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## Series Expansions **FREE**

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## SERIES EXPANSIONS

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There are three general approaches for understanding the critical behavior of systems that have not been solved exactly. One approach is approximation, e.g., mean-field theory and real-space renormalization-group techniques. However, such approximations often are unreliable in two and three dimensions and are difficult to extend in a controlled manner. A second approach is computer simulation. Simulations would give exact results if the system were infinite and if a sufficient number of independent configurations could be generated. Simulations have had an enormous impact in recent years, but accurate results often require large computer resources and sophisticated algorithms. In addition, it can be difficult to determine that a system has reached equilibrium and to extrapolate the results to the thermodynamic limit. Of course, a simulation is restricted to a particular model in a given spatial dimension at one time. The third general approach is a controlled expansion from a limit where the model can be solved exactly. An example is the momentum-space renormalization-group method, in which an expansion is made from a dimension where the model's critical behavior is known exactly. The method of interest in this column is the series-expansion method, in which a systematic expansion in a small parameter is made from either the ground state or the disordered state. In the series-expansion method, the system is intrinsically infinite, and the solution would be exact if all terms in the expansion were known. As we will see, even a finite number of terms can be usefully extrapolated into the critical region.

In general, the best way to study a model that cannot be solved exactly is to compare the results of simulations, series expansions, and other complementary approaches. Such comparisons have been made for many systems that undergo phase transitions and consistent results have been obtained from series expansions,  $\epsilon$  expansions (generated by the momentum-space renormalization group) and mean-field theory in higher dimensions, and exact results and simulations in lower dimensions.

The series method flowered from 1960 on and provided important input for the ideas of scaling and universality that underlie the renormalization group. Some unpopularity resulted from apparent violations of hyperscaling that were caused by inappropriate extrapolation techniques. The apparent extrapolation problems now are understood and several algorithmic breakthroughs have led to a revival of popularity of the series method.

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Although computers are essential for enumerating a worthwhile number of terms, a workstation usually is adequate. The increased availability of computer algebra, which is well suited for series studies, also has had a substantial impact on the present increased interest in the series approach.

There are many different approaches to the generation of the terms in a series. The generation and analysis stages can be done independently, and most series have been analyzed by several methods. Introductions to series methods for Ising models can be found in Refs. 1 and 2 and in Ref. 3 for percolation.

We have chosen site percolation<sup>3,4</sup> to describe the generation of a series. In site percolation each site is randomly occupied with probability  $p$  and is empty with probability  $q = 1 - p$ . Our goal is to determine the threshold value  $p_c$  at which an infinite (spanning) connected cluster of occupied nearest-neighbor sites occurs, and to describe the nature of the phase transition into the connected phase. A physical analogue of three-dimensional (3D) site percolation is a beaker containing a mixture of metal ball bearings and glass beads. In this case a metal ball bearing corresponds to an occupied site and a glass bead corresponds to a vacant site;  $p_c$  is the threshold at which a transition into the conducting phase occurs as the proportion of metal balls is increased.

We consider the percolation order parameter  $P(p)$ , where  $P(p)$  is the probability that a site belongs to the infinite cluster. The quantity  $P(p)$  is zero for  $p < p_c$  and behaves as  $A_p(p - p_c)^\beta$  for  $p > p_c$ . The exponent  $\beta$  is an example of a critical exponent. The critical exponent  $\gamma$  can be defined from the behavior of the mean cluster size  $S(p)$ , which behaves as  $|p - p_c|^{-\gamma}$  for  $p$  near  $p_c$ . Although there are exact results for  $\beta$  and  $\gamma$  for two dimensions,  $p_c$  is not known exactly for site percolation on the square lattice. The best current estimates of  $p_c$  from simulations<sup>5</sup> for the square lattice and for the simple cubic lattice are shown in Table I. Note that  $p_c$  is known exactly for site percolation on the triangular lattice and for bond percolation on the square lattice. There are no exact results for percolation in three dimensions.

We will see that the series for  $P(p)$  can be determined from a knowledge of  $n_s(p)$ , the mean number of  $s$  clusters per site for  $s = 1, 2, \dots$ . Here we first enumerate  $n_s(p)$  for small  $s$ . We consider a square lattice with  $N$  sites in the limit  $N \rightarrow \infty$ . To find  $n_1(p)$ , we required an occupied site to be surrounded by four vacant nearest-neighbor sites (a perimeter site). The total probability for this case is  $p q^4$ , the mean number of such cases is  $N p q^4$ . Hence the mean number of one site clusters per lattice site,  $n_1(p)$ , is  $p q^4$ . This

Table I. Best known estimates for critical exponents and percolation thresholds. Earlier estimates and results for other three-dimensional lattices are summarized in Ref. 17.

