

## New method for analyzing confluent singularities and its application to two-dimensional percolation

Joan Adler, Moshe Moshe, and Vladimir Privman

*Department of Physics, Technion-Israel Institute of Technology, Haifa, Israel*

(Received 16 December 1981)

Several persistent discrepancies between different results for critical exponents of statistical-mechanical models have recently been shown to originate from inappropriate treatment of confluent singularities. In this paper a new method for evaluating  $\Delta_1$ , the critical exponent of the confluent correction term, from relatively short series expansions is introduced and applied to  $d=2$  isotropic percolation to obtain estimates of both  $\Delta_1$  and  $\gamma$ . The discrepancies noted in the literature between values of  $\gamma$  are clearly shown to be removed by the application of our method.

Confluent singularities (CS) have often caused considerable difficulties in extracting critical exponents from series expansions.<sup>1</sup> For example, the long-standing problem<sup>2,3</sup> of the differences between critical exponents estimated from high-temperature series and from the renormalization group<sup>4</sup> (RG) in the  $d=3$  Ising model has been shown to be caused by improper treatment of CS. Another universality-violating puzzle that has apparently been remedied by a correct analysis of CS is the discrepancies between estimates of critical exponents obtained on different lattices for this model.<sup>2</sup> In this paper we propose a method for analyzing CS that is also adequate for relatively short series and apply it to  $d=2$  isotropic percolation.<sup>5</sup>

The area of percolation is of considerable interest for both its numerous applications<sup>6</sup> and as the  $q \rightarrow 1$  limit of the  $q$ -state Potts model.<sup>7</sup> The behavior of the mean cluster size  $S(p)$  and of  $\mu_0(p)$  the zeroth moment of the pair connectedness is governed by the exponent  $\gamma$ . One has

$$S(p), \mu_0(p) \sim C(p)(p_c - p)^{-\gamma} \text{ for } p \sim p_c^-, \quad (1)$$

where  $p$  is the probability that a bond (site) is occupied in the bond (site) percolation problem. The apparent nonuniversality of certain series estimates of  $\gamma$  and disagreement between RG and series analysis is a long-standing puzzle [the value of  $\gamma$  has been calculated by Monte Carlo,<sup>8</sup> series,<sup>9-11</sup> and RG (Ref. 12) methods]. Several low-density ( $p \rightarrow p_c^-$ )  $S(p)$  series estimates give values of  $\gamma \geq 2.40$ , typical "central" values being 2.42 and 2.43,<sup>9</sup> whereas the  $\mu_0(p)$  series (for the triangular-bond problem) gives  $\gamma = 2.38 \pm 0.02$  (Ref. 10) in

agreement with the high-density ( $p \rightarrow p_c^+$ ) series results.<sup>11</sup> The RG and Monte Carlo estimates may be summarized by the conjectured "exact" value of  $\gamma = 2.3888\dots$ ,<sup>12</sup> which is below the error bounds of several low-density series results.

In this paper we will show that the origin of the systematic errors in some of the series estimates of  $\gamma$  is due to the presence of CS and obtain series estimates of both  $\gamma$  and  $\Delta_1$  [the leading confluent exponent; see Eq. (2) below].

The analysis of CS for two-dimensional percolation might, at first glance, appear to be simpler than the analysis for  $d=3$  Ising models since the value of  $p_c$  is known exactly for several lattices.<sup>5</sup> However, there are several complications, and while we shall now show that some of these can be ignored, others have forced us to develop a special method of analysis for confluent corrections in models with characteristics as specified below.

*A priori*, there are several types of corrections to the leading singularity in Eq. (1). Let us firstly recall the possibility of logarithmic corrections<sup>13-15</sup> in  $d=2$  percolation, whose existence would complicate not only the leading critical behavior, but also the form of the leading CS (which will now involve double logarithms instead of powers<sup>16</sup>). We have chosen to ignore these corrections, following Refs. 14 and 15, and will show that a consistent picture is supported *a posteriori* by our calculations of the power confluent singularity. We consider the critical behavior to be of the form

$$f(p \rightarrow p_c^-) = C_0(p_c - p)^{-\gamma} [1 + a_1(p_c - p)^{\Delta_1} + b_1(p_c - p) + \dots], \quad (2)$$

