

## Critical amplitude of the Potts model: Zeroes and divergences

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(Received 24 October 1983)

The critical amplitude of the  $q$ -state Potts-model free energy is studied as a function of  $q$  in two dimensions and on the diamond hierarchical lattice. The amplitude diverges at an infinite number of  $q$  values,  $q_n$ , introducing logarithmic terms in the free energy. We expect that in each interval  $(q_n, q_{n+1})$  there is a value  $\hat{q}_n$  where the amplitude vanishes, affecting the singularity of the free energy as a function of temperature. Possible consequences for gelation and vulcanization of polymers are discussed.

### I. INTRODUCTION

The  $q$ -state Potts model has been extensively studied<sup>1</sup> in view of its connection to a variety of experimental systems undergoing phase transitions, ranging from percolation<sup>2</sup> to adsorption of noble gases on various substrates.<sup>3</sup> The nature of the transition between the low- and high-temperature phases changes from continuous for low values of  $q$ ,  $q \leq q_c$ , to discontinuous for high values of  $q$ ,  $q > q_c$ , thus enhancing the interest<sup>4</sup> in this model. In two dimensions, Baxter<sup>5</sup> has shown that  $q_c = 4$ , and den Nijs<sup>6</sup> proposed a formula which gives the thermal exponent as a function of  $q$  for  $q \leq 4$ . However, not much attention has been paid to the critical amplitude. It is the purpose of this paper to present a study of the  $q$  dependence of the critical amplitude of the Potts free energy.

A sequence of values of  $q$ ,  $\{q_n\}$ , starting with  $q_1 = 2$  (the Ising model) and converging towards zero, where the critical amplitude diverges, is calculated in Sec. II. For these values the power law is replaced by a logarithmic singularity. We present evidence which shows that between any two consecutive values  $q_n$  and  $q_{n+1}$  the amplitude varies monotonically between  $-\infty$  and  $+\infty$ . Hence there is a value  $\hat{q}_n$  in any interval  $(q_n, q_{n+1})$  where the critical amplitude is zero, Sec. III, and thus the expected leading singularity does not occur. We also obtain estimates for the  $\hat{q}_n$  values by using an expression for the  $q$  dependence of the critical amplitude which interpolates between known results.

In Sec. IV numerical estimates of the critical amplitudes of the two-dimensional  $q$ -state Potts and bond-percolation models are obtained by using Migdal-Kadanoff<sup>7</sup> renormalization group. These computations are, of course, approximations for the square lattice. However, they are exact when the models are defined on the diamond hierarchical lattice.<sup>8,9</sup> This is significant in view of the minimal amount of exact and detailed analysis of nontrivial models of phase transitions available.

These theoretical predictions may have experimental consequences, Sec. V, for polymer mixtures undergoing gelation and vulcanization processes which belong to the universality class of the Potts model with  $q$  between zero and one.<sup>10</sup> In this connection we analyze the critical

behavior of a bond-percolation process in the presence of a fugacity which controls the number of clusters.

### II. DIVERGENCE OF CRITICAL AMPLITUDE AND LOGARITHMIC SINGULARITIES

In this section we discuss the divergence of the critical amplitude of the Potts-model free energy at certain values of  $q$ , the number of states. The Potts Hamiltonian is

$$-\frac{\mathcal{H}}{kT} = 2J \sum_{\langle i,j \rangle} \delta_{s_i, s_j}, \quad (1)$$

where  $\delta$  is the Kronecker delta function,  $s_i = 1, 2, \dots, q$  is a spin variable located at site  $i$  of the lattice, and the sum is over nearest-neighbor sites. Throughout this paper  $q$  is a real variable.<sup>2,11</sup> The free energy per site  $f$ , close to the critical point, is the sum of a regular contribution  $f_{\text{reg}}$  and of a singular contribution  $f_{\text{sing}}$ ,

$$f = f_{\text{reg}} + f_{\text{sing}}, \quad (2)$$

$$f_{\text{sing}} \approx A_{\pm} |t|^{d/y}, \quad (3)$$

where  $A_{\pm}$  is the critical amplitude,  $t = (T - T_c)/T_c$  is the reduced temperature,  $d$  is the dimension, and  $y$  is the thermal exponent.