Two dimensions	$\gamma$	$\beta$	$p_c$
Exact	2.3888	1.3888-	
Square site:			
Simulation (Ref. 5)	...	...	0.5927460±0.0000
Series (dlog-Padé with exact exponents)			
$P(p)$ [Fig. 3(a)]	...	...	0.592
$S(p)$ [Fig. 3(b)]	...	...	0.5925
Series (including corrections to scaling all free parameters)			
$S(p)$ (Fig. 4)	2.38±0.05	...	0.59275±0.0001
Three dimensions			
Renormalization group (Ref. 18)	0.34	1.75,1.82	
Simple cubic site:			
Series (dlog-Padé) (Ref. 8)	0.403±0.008	1.73±0.03	0.3117±0.0003
Series (including corrections to scaling)			
Simple cubic bond			
Series (dlog-Padé) (Ref. 8)	0.452±0.018	1.74±0.10	0.2479±0.0004
Simulation (Ref. 5)	0.412±0.010	1.795±0.005	0.248810±0.0000
Series (Ref. 17)	0.405±0.025	1.805±0.02	0.2488±0.0002

configuration is drawn in Fig. 1(a). For a cluster of two connected sites, there are two possible orientations. Because there must be six perimeter sites, we have  $n_2(p) = 2p^2q^6$  [see Fig. 1(b)]. For three connected sites there are two possible shapes with eight and seven perimeter sites, respectively [see Fig. 1(c)]. The linear shape has two orientations and the other shape has four. Hence we obtain  $n_3(p) = 2p^3q^8 + 4p^3q^7$ .

The enumeration of all clusters for large  $s$  is a graph theoretical problem amenable to computer enumeration. (The clusters themselves are known as lattice animals and are of interest in many contexts. For example, see Refs. 3, 6, and 7 for their application to polymers.) To find the  $n_s$ , we need to know  $t$ , the number of perimeter sites needed to isolate a given cluster, and  $g(s,t)$ , the number of independent ways that a cluster of size  $s$  can be placed on the lattice. It is usual to express the result in terms of the perimeter polynomial,  $D_s(q) = \sum_t g(s,t)q^t$ . We write

$$n_s(p) = \sum_t g(s,t)p^s q^t = p^s D_s(q). \tag{1}$$

Perimeter polynomials  $D_s(q)$  have been tabulated for many lattices;<sup>8-10</sup> to the best of my knowledge they exist up to  $s=22$  for site percolation on the square lattice and up to  $s=13$  for site percolation on the simple cubic lattice. A FORTRAN program for the calculation of  $D_s(q)$  has been published by Mertens.<sup>9</sup>

We now show that the  $P(p)$  series can be derived directly from  $n_s(p)$ . For  $p < p_c$ , all occupied sites (probability  $p$ ) belong to finite clusters, and hence we have  $\sum_s s n_s(p) = p$ . [Check this sum rule to  $O(p^2)$  using the results given for  $n_s(p)$  for  $s=1,2,3$ . Remember to set  $q = 1 - p$ .] For  $p > p_c$ , an occupied site either belongs to the infinite cluster [there are  $NP(p)$  such sites] or to a finite cluster. Hence we have  $NP(p) + \sum_s s n_s = p$ , where the sum over  $s$  includes only finite clusters. Hence we obtain

$$P(p) = 1 - \frac{1}{p} \sum_s s n_s(p) = 1 - q^4 - 4q^6 - 8q^7 + \dots \tag{2}$$

The mean cluster size  $S(p)$  also can be expressed in terms of  $n_s(p)$  to generate a (low density) series in  $p$  for  $p < p_c$ , where  $p$  is the natural variable of expansion. We have<sup>3</sup>

$$S(p) = \frac{1}{p} \sum_s s^2 n_s(p). \tag{3}$$

$S(p)$  also has been studied for  $p > p_c$ , but because  $S(p > p_c)$  is not well-behaved, it will not be discussed here. See Ref. 8 for a discussion of the high-density  $S(q)$  series. The series coefficient<sup>8-10</sup> for  $P(p)$  and  $S(p)$  for the square lattice and the simple cubic lattice are given in Table II.

Let us now consider the analysis of the series in Table II. Although each series gives the first several terms of the