where the  $b_1$  term arises from the Taylor expansion of the analytic part of  $C(p)$  in Eq. (1). We are not aware of any series estimates of  $\Delta_1$  [for quantities whose critical behavior<sup>17</sup> is of the form of Eq. (1)], although RG field-theoretic<sup>18</sup> (FT) calculations of  $\omega = \Delta_1/\nu$  ( $\omega$  is the derivative of the  $\beta$  function at the fixed point) suggest  $\Delta_1 > 1$ , and a value of  $\Delta_1 = 1.1 \pm 0.3$  can be deduced from Ref. 14.

There are six parameters in Eq. (2) which must be estimated in order to parametrize the leading singularities of the critical behavior for  $d=2$  percolation. However, the available  $S(p)$  and  $\mu_0(p)$  series are relatively short, and this means that most of the series analysis methods that are usually used to study confluent corrections cannot be efficiently applied. We are forced to follow a somewhat less ambitious program and restrict our attention to those cases where exact  $p_c$  values are known.<sup>5</sup> These are the square bond (SQB,  $p_c = \frac{1}{2}$ ), the triangular site (TS,  $p_c = \frac{1}{2}$ ) and bond [TB,  $p_c = 2 \sin(\pi/18)$ ], and the honeycomb bond [HCB,  $p_c = 1 - 2 \sin(\pi/18)$ ] problems. The available series<sup>9,10</sup> are for  $S(p)$  on all four lattices and for  $\mu_0(p)$  in the TB case. We have

$$S(p), \mu_0(p) \simeq 1 + \sum_{r=1}^L b_r p^r, \quad (3)$$

and  $L = 14, 15, 10,$  and  $18$  for the SQB, TS, TB, and HCB problems, respectively (for the HCB case  $b_1 - b_5$  are zero). We also chose to consider the restricted form

$$f(p \rightarrow p_c^-) = C_0 (p_c - p)^{-\gamma} \times [1 + a_1 (p_c - p)^{\Delta_1} + \dots], \quad (4)$$

neglecting the influence of the  $b_1$  term, and thereby assuming that  $|a_1/b_1|$  is sufficiently large to ensure that the  $b_1$  term does not manifest itself in a short power series. This assumption is confirmed *a posteriori* by our results (as will be discussed below). Our last concession is the decision to concentrate our attention on methods that may provide information about the universal exponents  $\gamma$  and  $\Delta_1$ , rather than to elucidate the nonuniversal amplitude  $a_1$ .

In the cases like the  $d=3$  Ising model, where  $\Delta_1 \simeq 0.5$ , the nonanalytic confluent term  $(p_c - p)^{\Delta_1}$  has an appreciable influence on the estimates of the leading exponents. For the  $d=3$  Ising model a good FT estimate of  $\Delta_1$  was available and a suitable method is that of Roskies,<sup>3</sup> which suppresses the influence of the confluent term.<sup>3</sup> In cases

where  $\Delta_1$  is close to unity the confluent term does not appreciably influence the convergence of the usual  $D \log$  Padé and thus  $\gamma$  and  $p_c$  can be calculated rather accurately and then used as input to a procedure that cancels the leading singularity and concentrates on the confluent one. For example, one may construct<sup>19</sup> the series for

$$f_2(p) = (p_c - p) \frac{df(p)}{dp} - \gamma f(p), \quad (5)$$

whose logarithmic derivative has a pole at  $p_c$  with residue  $\Delta_1 - \gamma$  (if  $|a_1/b_1| \gg 1$  or  $\Delta_1 < 1$ ). A typical case where this method proved useful is that of the  $d=2$  directed bond percolation<sup>19</sup> (DBP), where  $\Delta_1 = 1.02 \pm 0.02$ .<sup>20</sup> The values of the DBP critical exponents agree very well with those derived in Reggeon FT (Ref. 21), which is in the same universality class.<sup>22</sup>