Logarithmic modifications of the power-law singularities can occur<sup>12</sup> when one of the scaling fields is marginal, e.g., at the upper critical dimension,<sup>13</sup> or when the critical exponents satisfy certain relationships.<sup>12</sup> We will elaborate on a particular example of the latter case which is important for the Potts model. When the ratio  $d/y$  is equal to an integer  $m_0$ ,  $d/y = m_0$ , the leading singularity of the free energy is not, in general,  $f_{\text{sing}} \sim |t|^{m_0}$ , but  $f_{\text{sing}} \sim t^{m_0} \ln |t|$ . The changeover from power law to logarithmic singularity can be traced back to a breakdown in the power (Taylor) expansion of the regular part of the free energy when  $d/y = m_0$ . Indeed, within a typical renormalization-group scheme, the free energy satisfies the functional equation

$$f(t) = g(t) + b^{-d} f(b^y t), \quad (4)$$

where  $g$  is an analytic function of the scaling field  $t$ , and  $b$  is the rescaling factor. The regular part of the free energy  $f_{\text{reg}}$  and  $g$  can be expanded in powers of  $t$ ,

$$f_{\text{reg}} = \sum_{m=0}^{\infty} f_m t^m, \quad g = \sum_{m=0}^{\infty} g_m t^m. \quad (5)$$

By using Eq. (4), the coefficients  $f_m$  can be expressed as

$$f_m = \frac{g_m}{1 - b^{-d+my}}. \quad (6)$$

However, if  $d/y = m_0$  the expansion of  $f_{\text{reg}}$  is not valid because  $f_{m_0}$ , from Eq. (6), diverges as  $(m_0 - d/y)^{-1}$ . In this case, the free-energy singularity is determined by the combined contributions of  $f_{m_0} t^{m_0}$  and the usual singular part  $A_{\pm} |t|^{d/y}$  in the limit  $d/y \rightarrow m_0$ ,

$$f_{\text{reg}} = \sum_{\substack{m=0 \\ m \neq m_0}}^{\infty} f_m t^m, \quad (7)$$

$$\begin{aligned} f_{\text{sing}} &= \lim_{d/y \rightarrow m_0} (f_{m_0} t^{m_0} + A_{\pm} |t|^{d/y}) \\ &= \lim_{d/y \rightarrow m_0} \{f_{m_0} t^{m_0} + A_{\pm} t^{m_0} (\text{sgnt})^{m_0} \\ &\quad \times [1 + (d/y - m_0) \ln |t|]\}, \end{aligned}$$

where  $\text{sgnt}$  is 1 if  $t > 0$  and  $-1$  if  $t < 0$ . By denoting

$$a = \lim_{d/y \rightarrow m_0} A_{\pm} (\text{sgnt})^{m_0} (d/y - m_0), \quad (8)$$

$$c_{\pm} = \lim_{d/y \rightarrow m_0} [A_{\pm} + f_{m_0} (\text{sgnt})^{m_0}],$$

and assuming the existence of these limits, we can rewrite  $f_{\text{sing}}$  as

$$f_{\text{sing}} = a t^{m_0} \ln |t| + c_{\pm} |t|^{m_0}. \quad (9)$$

Equation (8) and the assumption that  $c_{\pm}$  is finite imply

$$a = - \lim_{d/y \rightarrow m_0} f_{m_0} (d/y - m_0), \quad (10)$$

which shows that the amplitude  $a$  is the same above ( $t > 0$ ) and below ( $t < 0$ ) the critical temperature.<sup>14</sup> It also follows, Eq. (8), that  $A_{\pm}$  diverges as

$$A_{\pm} \sim (d/y - m_0)^{-1} \text{ for } d/y \rightarrow m_0. \quad (11)$$

These results, Eqs. (8)–(11), though discussed here in the context of the Potts model are more general. Indeed, they are confirmed by the exact solutions of the eight-vertex model<sup>15</sup> and of the Ising model on a Cayley tree.<sup>16</sup> For both models a symmetry, duality in the former and time reversal in the latter, forbids the occurrence of odd powers of the scaling field in  $f_{\text{sing}}$ , thus allowing logarithmic modifications of the power law only when  $d/y$  is an even integer. The same holds for the Potts model which is self-dual when defined on the square lattice. The self-duality also implies that the amplitudes  $A_{\pm}$  and  $c_{\pm}$  are the same above and below the critical temperature,

$$A_+ = A_-, \quad c_+ = c_-$$

and (12)

$$a = 0 \text{ if } d/y \text{ is an odd integer.}$$

den Nijs has conjectured<sup>6</sup> that the thermal exponent  $y$  of the  $q$ -state Potts model in two dimensions varies with  $q$  as

$$y = 3 \frac{1-u}{2-u}, \quad (13)$$

where  $0 \leq u = (2/\pi) \cos^{-1}(\sqrt{q}/2) \leq 1$  and  $0 \leq q \leq 4$ . According to this conjecture which has been verified numerically<sup>4,17</sup> and analytically,<sup>18</sup> and agrees with all known results,  $d/y$  decreases monotonically from  $+\infty$  at  $q=0$  to  $\frac{4}{3}$  at  $q=4$ , thus spanning all integers larger than unity. The values of  $q$  for which  $d/y = 2m$ ,  $m=1,2,\dots$ , and where logarithmic singularities occur, Eq. (9), can be obtained from Eq. (13),