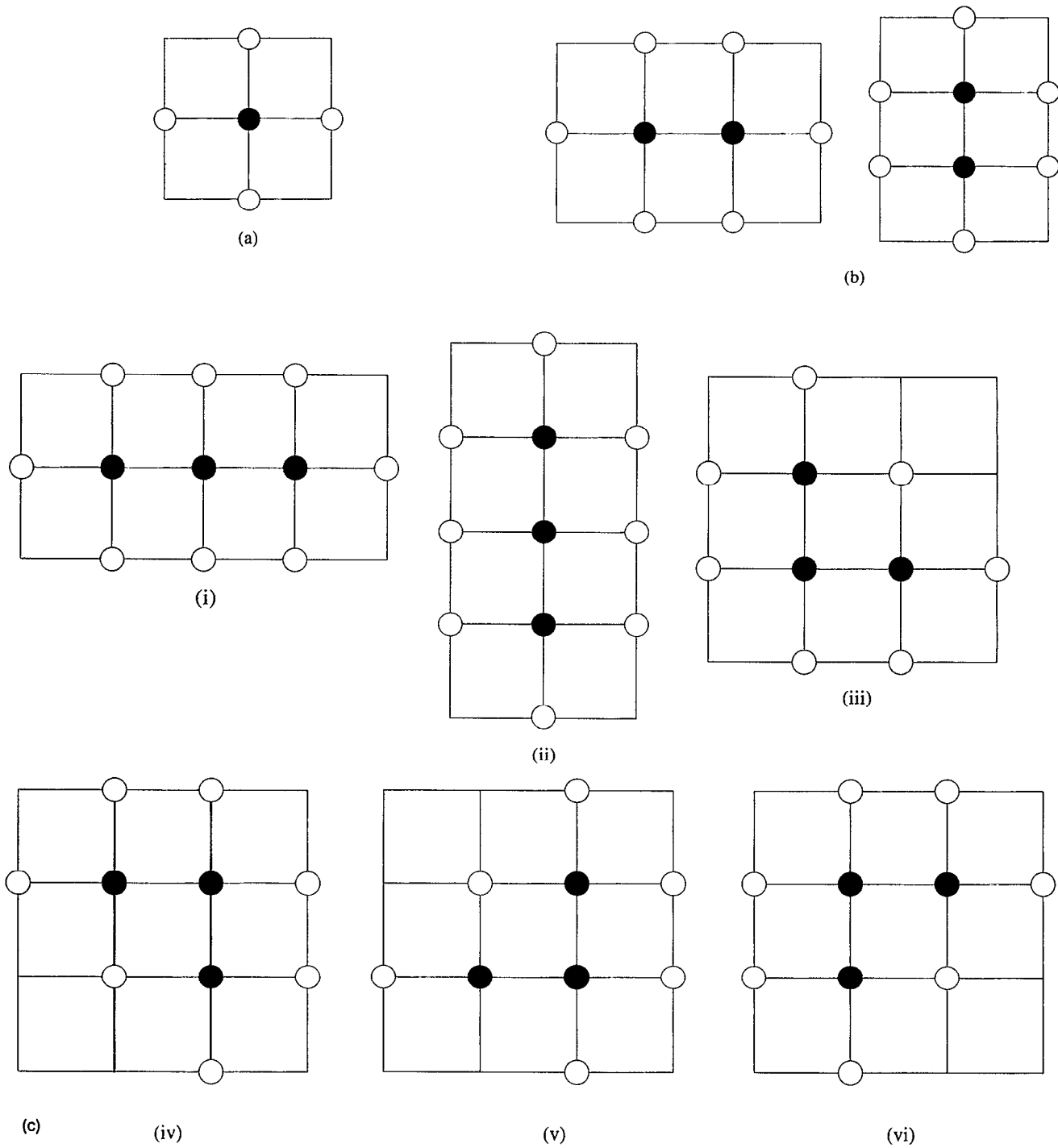


Figure 1. The  $s$  clusters per site for  $s \leq 3$  for the square lattice. Occupied sites are indicated by a filled circle and unoccupied sites by an empty circle. (a) An isolated occupied site corresponding to  $n_1(p) = pq^4$ . (b) The two clusters with two occupied sites. (c) The six clusters with three occupied sites.

exact solution, a simple graph of the series for different values of  $p$  does not give an unambiguous indication of the critical behavior (see Fig. 2). If we compare Fig. 2(a) for  $P(p)$  with Fig. 2(b) for  $S(p)$ , we see that  $S(p)$  has a maximum suggesting a divergence above  $p = 0.6$ , but  $P(p)$  in-

dicates a transition closer to  $p = 0.5$ . A more reliable evaluation is possible by identifying the critical point with the radius of convergence of the series. The usual procedure is to determine the location and nature of the critical point using the logarithmic derivative (dlog) of the series. It is

Table II. The series coefficients for  $P(p) = \sum_n a_n q^n$  and  $S(p) = \sum_n b_n p^n$  for the square lattice, and  $P(p) = \sum_n c_n q^n$  and  $S(p) = \sum_n d_n p^n$  for the simple cubic lattice. The results are taken from Refs. 8-10.

$n$	$a_n$	$b_n$	$c_n$	$d_n$
0	1	1	1	1
1	0	4	0	6
2	0	12	0	30
3	0	24	0	114
4	-1	52	0	438
5	0	108	0	1542
6	-4	224	-1	5754
7	-8	412	0	19574
8	-23	844	0	71958
9	-28	1528	0	233574
10	-186	3152	-6	870666
11	48	5036	6	2696274
12	-1301	11984	0	10375770
13	1412	15040	-36	30198116
14	-12292	46512	63	122634404
15	30384	34788	-50	
16	-142441	197612	-117	
17		4036	360	
18		929368	-602	
19		-702592	654	
20		4847552	-1035	
21		-7033956	1940	
22		27903296	-2789	
23		-54403996	354	
24			9425	
25			-32384	
26			71838	
27			-131188	
28			196124	
29			-196560	
30			-22889	
31			602852	
32			-1714585	
33			4104136	

based on the idea that if we take the dlog of a function, say  $S(p)$ ,

$$\frac{d}{dp} \left( \ln \sum_n b_n p^n \right) \propto \frac{\gamma}{(p_c - p)}, \quad (4)$$

then the right-hand side of Eq. (4) will have a pole at  $p = p_c$  with a residue of  $\gamma$ .

