asymptotic expansion of  $\Sigma_+$ . Most of the contribution to the integral for  $\Sigma_+$  comes from the region around the extremum  $z_1$  and the value of the exponent in this region is well approximated by a Taylor series

$$\begin{aligned}
 g(z) &= g(z_1) + \frac{g''(z_1)}{2} (z - z_1)^2 + \frac{g'''(z_1)}{6} (z - z_1)^3 \dots \\
 &= g(z_1) + u + iv
 \end{aligned}
 \tag{B12}$$

Again the path through the extremum is chosen such that  $\text{Im}(g - g(z_1)) = 0$  and  $\text{Re}(g - g(z_1)) = u < 0$ .

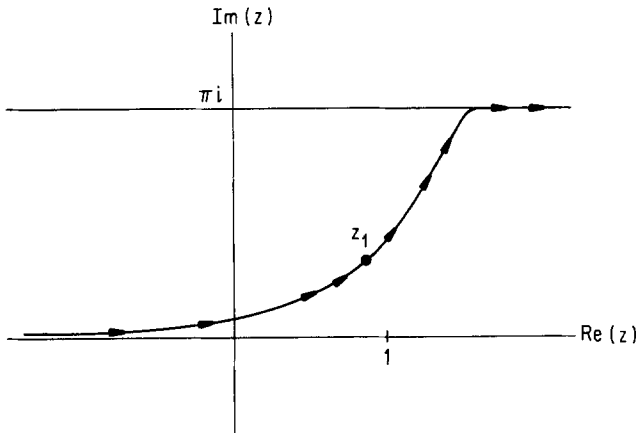


Fig. 8. Steepest-descent path used to evaluate the integral  $\Sigma(c)$  for the case  $J < 1$ .

This leads to the following equation for the path of integration through the extremum at  $z_1$

$$X = Y \left[ \frac{Y/3 + N^{-1/3}(2A)^{1/2}}{Y + N^{-1/3}(2A)^{1/2}} \right]^{1/2}$$

which is depicted in Fig. 8.

The corrections to the Gaussian result are now easily obtained.

### APPENDIX C

Here we show how the sum rule discussed in Section 4 is recovered. Using the fact that  $F$  is the coefficient of  $c^N/N!$  in (16) (multiplied by the factor  $\exp[(-NJ/2) + Nh]$ ) we have

$$F = \frac{N!}{2\pi i} \oint \frac{1}{c^{N+1}} \left( \frac{N}{2\pi J} \right)^{1/2} \sum (ce^{-h}) \left\{ \frac{1}{2} \ln \left( \frac{N}{2\pi} J \right) + \ln \sum (c) \right\} \exp \left[ \left( \frac{-NJ}{2} \right) + h \right] dc \tag{C1}$$

where the integral is over a contour just surrounding the origin. Replacing  $c$  by  $ce^h$  we find that the only  $h$ -dependent contribution to  $F$  is

$$\exp \left( - \frac{NJ}{2} \right) \frac{N!}{2\pi i} \oint \frac{1}{c^{N+1}} \left( \frac{N}{2\pi J} \right)^{1/2} \sum (c) \ln \left[ \sum (ce^h) \right] dc \tag{C2}$$

If now we take the derivative with respect to  $h$  of this expression we obtain

$$\exp \left( - \frac{NJ}{2} \right) \frac{N!}{2\pi i} \oint \frac{1}{c^{N+1}} \left( \frac{N}{2\pi J} \right)^{1/2} \frac{\sum(c)}{\sum(ce^h)} \sum' (ce^h) ce^h dc \tag{C3}$$

Setting  $h = 0$

$$\exp \left( - \frac{NJ}{2} \right) \frac{N!}{2\pi i} \oint \frac{1}{c^{N+1}} \left( \frac{N}{2\pi J} \right)^{1/2} \sum' (c) \cdot c dc \tag{C4}$$

Since

$$\sum' (c) = \int \exp \left( - \frac{N}{2J} y^2 + ce^y + y \right) dy \tag{C5}$$

we can perform the contour integral over  $c$  immediately. We obtain

$$\exp\left(-\frac{NJ}{2}\right) \frac{N!}{(N-1)!} \left(\frac{N}{2\pi J}\right)^{1/2} \int \exp\left(-\frac{N}{2J}y^2 + Ny\right) dy = N \quad (\text{C6})$$

This result is independent of the quantity  $J$ , and is the correct right-hand side of the sum rule.

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