$$q_m = 4 \sin^2 \frac{\pi}{6m-2}, \quad m=1,2,3,\dots \quad (14)$$

This sequence starts with  $q_1=2$ , corresponding to the Ising model which exhibits a logarithmically divergent specific heat,<sup>19</sup> and the next following values are in the interval  $(0,1)$ :  $q_2=0.3820$ ,  $q_3=0.1218$ ,  $q_4=0.0810$ , etc. For large  $m$ , Eq. (14) is approximated by  $q_m \approx \pi^2/9m^2$  and the accumulation point of this sequence is 0.

When  $d/y = 2m+1$ ,  $m=1,2,3,\dots$ , corresponding to the following  $q$  values,

$$\bar{q}_m = 4 \sin^2 \frac{\pi}{6m+1}, \quad m=1,2,3,\dots \quad (15)$$

there is no logarithmic contribution because the amplitude  $a$  is zero, Eq. (12). In this case

$$f_{\text{sing}} \simeq c_{\pm} |t|^{2m+1}, \quad m=1,2,3,\dots \quad (16)$$

and thus the  $(2m+1)$ th derivative of the free energy with respect to  $t$  is discontinuous at the critical point  $t=0$ , i.e., the transition is of  $(2m+1)$ th order in Ehrenfest's sense.<sup>20</sup>

### III. CRITICAL AMPLITUDE DEPENDENCE ON $q$

#### A. Monotonicity ansatz

In this section we make the ansatz that the critical amplitude of the two-dimensional Potts free energy is a piecewise monotonic function of  $q$ , and we discuss the consequences of the ansatz. The exact solution of the eight-vertex model<sup>15</sup> has proven to be useful for acquiring information on the Potts model. Indeed, Baxter,<sup>5</sup> using a mapping between the two models, has shown that for  $q \leq 4$  the transition is continuous while for  $q > 4$  the Potts transition is discontinuous. Moreover, den Nijs's conjecture,<sup>6</sup> which determines the thermal exponent of the Potts model, is a relationship between the exponents of this model and the eight-vertex model. It is then plausible that insight can also be gained on the critical amplitude of the Potts model by examining the exactly known critical amplitude of the eight-vertex model.

The critical amplitude of the eight-vertex free energy diverges when  $d/y$  ( $\pi/\mu$  in Baxter's notation<sup>15</sup>) is equal to even integers (consistent with our discussion in Sec. II), and in between two such values it varies monotonically between  $-\infty$  and  $+\infty$ . By analogy with the eight-vertex model we make the ansatz that the critical amplitude of the Potts model is a *piecewise monotonic* function of  $d/y$  where  $y$  is the Potts-model thermal exponent and  $d=2$ . Since  $d/y$  is a monotonic function of  $q$ , Eq. (13), the amplitude also varies monotonically with  $q$ . We verified this ansatz by computing the  $q$  dependence of the amplitude within the Migdal-Kadanoff<sup>7</sup> renormalization-group scheme, and the results are presented below in Sec. IV.

For  $2 < q \leq 4$  the specific heat, which is a positive quantity, diverges with an exponent  $\alpha = 2 - d/y > 0$  [Eq. (13)], and thus for small  $t$  it can be approximated by its singular contribution,

$$C \approx A(2-\alpha)(1-\alpha) |t|^{-\alpha} > 0, \quad (17)$$

where  $A \equiv A_+ = A_-$ . Equation (17) implies that  $A > 0$ . Hence as  $q \rightarrow q_1^+ = 2^+$ , the amplitude  $A \rightarrow +\infty$ , while for  $q \rightarrow q_1^- = 2^-$  it diverges to  $-\infty$  according to Eq. (11). At  $q=1$  the Potts model is trivial; the free energy  $f$  is proportional to the coupling  $J$ . This is consistent with Eqs. (2) and (3), provided that the critical amplitude  $A=0$  at  $q=1$ . Decreasing  $q$  still further,  $A$  increases and as  $q \rightarrow q_2^+ = 0.3820^+$  it diverges to  $+\infty$ , while at  $q \rightarrow q_2^-$ ,  $A \rightarrow -\infty$ . The qualitative dependence of  $A$  on  $d/y$  and  $q$  is shown in Fig. 1.