Because calculating the pole and the residue of the series directly is not successful in general, Padé approximants and their poles and residues are calculated.<sup>11</sup> Padé approximants are polynomial ratios that are used in many contexts,<sup>12</sup> and in general work better than we might expect. The  $[L, M]$  Padé approximant ( $L + M \leq N$ ) to a series of

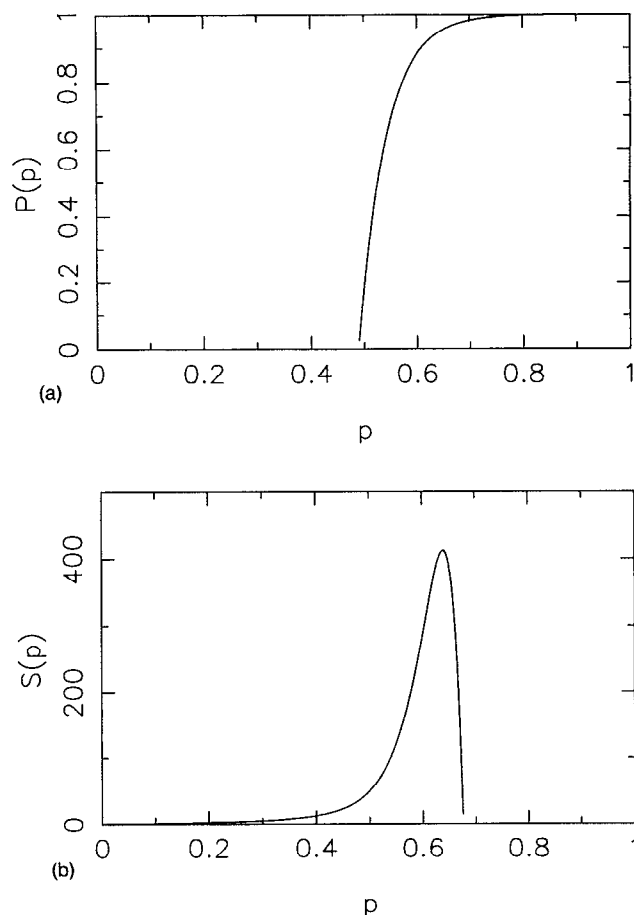


Figure 2. Sum of the terms in the series for  $P(p)$ , part (a), and  $S(p)$ , part (b), as functions of  $p$ . Note that it is difficult to determine both the exponents and the threshold for the critical behavior from these plots.

order  $N$  is the ratio of a polynomial of order  $L$  to a polynomial of order  $M$ , such that when the denominator of the approximant is divided into the numerator, the first  $L + M + 1$  terms of the expansion of the Padé approximant match the first  $L + M + 1$  terms of the series. The approximants can be calculated using standard computer languages such as Fortran or using computer algebra packages such as MATHEMATICA and MAPLE. The Fortran approach is more efficient, but requires many more lines of code.

We give in Table III a sample program for calculating Padé approximants using MATHEMATICA. The program is simple enough for someone with no prior MATHEMATICA experience. In this program the series is denoted by "t," and the variable  $p$  or  $q$  is denoted by "K." This choice of notation leads to minimal confusion with reserved words in MATHEMATICA. The code given in Table III inputs the series, uses certain built-in MATHEMATICA commands for handling Padé approximants, gives the order of the series, calculates the logarithmic derivative, obtains the roots of the denominator of the Padé approximant, defines an expression for the numerator, and defines an expression for the



**Table III. MATHEMATICA program for the evaluation of Padé approximants.**

```
t = 1.0 + 4.0*K + 12.0*K^2 + 24.0*K^3 + 52.0*K^4 +
108.0*K^5 + 224.0*K^6 + 412.0*K^7 + 844.0*K^8 +
1528.0*K^9 + 3152.0*K^10 + 5036.0*K^11 + 11984.0*K^12 +
15040.0*K^13 + 46512.0*K^14 + 34788.0*K^15 + 197612.0*K^16 +
4036.0*K^17 + 929368.0*K^18 -702592.0*K^19 + 4847552.0*K^20 -
7033956.0*K^21 + 27903296.0*K^22 -54403996.0*K^23

<<"Calculus'Padé"

order=23;

ft=N[Collect[D[Normal[Series[Log[t],{K,0,order}]],K],K],60];

pp[l_,m_] :=Roots[Denominator[Padé[ft,{K,0,1,m}]]==0,K];
qq[l_,m_] :=Numerator[Padé[ft,{K,0,1,m}]];
rr[l_,m_] :=D[Denominator[Padé[ft,{K,0,1,m}]],K];
```

derivative of the denominator. The program can be used to calculate different approximants interactively. We have selected the series for the square lattice  $S(p)$  from Table II. The following instructions are for a Unix system. Copy the program in Table III to a file called "mpad," enter the MATHEMATICA program (type 'math'), and type '<<mpad' in response to the prompt 'In[1]:='. In response to 'In[2]:= ', the roots for the  $[L, M]$  approximant, a good first choice can be found by entering 'pp[10,10]' ( $L=M=10$ ).