In isotropic percolation at  $d=2$ ,  $\Delta_1$  is expected to differ from unity<sup>18</sup> and thus we have a case where the calculation of the leading exponents is appreciably influenced by the  $(p_c - p)^{\Delta_1}$  confluent term. However, we do not have an accurate independent estimate of  $\Delta_1$ , and we have the problem that the series are relatively short. To develop a method to overcome these problems we first follow Ref. 3 and transform the series to an expansion in powers of

$$y = 1 - (1 - p/p_c)^\Delta. \quad (6)$$

However, unlike Ref. 3, we take  $\Delta$  to be variable in what follows and study

$$\begin{aligned} F_\Delta(y) &= f(p(y)) \\ &= p_c^{-\gamma} (1-y)^{-\gamma/\Delta_1} \\ &\quad \times [1 + a_1 p_c^{\Delta_1} (1-y)^{\Delta_1/\Delta} + \dots], \end{aligned} \quad (7)$$

using the biased  $D \log$  Padé method. We analyze

$$\begin{aligned} G_\Delta(y) &= \Delta(y-1) \frac{d}{dy} \ln F_\Delta(y) \\ &= -\gamma + \frac{\tilde{a}_1 \Delta_1 (1-y)^{\Delta_1/\Delta}}{1 + \tilde{a}_1 (1-y)^{\Delta_1/\Delta}}, \end{aligned} \quad (8)$$

where  $\tilde{a}_1 = a_1 p_c^{\Delta_1}$ . This function enables the calculation of curves of  $-G_\Delta(1) = \gamma_{\text{output}}$  as a function of the input  $\Delta$  in the  $(\Delta, \gamma)$  plane.

In the event that  $\Delta = 1$ , we have

$$G_1(y) = -\gamma + \frac{\tilde{a}_1 \Delta_1 (1-y)^{\Delta_1}}{1 + \tilde{a}_1 (1-y)^{\Delta_1}}$$

$$\stackrel{y \sim 1}{\simeq} -\gamma + \tilde{a}_1 \Delta_1 (1-y)^{\Delta_1}, \quad (9)$$

and the calculation of  $G_1(1)$  is simply the usual biased  $D \log$  Padé analysis of  $f(p)$ . The nonanalytic correction term is zero at  $y=1$ ; however, when Padé approximants are formed to a *finite* power series this nonanalytic term causes systematic deviations in the value of  $\gamma$ .

Let us now analyze the case where the input value of  $\Delta$  is very close to the correct  $\Delta_1 \neq 1$ . We linearize  $G_\Delta(y)$  in the difference  $\Delta - \Delta_1$  and retain the leading terms when  $y \rightarrow 1$ . One finds

$$G_\Delta(y) \simeq -\gamma - \tilde{a}_1 (1-y) \ln(1-y) (\Delta - \Delta_1) + O((1-y)), \quad (10)$$

and again there is a nonanalytic term (which vanishes as  $y \rightarrow 1$ ) and which may give small, systematic nonzero contributions to the Padé approximants of the finite power series. However, the effect of these contributions will now be to change the relative *slope* of the curves of the output  $-G_\Delta(1) = \gamma(\Delta)$  values as functions of  $\Delta$ . The curves  $\gamma(\Delta)$ , when evaluated with different Padé approximants, will be linear functions with small slopes when  $\Delta \simeq \Delta_1$ . The different  $\gamma(\Delta)$  curves should intersect at the correct value of  $\gamma$  and  $\Delta_1$ . Of course, in practice, for relatively short series, the  $b_1$  term of Eq. (3) as well as additional finite series effects alters this ideal situation. Thus, we expect the different Padé approximants to produce curves  $\gamma(\Delta)$  that converge near the correct values of  $\gamma$  and  $\Delta_1$ . The only input required in this method is  $p_c$ , which is known exactly in our case.