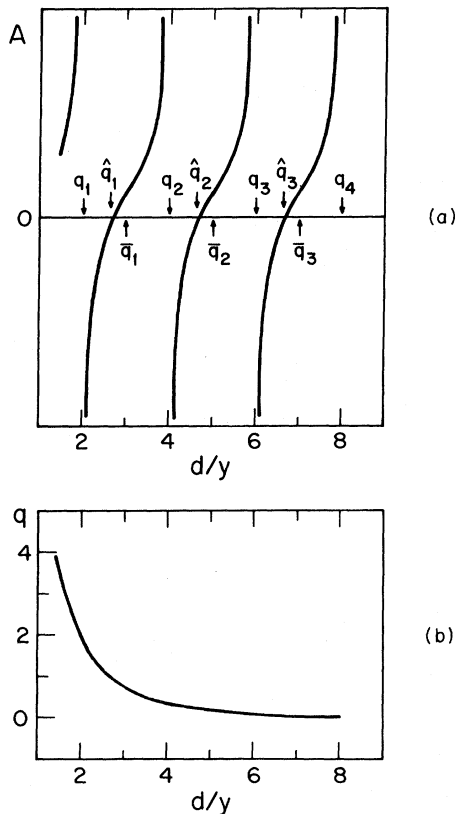


FIG. 1. (a) Qualitative dependence of the amplitude on  $d/y < 8$ ,  $d=2$ . The special values  $q_n$ ,  $\bar{q}_n$ , and  $\hat{q}_n$  are marked. (b)  $q$  dependence on  $d/y$  from den Nijs's conjecture.

Figure 1 is in agreement with results obtained for bond percolation which is related<sup>2</sup> to the  $q$ -state Potts model with  $q \rightarrow 1$ . The mean number of clusters  $G$  is equal to the derivative of  $f$  with respect to  $q$  evaluated at  $q=1$ ,

$$G = \left. \frac{\partial f}{\partial q} \right|_{q=1}. \quad (18)$$

Then,

$$G_{\text{sing}} \approx \left. \frac{\partial}{\partial q} (A |t|^{d/y}) \right|_{q=1} = \left[ \left. \frac{dA}{dq} |t|^{d/y} + A \frac{\partial}{\partial q} |t|^{d/y} \right] \right|_{q=1}. \quad (19)$$

Since  $A(q=1)=0$ , it follows that the percolation amplitude is  $dA/dq|_{q=1}$ . According to our analysis, this is a negative quantity (Fig. 1) in agreement with series expansions<sup>21</sup> for bond percolation.

An important consequence of the  $q$  dependence of  $A$ , as shown in Fig. 1, is that there is a sequence of values  $\{\hat{q}_n\}$ , with  $q_{n+1} < \hat{q}_n < q_n$  [ $q_n$  are given in Eq. (14)], starting with  $\hat{q}_1=1$ , where  $A$  is zero,  $A(q=\hat{q}_n)=0$ . Hence for these values the free energy does not exhibit the singularities prescribed by den Nijs's conjecture.

#### B. Interpolation formula for $A(q)$

The solution of the eight-vertex model suggests an expression for the dependence of the Potts-model critical amplitude on  $q$ . In the eight-vertex model, the critical amplitude<sup>15</sup> is proportional to  $\cot(\pi/y)$ , where  $y$  is the thermal exponent. By analogy we propose the following form for the Potts amplitude:

$$A = -b(q) \left[ \cot \frac{\pi}{y(q)} - \frac{1}{\sqrt{3}} \right], \quad (20)$$

where  $y(q)$  is the Potts thermal exponent and  $b(q)$  is a slowly varying positive function of  $q$ . The sign of  $b(q)$  was chosen so that  $A > 0$  for  $q > 2$ . Equation (20) interpolates between all exact or accepted results as follows: (i)  $A$  diverges whenever  $d/y = 2/y$  is an even integer and (ii)  $A$  is zero for  $q=1$  ( $y = \frac{3}{4}$ ). It is interesting to note that by using Eqs. (13) and (20) we obtain

$$\hat{q}_m = 4 \sin^2(\pi/6m), \quad m = 1, 2, 3, \dots \quad (21)$$

as the values of  $q$  where  $A=0$ . The sequence starts with  $\hat{q}_1=1$  and continues with the following values in the interval  $(0,1)$ :  $\hat{q}_2=0.2679$ ,  $\hat{q}_3=0.1206$ ,  $\hat{q}_4=0.0681$ , etc.