For the choice pp[10,10] and the choices of  $L, M$ , there are usually many roots, most of them complex. The one of interest usually is the smallest positive real root. (Sometimes there are very small positive real poles, known as "defective poles," but the physical root corresponding to the percolation transition is usually the smallest real root.) For  $L=M=10$ , the smallest positive real root is 0.590317, i.e., the [10,10] approximant gives an estimate of  $p_c=0.590317$ . In response to the next prompt, 'In[3]:= ', the residue for the [10,10] case can be calculated by entering the command 'qq[10,10]/rr[10,10] / K--0.590317', to which a response of '-2.27629' should be found, indicating an estimate of  $\gamma=2.27629$ . (The minus sign in the response from MATHEMATICA is due to the fact that the derivative with respect to  $p$  of the denominator in Eq. (4) is  $-1$ .) A set of approximants can be found by evaluating pp and qq/rr for different values of  $L$  and  $M$ . Approximants are usually selected to have high  $L$  and  $M$  values, with  $L \approx M$ . For example, results for  $(L, M, p_c, \gamma)$  are (10, 11, 0.593286, 2.42996) and (11, 11, 0.592045, 2.35476).

The MATHEMATICA program in Table III requires some extensions to enable a large number of poles and residues to be tabulated and sorted so that the physical root can be selected and then plotted. More efficient FORTRAN programs for series analysis are available from several sources. These programs include subroutines for the input of the terms of the series, the calculation of the desired Padé approximants, subroutines for the calculation of the poles and residues, and subroutines for tabular and graphical output. A good general reference to series analysis (with programs available on diskette) is by Guttman.<sup>13</sup> If there are complications

such as more than one expansion variable, more sophisticated approximants must be considered. Differential and partial-differential approximants are two such methods. Some excellent partial-differential approximant routines are described in Ref. 15. For the square site  $S(p)$  series, pole-residue values for  $L=M \geq 8$  are given in Table IV.

Once the individual poles and residues have been obtained, we must decide how to deduce the overall estimate for  $p_c$  and the exponents. Simple averaging is not always desirable and the usual first step is to graph all the residues as functions of the pole location for a range of physical poles that fall reasonably close together. Examples of such pole-residue plots for the  $P(p)$  and  $S(p)$  square site series are given in Fig. 3. Note the clustering near certain values of  $p_c$  and  $\gamma$  and the tendency of these values to fall on a reasonably straight line. When the exact exponents are known (see Table III), we can evaluate the threshold by reading off the  $p$  value that corresponds to the exact exponent. An approach that is useful for evaluating exponents in cases, where the threshold is known exactly or to high precision from simulations is to take threshold-biased approximants. This approach can be implemented by multiplying both sides of Eq. (4) by  $p-p_c$ , calculating Padé approximants, and then evaluating them at  $p=p_c$  to give a direct estimate of  $\gamma$ .

The exact values, the best known values from series,<sup>17</sup> simulations,<sup>5</sup> and estimates from the plots of Fig. 3 are compared in Table I. For completeness, some results from the series for bond percolation also are given. We have discussed site rather than bond percolation because the generation of series for site percolation is easier to explain. However, in general, the series for bond percolation are better behaved. Discussions of bond-percolation series (the generation of the series from perimeter polynomials and the dlog Padé analysis) in lower dimensions are given in Refs. 8 and 10. The generation of low-density bond-percolation series for all dimensions simultaneously using the No-Free-End graph approach<sup>16</sup> is discussed in Ref. 17. A comparative analyses of these series and other bond-percolation series,<sup>10</sup> results from simulations,<sup>5</sup> and renormalization-group studies<sup>18</sup> cited in Table I also are discussed in Ref. 17.

From Table I we see that the agreement of the simple dlog Padé results with the other estimates shown is good, but there is uncertainty in cases where there is no independent determination of the exponent or the threshold. There also are small discrepancies which were sufficient to lead to violations of hyperscaling in early bond-percolation and three-dimensional Ising analyses. Improved exponent and  $p_c$  estimates can be found from the series of Table II by extending the analysis techniques. These extensions are based on noting that the critical behavior is more complex than a single power-law divergence and has additional confluent (same-place) singularities.<sup>19</sup> The idea is to replace the simple form,  $S(p) \sim (p_c - p)^{-\gamma}$ , by  $S(p) \sim (p_c - p)^{-\gamma} [1 + a(p_c - p)^{\Delta}]$ , and to transform the series to minimize the interference of the additional terms prior to calculating the approximants. One method, which is a variant of the threshold-biased dlog Padé, has been extensively applied to percolation.<sup>19,20</sup> The method is based on a gen-

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Table IV. Results of dlog Padé analysis for the  $S(p)$  using the MATHEMATICA program in Table III. A pole of  $0.1E+10$  indicates that no real pole was found, and an  $s$  following the residue indicates a defective pole.