Using this new algorithm we calculated  $\gamma = -G_\Delta(1)$  as a function of  $\Delta$  for a suitable range of  $\Delta$  values. We evaluated the nine central  $[L, M]$  (largest  $L + M$  and closest to diagonal) Padé approximants for each of the five above-mentioned series. For the SQB, TS, and TB  $S(p)$  and the TB  $\mu_0(p)$  series the results are presented in Figs. 1, 2, 3, and 4, respectively. In these four cases we found the expected behavior: a more or less well-defined linear region of convergence of the different  $\gamma(\Delta)$  curves. These regions are enclosed by the broken line boxes in Figs. 1–4. The effect of CS was not taken into account in past analyses; here we may clearly observe the influence of the confluent terms on the  $\gamma$  estimates. With  $\Delta = 1$

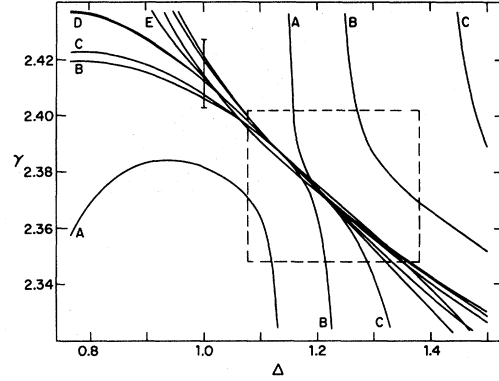


FIG. 1.  $\gamma(\Delta)$  curves for the  $S(p)$  series for the bond percolation problem on the square lattice. The different  $[L, M]$  Padé approximants give curves which are labeled as follows: A, [5,8]; B, [6,6]; C, [5,7]; D, [6,7] and [5,6], and E, [7,6], [8,5], [7,5], and [6,5].

(which is equivalent to ignoring the nonanalytic confluent terms) we see (from the bars in Figs. 1–4) that we would have obtained  $\gamma \geq 2.40$  from the  $S(p)$  series but  $\gamma \sim 2.38$  for the  $\mu_0(p)$  series, consistent with Refs. 9–11. The correct estimates from the boxes are

$$\gamma = 2.375 \pm 0.015, \quad (11)$$

$$\Delta_1 = 1.25 \pm 0.15. \quad (12)$$

The  $\gamma$  estimate is consistent with the exact conjecture, Monte Carlo, and RG results, and with the range of  $\gamma$  values which is consistent with the absence of logarithmic corrections (see Ref. 15). The  $\Delta_1$  value is consistent with the RG FT estimate and the estimate of Ref. 14, justifying the neglect

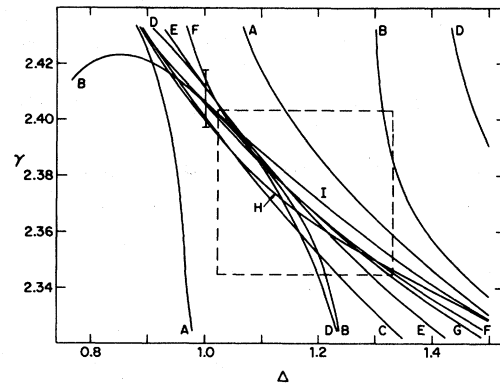


FIG. 2.  $\gamma(\Delta)$  curves for the  $S(p)$  series for the site percolation problem on the triangular lattice. The curves obtained using the [8,5], [5,9], [7,6], [5,8], [6,7], [6,8], [7,7], [9,5], [8,6] Padé approximants are indicated by the letters A, B, C, D, E, F, G, H, I, respectively.

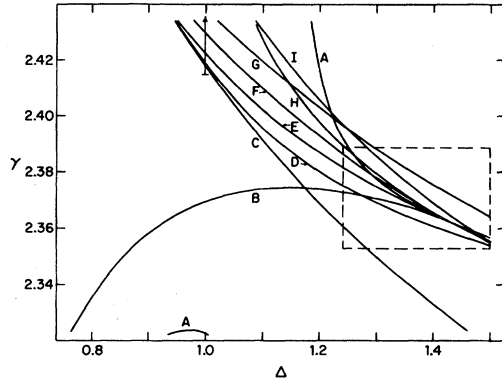


FIG. 3.  $\gamma(\Delta)$  curves for the  $S(p)$  series for the bond percolation problem on the triangular lattice. The curves obtained using the  $[3,6],[4,5],[4,3],[6,3],[5,4],[4,4],[5,3],[3,5],[3,4]$  Padé approximants are indicated by the letters  $A, B, C, D, E, F, G, H, I$ , respectively. The range of values for  $\Delta=1$  extends up to  $\gamma \sim 2.445$ .

of the influence of the  $b_1$  term.