#### V. NUMERICAL COMPUTATIONS USING THE MIGDAL-KADANOFF RENORMALIZATION GROUP

In this section we present numerical computations of the Potts critical amplitude and bond-percolation related quantities. We use the Migdal-Kadanoff renormalization-group method<sup>7</sup> with rescale factor  $b=2$ , which is an approximation for two-dimensional lattices. At the

same time this scheme is *exact for the diamond hierarchical lattice*.<sup>8,9</sup> This lattice is constructed, Fig. 2, in the following iterative way: four bonds such as the one in Fig. 2(a) are aggregated to form a diamond and then, four diamonds such as in Fig. 2(b) are aggregated to form a diamond of diamonds; by repeating this process *ad infinitum* we generate the diamond hierarchical lattice.

### A. Potts critical amplitude

The free energy per site for the Potts model, Eq. (1), on the diamond hierarchical lattice is given by the convergent<sup>9</sup> series

$$f = \sum_{n=0}^{\infty} 4^{-n} g(J^{(n)}), \quad (22)$$

where<sup>22</sup>

$$g = \frac{3}{4} \ln[2 \exp(2J) + q - 2]. \quad (23)$$

The recursion equation for the exchange coupling is

$$J^{(n+1)} = \ln \left[ \frac{\exp(4J^{(n)}) + q - 1}{2 \exp(2J^{(n)}) + q - 2} \right], \quad (24)$$

and  $J^{(0)} = J$  [the original coupling appearing in Eq. (1)].

In order to find the critical amplitude of  $f_{\text{sing}}$ , the regular part  $f_{\text{reg}}$  was subtracted from the free energy,  $f_{\text{sing}} = f - f_{\text{reg}}$ . The free energy  $f$  is obtained from Eqs. (22)–(24) while  $f_{\text{reg}} = \sum_m f_m (J - J^*)^m$ , with coefficients  $f_m$  calculated by differentiating  $m$  times the equation  $f(J) = g(J) + \frac{1}{4} f(J^{(1)})$  at the fixed point  $J^{(1)} = J = J^*$ . We then computed the amplitude from  $A_{\pm} = f_{\text{sing}}(J) |J - J^*|^{-d/y}$ , with  $d=2$ , for several values of  $J$  close to  $J^*$  until good numerical stability was achieved. The numerical results in Fig. 3 support the ansatz of Sec. III, i.e., the amplitude is a piecewise monotonic function of  $q$ . We find that when  $d/y=2$  and 4 (even integers), corresponding to  $q_1=6.82$  and  $q_2=0.54$ , the amplitude diverges. At  $q=\hat{q}_1=1$  the amplitude is zero, which is a consequence of the fact that for any lattice  $f \sim J$ . A second zero occurs at  $q=\hat{q}_2 \simeq 0.26$ . We also find the following: (i) for any  $q$ ,  $A_+ = A_-$ , and (ii) for  $d/y=3$  and 5 (odd integers), corresponding to  $\bar{q}_1=1.33$  and  $\bar{q}_2=0.29$ , the amplitude does not diverge. This exact result, which is a consequence of duality, is discussed elsewhere.<sup>23</sup> On

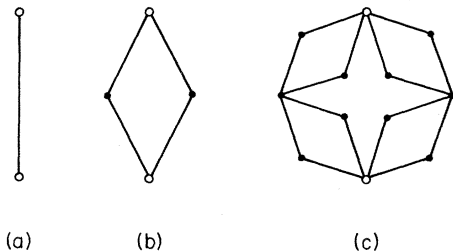


FIG. 2. Diamond hierarchical lattice construction. Iteration levels 0, 1, and 2 are shown in (a), (b), and (c), respectively.

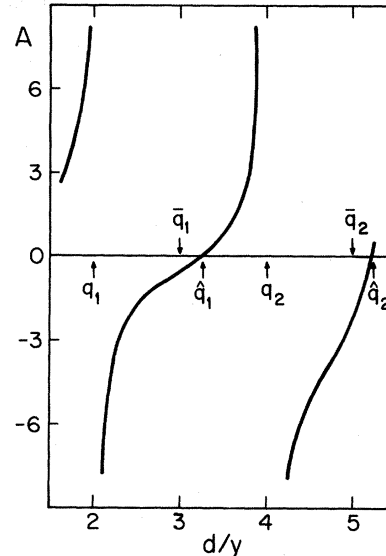


FIG. 3. Amplitude dependence on  $d/y(q)$  for the Potts model on the diamond hierarchical lattice (Migdal-Kadanoff renormalization group,  $b=d=2$ ). The special values  $q_n$ ,  $\bar{q}_n$ , and  $\hat{q}_n$  are marked. Numerical results are displayed for  $1.6 < d/y < 5.3$ .

hierarchical lattices, for fixed  $q$ , the critical amplitude is equal to a constant plus a numerically small periodic function<sup>24</sup> of  $\ln |J - J^*|$ . In the cases we analyzed, the periodic part of the amplitude is very small, about  $10^{-5}$  of the constant part, and does not effect the results quoted in this paper. This is also true for the percolation amplitude which is discussed next.