Residues and Poles of the Logarithmic derivative:		Pole	Residue
$L = 8$	$M = 8$ :	$0.5856313648E+00$	$-0.2118336235E+01$
$L = 9$	$M = 8$ :	$0.5925216637E+00$	$-0.2374458407E+01$
$L = 10$	$M = 8$ :	$0.5856835174E+00$	$-0.2054507444E+01$
$L = 11$	$M = 8$ :	$0.5925495961E+00$	$-0.2382779636E+01$
$L = 12$	$M = 8$ :	$0.5926821075E+00$	$-0.2389494843E+01$
$L = 13$	$M = 8$ :	$0.5923431576E+00$	$-0.2371047262E+01$
$L = 14$	$M = 8$ :	$0.5920057326E+00$	$-0.2351559017E+01$
$L = 8$	$M = 9$ :	$0.6003582740E+00$	$-0.2896518869E+01$
$L = 9$	$M = 9$ :	$0.5906550721E+00$	$-0.2289691929E+01$
$L = 10$	$M = 9$ :	$0.5911466232E+00$	$-0.2312226265E+01$
$L = 11$	$M = 9$ :	$0.5926957737E+00$	$-0.2390243512E+01$
$L = 12$	$M = 9$ :	$0.5925816595E+00$	$-0.2384314229E+01$
$L = 13$	$M = 9$ :	$0.5942965791E+00$	$-0.2438870213E+01$ s
$L = 8$	$M = 10$ :	$0.1000000000E+10$	$0.0000000000E+00$ s
$L = 9$	$M = 10$ :	$0.5912777153E+00$	$-0.2318862152E+01$
$L = 10$	$M = 10$ :	$0.5903165650E+00$	$-0.2276293146E+01$ s
$L = 11$	$M = 10$ :	$0.5923064527E+00$	$-0.2369246659E+01$
$L = 12$	$M = 10$ :	$0.5909769253E+00$	$-0.2281835245E+01$
$L = 8$	$M = 11$ :	$0.5951643941E+00$	$-0.2541617662E+01$
$L = 9$	$M = 11$ :	$0.5929326371E+00$	$-0.2408101614E+01$
$L = 10$	$M = 11$ :	$0.5932862204E+00$	$-0.2429955025E+01$
$L = 11$	$M = 11$ :	$0.5920447450E+00$	$-0.2354762283E+01$
$L = 8$	$M = 12$ :	$0.5941071468E+00$	$-0.2478668789E+01$
$L = 9$	$M = 12$ :	$0.5931901997E+00$	$-0.2423632990E+01$
$L = 10$	$M = 12$ :	$0.5929826282E+00$	$-0.2410954786E+01$
$L = 8$	$M = 13$ :	$0.5887310758E+00$	$-0.2060213296E+01$
$L = 9$	$M = 13$ :	$0.5214158748E+00$	$-0.2359175878E-01$
$L = 8$	$M = 14$ :	$0.5973578638E+00$	$-0.2599570038E+01$ s

eralization of the Roskies transform. In the method the series in  $p$  is transformed to one in the variable  $y = 1 - (1 - p/p_c)^{\Delta_1}$ . We obtain Padé approximants to the series  $G(y) = \Delta_1(y-1)d[\ln S(p)]/dp$ . At the correct value of  $\Delta_1$ , a set of different high and near-diagonal threshold-biased approximants of  $G(y)$  all should give the correct  $\gamma$ . It can be shown<sup>19</sup> that deviations from the correct value will be seen as changes in the slope of the  $\gamma$  estimates plotted as a function of the input value of  $\Delta_1$ . Such a plot leads to an intersection region near the correct  $(\Delta_1, \gamma)$  point. A related method involves calculating the logarithmic derivative of  $B(p) = \gamma S(p) - (p_c - p)d[S(p)]/dp$ , which has a pole at  $p_c$  with residue  $\gamma - \Delta_1$ . Again threshold-biased approximants are calculated and graphed, and an intersection region is found near the correct  $(\Delta_1, \gamma)$  point. Such a plot for the square-site  $S(p)$  series of Mertens<sup>9</sup> is given in Fig. 4. Interactive graphics subroutines are very useful for these methods and are available from PINET (see below).<sup>14</sup> The methods were used<sup>19,20</sup> to show that although some dlog Padé exponent estimates from two-dimensional percolation series violate hyperscaling, an allowance for confluent cor-

rections gives exponent estimates that agree with hyperscaling and exact results. If the value of  $p_c$  is not known, different trial values are tested and convergence in the three-dimensional  $p_c, \gamma, \Delta_1$  space is sought. For the series in Table II, improved estimates from these methods and other more sophisticated analyses<sup>14</sup> are shown in Table I.

The range of physics that can be studied with series expansions is very broad. In addition to disordered systems<sup>21</sup> such as random resistor networks, phase transitions in polymers and a wide variety of magnetic systems are amenable to series expansion study. Current research includes Ising models in random fields,<sup>22</sup> Heisenberg and  $xy$  systems,<sup>23</sup> quantum magnetism,<sup>24</sup> spin glasses of different kinds,<sup>25,26</sup> and crystal growth.<sup>27</sup> In many cases simulation and series studies are being done, leading to a much more reliable overview than either method would give alone.<sup>28</sup> Series expansions also can help ensure the reliability of simulations away from the critical region by comparing the results of simulations to the estimates made from the sum of the first few terms of a series. References that are accessible to novices on different aspects of series generation and