For the HC bond  $S(p)$  series we did not find any systematic trend in the  $\gamma(\Delta)$  curves. This may be explained by the fact that the transformation of Eq. (16) affects the distances of different singularities from the origin in different ways. It is known<sup>9</sup> that there are unphysical singularities near the origin in this model. We suspect that these singularities cause the irregular Padé results here (see also Ref. 3).

We note that the overall slope of the different curves for each series is proportional to the amplitude  $a_1$  [compare Eq. (10)]. We speculate that  $a_1$  has similar values for the three  $S(p)$  series, but  $|a_1(\mu_0)/a_1(S)| \ll 1$ .

The above results concern the intersection of the  $\gamma_{\text{output}}(\Delta_{\text{input}})$  curves defined by the different Padé approximants to  $G_\Delta(1)$  of Eq. (8). It is possible to extend the method of Ref. 19. [Eq. (8)] in a similar manner and obtain  $\Delta_{\text{output}}(\gamma_{\text{input}})$  curves in the  $(\gamma, \Delta)$  plane. An analysis similar to that leading to Eq. (10) may again be performed, giving to leading order in  $p_c - p$

$$D_{\gamma_i}(p) = (p - p_c) \frac{f'_2(p)}{f_2(p)} + \gamma_i$$

$$\stackrel{p \sim p_c^-}{\simeq} \Delta - (\gamma_i - \gamma)(p_c - p)^{-\Delta/a_1}, \quad (13)$$

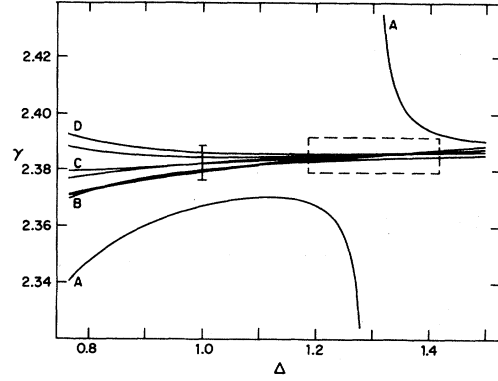


FIG. 4.  $\gamma(\Delta)$  curves for the  $\mu_0(p)$  series for the bond percolation problem on the triangular lattice. The different  $[L, M]$  Padé approximants give curves which are labeled as follows:  $A, [6,3]$ ;  $B, [3,6], [5,4]$ , and  $[4,3]$ ;  $C, [5,4], [4,4]$ , and  $[4,5]$ , and  $D, [3,5]$  and  $[5,3]$ .

where  $\gamma_i = \gamma_{\text{input}}$ ,  $\Delta_{\text{output}} = D_{\gamma_i}(p_c) = \Delta(\gamma_i)$ . The intersection of the different finite series Padé  $\Delta(\gamma_i)$  curves (which have *large* slopes) is expected to be at  $\gamma_i = \gamma$ ,  $\Delta = \Delta_1$ . We have carried out an analysis for all five series with exactly known  $p_c$  values by this technique, but the results are less conclusive than those presented above. The range of spread of the different curves in the  $(\gamma, \Delta)$  plane was similar, but a clear intersection region was only observed for the SQB series, where the  $(\gamma, \Delta)$  range was consistent with Eqs. (11) and (12).

In summary, our analysis provides an explicit example of how the presence of confluent terms introduces severe systematic errors in the values of the leading critical exponents.<sup>23</sup> The technique presented here enables consistent results for confluent exponents to be found from relatively short series. It explains and resolves the “puzzle” of the inconsistent  $\gamma$  estimates in  $d=2$  percolation. We may contrast the current situation with the outlook of Ref. 9 and suggest that longer percolation series may be of use in obtaining more accurate values for both  $\gamma$  and  $\Delta_1$  and to determine the critical amplitude of the correction term.

One of us (J.A.) would like to acknowledge the support of the Lady Davis Fellowship Foundation.