### B. Bond percolation

The mean number of clusters per lattice site  $G$  for bond percolation is obtained by differentiating the Potts-model free energy per site with respect to  $q$  at  $q=1$ , Eq. (18). By also using<sup>22</sup>  $f(q=1) = 3J$  we find

$$G = \frac{3}{4} \sum_{n=0}^{\infty} 4^{-n} (1 - p_n)^2, \quad (25)$$

where  $p_n = 1 - \exp(-2J^{(n)})$  is the occupation probability for a bond of order  $n$ . The recursion equation for  $p_n$  is

$$p_{n+1} = 2p_n^2 - p_n^4, \quad (26)$$

and  $p_0 = p$  is the occupation probability for the primitive<sup>9</sup> bonds of the lattice. This equation<sup>25</sup> is derived either by setting  $q=1$  in Eq. (24), or alternatively by calculating the probability  $p_{n+1}$  to connect the boundary<sup>9</sup> sites (open circles in Fig. 2) given that a  $n$ th-order bond is present with a probability  $p_n$ . The recursion equation (26) has three fixed points:  $p=0$ , which governs the “nonpercolating phase,”  $p=1$ , which governs the “percolating phase,” and  $p^* = (\sqrt{5}-1)/2 \simeq 0.618$ , which is the percolation threshold on the diamond hierarchical lattice. The “thermal” exponent, corresponding to a singularity  $G_{\text{sing}} \sim |p - p^*|^{2/y}$ , is  $y=0.6115$ , which is compared with den Nijs’s prediction for two-dimensional bond percolation  $y = \frac{3}{4}$ . The dependence of  $G$  on  $p$ , computed by using

Eqs. (25) and (26), is shown in Fig. 4.<sup>26</sup>

We also computed the critical amplitude  $\hat{A}_\pm$  defined through

$$G_{\text{sing}} = \hat{A}_\pm |p - p^*|^{2/\gamma} = G - G_{\text{reg}}, \quad (27)$$

where  $G_{\text{reg}} = \sum_m g_m (p - p^*)^m$ . We find  $\hat{A}_+ = \hat{A}_- \simeq -6.3$  to be compared with series expansions for square-lattice bond percolation<sup>21</sup>  $\hat{A}_+ = \hat{A}_- = -4.24 \pm 0.015$ .

### V. BOND PERCOLATION WITH A FUGACITY WHICH CONTROLS THE NUMBER OF CLUSTERS

In this section we consider bond-percolation processes in the presence of a fugacity which controls the number of clusters. Since the  $q$ -state Potts model is related to this process, as is shown next, we will use the results of Secs. II and III to analyze the singularities of the mean number of clusters as a function of the bond-occupation probability.

This study may be relevant for polymer mixtures undergoing gelation and vulcanization. Indeed, gelation and vulcanization are percolation processes.<sup>27</sup> Moreover, it has been argued<sup>10</sup> that an appropriate choice of polyfunctional units in polymer mixtures amounts to controlling the number of loops in the allowed configurations. Then, it seems plausible that a simple model for these processes is bond percolation in the presence of a fugacity which controls the number of clusters or equivalently the number of loops, since for a lattice of  $N$  sites, and for any graph with  $b$  bonds, the number of loops  $c$  is determined by the number of clusters  $n$ , according to Euler's formula  $c = b + n - N$ .

For reasons which become clear later, we denote the cluster fugacity by  $q$  and the bond occupation probability by  $p$ . As usual, two sites connected through a chain of occupied bonds belong to the same cluster, and single-site clusters are considered also. The mean number of clusters per site is

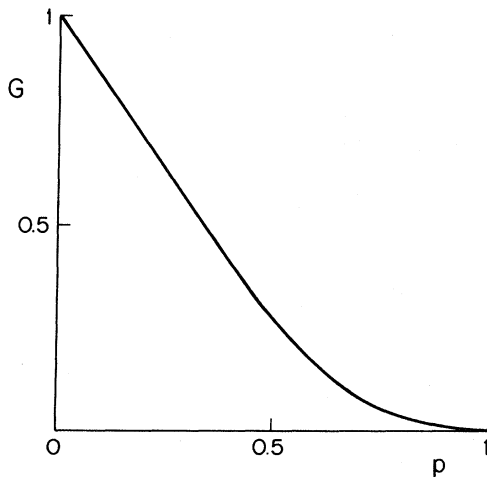


FIG. 4. Mean number of clusters per site  $G$  as a function of the bond-occupation probability  $p$  for the diamond hierarchical lattice (Migdal-Kadanoff renormalization group,  $b = d = 2$ ).