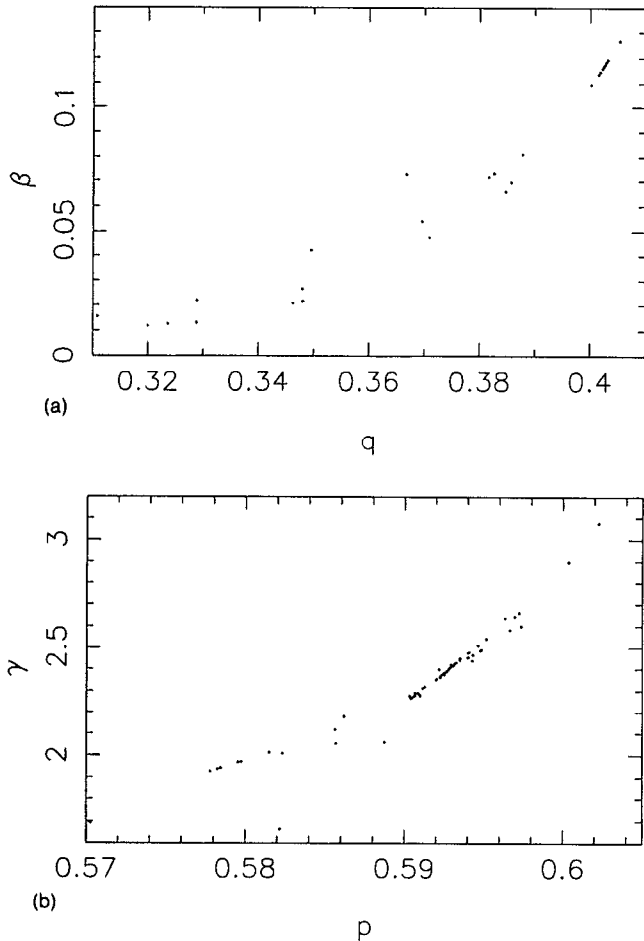


Figure 3. (a) Pole-residue plots for the residue  $\beta$  as a function of the pole  $q$  from the  $P(p)$  series. (b) The residue  $\gamma$  as a function of the pole  $p$  from the  $S(p)$  series. The exact exponent values are indicated by asterisks.

analysis were given above<sup>1-3,13-15</sup> and also include Ref. 25, where star graphs, which are a powerful method for series generation, are discussed. In general, the advantages of series expansions relative to simulations are that they often can be calculated simultaneously for all dimensions and all values of a physical parameter such as magnetic field. Their disadvantage is that they are less versatile than simulations and cannot be adapted quickly to a minor change in the functional form of a Hamiltonian.

### Suggestions for further study

1. Implement the MATHEMATICA program of Table III and collect estimates to draw a pole-residue plot similar to that of Fig. 3 for the  $S(p)$  series given in Table II.
2. Do a hand calculation or use the program of Mertens<sup>9</sup> to obtain several additional perimeter polynomials and  $n_s$  values for square and simple-cubic site percolation. Then obtain some further terms for the  $P(p)$  and  $S(p)$  series and compare your results with Table II.

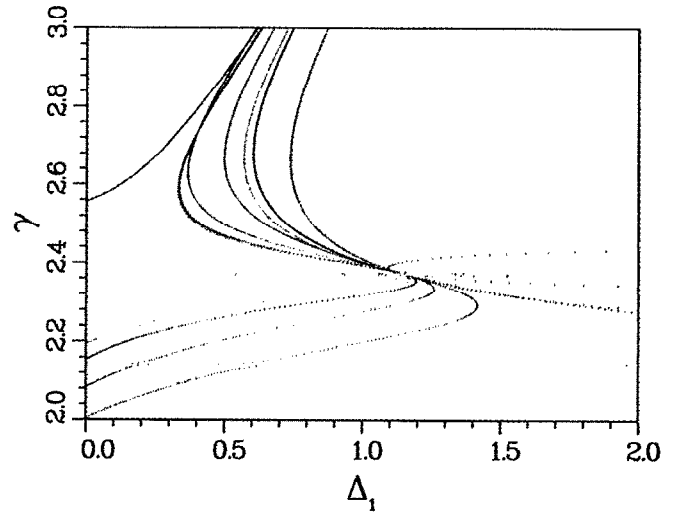


Figure 4. Estimates of  $\gamma$  and  $\Delta_1$  from Padé approximants of the function  $B(p) = \gamma S(p) - (p_c - p)d[S(p)]/dp$  for the square-site  $S(p)$  series.

3. (more difficult) An extended  $P(p)$  series can be calculated from the additional perimeter polynomials.<sup>9</sup> To my knowledge this extended series and its analysis have not been published. This author would be happy to hear from anyone completing this analysis.

4. Extend the MATHEMATICA program in Table III (or write a FORTRAN program) to prepare a full table of poles and residues for the  $S(p)$  and  $P(p)$  series. (Generate the table of values in a single program using suitable loops.) Compare the exponent results obtained in this way to those obtained from threshold-biased approximants. Threshold-biased approximants for  $\gamma$  can be calculated by taking Padé approximants of the series for  $d(\ln \sum_n b_n p^n)(p_c - p)/dp$  (see Table II) and evaluating the approximants at the best known values for  $p_c$ .

5. MAPLE is a computer algebra package that also can be used for series generation and analysis. A MAPLE program equivalent to the one in Table III and the steps described in the text for the  $[10,10]$  approximant are listed in Table V.