- <sup>1</sup>*Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1974) Vol. 3.
- <sup>2</sup>M. Ferer, *Phys. Rev. B* **16**, 419 (1977); J. J. Rehr, *J. Phys. A* **12**, L179 (1979); S. McKenzie, *ibid.* **12**, L185 (1979).
- <sup>3</sup>R. Z. Roskies, *Phys. Rev. B* **24**, 5305 (1981).
- <sup>4</sup>J. C. LeGuillou and J. Zinn-Justin, *Phys. Rev. B* **21**, 3976 (1980).
- <sup>5</sup>J. W. Essam, *Rep. Prog. Phys.* **43**, 833 (1980); D. Stauffer, *Phys. Rep.* **54**, 1 (1979).
- <sup>6</sup>P. Pfeuty and E. Guyon (unpublished).
- <sup>7</sup>P. W. Kasteleyn and C. M. Fortuin, *J. Phys. Soc. Jpn. Suppl.* **26**, 11 (1969); *Physica (Utrecht)* **57**, 536 (1972).
- <sup>8</sup>*Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Heidelberg, 1979).
- <sup>9</sup>M. F. Sykes, D. S. Gaunt, and M. Glen, *J. Phys. A* **9**, 97 (1976); M. F. Sykes and M. Glen, *ibid.* **9**, 87 (1976).
- <sup>10</sup>A. G. Dunn, J. W. Essam, and D. S. Ritchie, *J. Phys. C* **8**, 4214 (1975).
- <sup>11</sup>C. Domb and C. J. Pearce, *J. Phys. A* **9**, L137 (1976).
- <sup>12</sup>M. P. M. den Nijs, *J. Phys. A* **12**, 1857 (1979); M. P. Nightingale and H. W. J. Blote, *Physica* **104A**, 352 (1980).
- <sup>13</sup>D. Andelman and A. N. Berker, *J. Phys. A* **14**, L91 (1981).
- <sup>14</sup>D. Stauffer, *Phys. Lett.* **83A**, 404 (1981).
- <sup>15</sup>J. Adler and V. Privman, *J. Phys. A* **14**, L463 (1981).
- <sup>16</sup>A. Z. Patashinskii and V. L. Pokrovskii, *Usp. Fiz. Nauk.* **121**, 55 (1977) [*Sov. Phys.—Usp.* **20**, 31 (1977)].
- <sup>17</sup>Estimates for the confluent correction to the “magnetic field” singularity have been made by D. S. Gaunt and M. F. Sykes [*J. Phys. A* **9**, 1109 (1976)] and for the singularity in the generating function for the total number of clusters with  $s$  sites by D. S. Gaunt, M. F. Sykes, and H. Ruskin [*J. Phys. A* **9**, 1899 (1976)].
- <sup>18</sup>A. Houghton, J. S. Reeve, and D. J. Wallace, *Phys. Rev. B* **17**, 2956 (1978).
- <sup>19</sup>J. Adler, M. Moshe, and V. Privman, *J. Phys. A* **14**, L363 (1981).
- <sup>20</sup>Both directed and isotropic percolation have high upper critical dimensions ( $d_c = 5, 6$ , respectively) and we observe that in both cases  $\Delta_1$  increases as  $\epsilon = d_c - d$  increases. We speculate that large values of  $\Delta_1$  may well be found for other systems with high  $d_c$ .
- <sup>21</sup>R. C. Brower, M. A. Furman, and M. Moshe, *Phys. Lett.* **76B**, 213 (1978). The critical exponent  $\lambda = \omega = \Delta_1/\nu$  was first introduced in RFT by W. R. Frazer and M. Moshe, *Phys. Rev. D* **12**, 2370 (1975). For a review of lattice formulation and calculations in RFT see M. Moshe, *Phys. Rep.* **37C**, 255 (1978).
- <sup>22</sup>J. L. Cardy and R. L. Sugar, *J. Phys. A* **13**, L42 (1980).
- <sup>23</sup>We have also applied our method to several  $d = 3$  Ising series. The results which will be presented in the future, are consistent with Ref. 3, and show that  $\nu(\text{series}) = \nu(\text{RG})$  is obtained with a large range of input  $\Delta$  values. [J. Adler, M. Moshe, and V. Privman *Phys. Rev. B* (in press).]