$$G(p, q) = \frac{1}{N} \frac{\sum_{\mathcal{G}} p^{b(\mathcal{G})} (1-p)^{N_b - b(\mathcal{G})} q^{n(\mathcal{G})}}{\sum_{\mathcal{G}} p^{b(\mathcal{G})} (1-p)^{N_b - b(\mathcal{G})} q^{n(\mathcal{G})}}, \quad (28)$$

where the summation is over all possible graphs  $\mathcal{G}$  compatible with the lattice and  $N_b$  is the total number of lattice edges. The fugacity  $q$  controls the number of clusters in the sense that graphs with the same number of bonds  $b$  but with different number of clusters get different weights. When  $q < 1$  the graphs with a smaller number of clusters, or loops, are favored over graphs with greater such numbers, while the reverse holds when  $q > 1$ . When  $q = 1$ , since

$$\sum_{\mathcal{G}} p^{b(\mathcal{G})} (1-p)^{N_b - b(\mathcal{G})} = 1,$$

Eq. (28) reduces to the expression for the mean number of clusters in the regular bond-percolation problem.<sup>1</sup>

The bond-percolation process with a fugacity  $q$  which controls the number of clusters is related to the  $q$ -state Potts model. Indeed, a high-temperature expansion<sup>1</sup> for the partition function is

$$Z = \exp(Nf) = \sum_{\mathcal{G}} \left[ \frac{p}{1-p} \right]^{b(\mathcal{G})} q^{n(\mathcal{G})}, \quad (29)$$

where  $p = 1 - \exp(-2J)$  and  $N$  is the total number of lattice sites. A consequence of Eqs. (28) and (29) is that the mean number of clusters per site as a function of bond-occupation probability  $p$  and fugacity  $q$  is related to the  $q$ -state Potts free energy per site  $f$  according to

$$G = q \frac{\partial f}{\partial q}. \quad (30)$$

This also justifies our notation for fugacity. When  $q = 1$ , Eq. (30) is the usual relationship<sup>1,2</sup> between bond percolation and Potts model with  $q \rightarrow 1$ .

The singularity of  $G$  as a function of  $t(q) \equiv p - p^*(q)$ , where  $p^*(q)$  is the threshold probability, is given by  $G_{\text{sing}} = q \partial f_{\text{sing}} / \partial q$ . For  $\Delta(q) \equiv d/\gamma(q)$  noninteger,  $f_{\text{sing}} \simeq A_{\pm}(q) |t(q)|^{\Delta(q)}$  and

$$G_{\text{sing}} \simeq -q A_{\pm} \Delta \frac{dp^*}{dq} (\text{sgnt}) |t|^{\Delta-1} + q A_{\pm} \frac{d\Delta}{dq} |t|^{\Delta} \ln |t| + q \frac{dA_{\pm}}{dq} |t|^{\Delta}, \quad (31)$$

where  $\text{sgnt}$  equals 1 if  $t > 0$  and  $-1$  if  $t < 0$ . Hence the leading singularity is  $|t|^{\Delta-1}$ . Moreover, in two dimensions  $A_+ = A_-$  so that the amplitudes for  $G_{\text{sing}}$  [Eq. (31)] have opposite signs below and above the threshold probability. However, there is a sequence of  $q$  values,  $\hat{q}_n$  (Sec. III), starting with  $\hat{q}_1 = 1$  where  $A_{\pm} = 0$  and as a consequence

$$G_{\text{sing}} \simeq q \frac{dA_{\pm}}{dq} |t|^{\Delta}.$$

In two dimensions  $dA_+/dq = dA_-/dq < 0$ , Sec. II, so that the amplitude of  $G_{\text{sing}}$  for these special values of  $q$  is the same negative quantity below and above the threshold probability.

When  $\Delta=d/y$  is an integer  $m_0$ , the singularity of  $f$  is the result of the combined contributions  $A_{\pm}|t|^{\Delta}$  and  $f_{m_0}t^{m_0}$  (Sec. II),

$$\begin{aligned} G_{\text{sing}} &\simeq q \lim_{\Delta \rightarrow m_0} \frac{\partial}{\partial q} (f_{m_0} t^{m_0} + A_{\pm} |t|^{\Delta}) \\ &= \hat{a} t^{m_0-1} \ln |t| + \hat{c}_{\pm} |t|^{m_0-1} \\ &\quad + \hat{b} t^{m_0} (\ln |t|)^2 + \hat{e}_{\pm} |t|^{m_0} \ln |t| + \hat{d}_{\pm} |t|^{m_0}, \end{aligned} \quad (32)$$