Table V. MAPLE program for the evaluation of Padé approximants. The series coefficients are taken from Ref. 29.

```
Digits:=60;
t := 1.0 + 4.0*K + 12.0*K^2 + 24.0*K^3 + 52.0*K^4\
+ 108.0*K^5 + 224.0*K^6 + 412.0*K^7 + 844.0*K^8\
+ 1528.0*K^9 + 3152.0*K^10 + 5036.0*K^11 + 11984.0*K^12\
+ 15040.0*K^13 + 46512.0*K^14 + 34788.0*K^15 + 197612.0*K^16\
+ 4036.0*K^17 + 929368.0*K^18 -702592.0*K^19 + 4847552.0*K^20\
-7033956.0*K^21 + 27903296.0*K^22 -54403996.0*K^23;

c := collect(diff(normal(series(ln(t),K=0,23)),K),K);
pade := convert(c,ratpoly,10,10);
pc := fsolve(denom(pade)=0,K);
residue := numer(pade)/diff(denom(pade),K);

gg := subs(K=.5903165654,residue);
```

Table VI. Series coefficients for the Ising model susceptibility (Ref. 29)  $\chi(v) = \sum_n a_n v^n$  for the square lattice and  $\chi(v) = \sum_n b_n v^n$  for the bcc lattice, where  $v = \tanh(J/kT)$  is the high temperature expansion parameter. The last column gives the directed percolation series  $S(p) = \sum_n c_n p^n$  for the square lattice (Ref. 31).

$n$	$a_n$	$b_n$	$c_n$
0	1	1	1
1	4	8	2
2	12	56	4
3	36	392	8
4	100	2648	15
5	276	17864	28
6	740	118760	50
7	1972	789032	90
8	5172	5201048	156
9	13492	34268104	274
10	34876	224679864	466
11	89764	1472595144	804
12	229628	9619740648	1348
13	585508	62823141192	2300
14	1486308	409297617672	3804
15	3763460	2665987056200	6450
16	9497380	17333875251192	10547
17	23918708	112680746646856	17784
18	60080156	731466943653464	28826
19	150660388	4747546469665832	48464
20	377009364	30779106675700312	77689
21	942106116	199518218638233896	130868
22	2350157268		207308
23	5855734740		350014
24	14569318492		548271
25	36212402548		931584
26	89896870204		1433966
27	222972071236		2469368
28	552460084428		3725257
29	1367784095156		6510384
30	3383289570292		9590838
31	8363078796612		17192714
32	2065605460804		24357702
33	50987841944612		42428434
34	125771030685740		62388268
35			119938514

Do any of the above problems using MAPLE and compare your results. Suggestions: Copy the program in Table V into a file called "mappad." We use " " quotes around a filename and ' ' quotes around a computer command. The type of quote in MAPLE in certain commands such as read must be entered exactly as written below. The "mappad" file can be accessed by typing maple and then responding to the >prompt and 'read 'mappad';'. It also is possible to use the symbolic toolbox of Matlab. I found that it was necessary to break the long definition of the series into several

parts, each a line long and to add an 'end;' statement. If the modified file is called "mappad.m," enter Matlab and write 'procread('mappad.m')'. Enter the file into the Maple toolbox, and then ask questions such as 'maple('pc')' or 'maple('gg')'. The routines used for the evaluation of polynomials in the most recent version, MAPLE V, version II, which is the MAPLE kernel in Matlab 4.1.1, differ from previous versions. In the new version be careful to use integers for the series coefficients. Because this is not always possible, define `Digits` explicitly when working with the routine `convert(ratpoly)`.

6. The high-temperature Ising-model susceptibility series<sup>29</sup> is shown in Table VI for the square lattice. In this case the exact values of  $T_c$  and  $\gamma$  can be reproduced easily. Determine how many terms in the series you need to obtain agreement to two significant figures with the exact values. (more difficult) Series of any length for the low-temperature susceptibility and magnetization can be generated with MATHEMATICA or MAPLE from the exact solution for the Ising model in two dimensions. Generate these series to 10th, 20th, and 30th order and analyze them. Compare your results with the exact values and with the high temperature series results.

7. (more difficult) Confirm the result that the bcc Ising series of Table VI yields exponent estimates that violate hyperscaling and disagree with simulation and renormalization-group results if analyzed with dlog Padé methods. Then use one of the transforms that allows for corrections to scaling to obtain results that agree with the renormalization-group estimate of  $\gamma \approx 1.238$ . Compare your results to those in Ref. 30, where a summary of results for the bcc and other lattices are listed.

8. Series for directed percolation are given in Ref. 31 and reproduced in Table VI. Analyze these series and determine  $p_c$  and critical exponents for directed percolation. Are the values higher or lower than for usual (isotropic) percolation?

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search. Information on this workshop and subscription to the associated listserv information list can be obtained by email to series94@phjoan.technion.ac.il.

*From the editors.* A version of the FORTRAN program called magpole.for, used to generate Table IV, and some of the interactive programs from Ref. 14 are available by FTP, using a special password (see p. 254). To obtain these programs, FTP to "pinet.aip.org" and go to the subdirectory "cip/sourcecode." For more information on this service, contact [pum@aip.org](mailto:pum@aip.org). We currently are working on the second edition of our undergraduate text on computer simulation and would especially appreciate any suggestions you might have for its improvement. We also will present a workshop on "Teaching a Computer Simulation Laboratory for students with diverse backgrounds and interests" at the summer AAPT meeting, University of Notre Dame, 8–13 August 1994. Please send comments and suggestions to [hgould@clarku.edu](mailto:hgould@clarku.edu) or [jant@kzoo.edu](mailto:jant@kzoo.edu).

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