where

$$\begin{aligned} \hat{a} &= -q m_0 \frac{dp^*}{dq} a, \\ \hat{c}_{\pm} &= -q m_0 \frac{dp^*}{dq} (\text{sgnt}) c_{\pm}, \\ \hat{b} &= q \frac{d\Delta}{dq} a, \\ \hat{d}_{\pm} &= \lim_{\Delta \rightarrow m_0} \left[ q \frac{df_{m_0}}{dq} (\text{sgnt})^{m_0} + q \frac{dA_{\pm}}{dq} \right], \\ \hat{e}_{\pm} &= \lim_{\Delta \rightarrow m_0} \left[ q (\Delta - m_0) \frac{dA_{\pm}}{dq} + q \frac{d\Delta}{dq} A_{\pm} \right], \end{aligned} \quad (33)$$

and  $a$  and  $c_{\pm}$  are given in Eq. (8). The leading singularity is  $G_{\text{sing}} \sim t^{m_0-1} \ln |t|$ , provided  $\hat{a} \neq 0$ . For the square lattice  $a=0$  when  $m_0$  is odd, Sec. II, and thus  $\hat{a}=\hat{b}=0$ . Moreover,  $c_+=c_-$ , Eq. (12), which implies  $\hat{c}_+=-\hat{c}_-$ . Hence in these cases the leading singularity is  $G_{\text{sing}} \sim \hat{c}_{\pm} \text{sgnt} |t|^{m_0-1}$ , i.e., the percolation transition is of  $(m_0-1)$ th order,  $m_0-1=2,4,6,\dots$ , in Ehrenfest's classification.<sup>20</sup>

The simple model for gelation and vulcanization of this section, bond percolation with a cluster fugacity, is consistent with the field-theoretical approach<sup>10</sup> prediction that these processes are in the Potts universality class with  $q$  between zero and one. Our analysis, however, shows that for (most) fugacity values the mean number of clusters singularity is not  $G \sim |t|^{d/y(q)}$ , with  $y(q)$  the  $q$ -state Potts thermal exponent, but  $G \sim |t|^{[d/y(q)-1]}$ . On the other hand, there is a sequence of values of the fugacity  $\hat{q}_n$  [ $A(\hat{q}_n)=0$ ], where the singularity of  $G$  is indeed given by  $d/y(q)$ , and this includes the  $q=1$  case of the usual bond percolation.

## VI. CONCLUSIONS

We presented a study of the two-dimensional Potts-model critical-amplitude dependence on  $q$ . There is a sequence of  $q$  values,  $\{q_n\}$ , given in Eq. (14), at which the critical amplitude diverges and the power-law singularity of the free energy is modified by logarithms. There is evidence for the existence of another sequence of  $q$  values,  $\{\hat{q}_n\}$ , where the critical amplitude vanishes and thus the free energy of the corresponding Potts model does not exhibit the expected singularity. An interesting question is whether there is any singularity at all for the special values  $q=\hat{q}_n$  with  $n>1$ . Estimates for  $\hat{q}_n$ , Eq. (21), were obtained by using Eq. (20), which interpolates between the known divergences of the amplitude at  $q_n$ . We also studied the Potts critical amplitude and bond percolation on the diamond hierarchical lattice.

Our work deals with two-dimensional and hierarchical lattices, but it may be that the main results, such as the generic dependence of the critical amplitude on  $q$ , Fig. 1, will hold in three dimensions, with shifted values for  $q$ . Thus there may be three-dimensional experimental realizations, e.g., for polymer mixtures undergoing gelation and vulcanization. It is also interesting to note that, in general,  $A_+ \neq A_-$  for three-dimensional systems. Hence different singularities could occur above and below the critical temperature at certain values of  $q$  where only one amplitude ( $A_+$  or  $A_-$ ) is zero.<sup>28</sup>

Irrelevant fields and nonlinearities in scaling fields generate corrections to scaling<sup>12,29</sup> which are not discussed in this paper. Further studies of critical amplitudes, perhaps by means of Nightingale's phenomenological renormalization-group<sup>17</sup> or series expansions, are necessary to verify our findings.

## ACKNOWLEDGMENTS

We benefited from discussions with M. Kardar, especially in connection with the interpolation formula for the amplitude. We thank A. N. Berker for numerous comments. We are grateful to A. Aharony, D. Blankschtein, H. Nakanishi, and S. Redner for correspondence and discussions. This research was supported by the Joint Services Electronics Program under Contract No. DAAG29-83-K0003. One of us (M. K.) is the recipient of a Bantrell Fellowship.

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