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# **Directed percolation: series expansions for some** three-dimensional lattices

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Abstract. Low density series expansions have been obtained for the directed cubic lattice bond problem and the directed cubic and body centred cubic lattice site problems. Estimates of the critical probabilities and critical exponents  $\gamma$ ,  $\gamma_0$ ,  $\nu_{\parallel}$ ,  $\nu_{\perp}$  for these problems are obtained. The exponent values are found to be consistent with the universality of directed percolation and Reggeon field theory and the hyperscaling relation  $\beta = (D\nu_{\perp} + \nu_{\parallel} - \gamma)/2$ .

### 1. Introduction

Recently there has been considerable interest in the directed percolation problem which was first formulated by Broadbent and Hammersley (1957) in terms of fluid flowing through a random medium. In this paper we consider models in which there is some (cartesian) axis such that the fluid flow always has a positive component along this axis (the 'preferred' axis or direction). Models with this property are in a different universality class from isotropic percolation (Blease 1977a,b,c, Obukhov 1980); however, Cardy and Sugar (1980) showed them to be in the same universality class as Reggeon field theory. These models have two connectedness lengths  $\xi_{\parallel}$  and  $\xi_{\perp}$ (Kinzel and Yeomans 1981), and based on the equivalence with Reggeon field theory Cardy and Sugar (1980) proposed a scaling form for the pair connectedness of a site at *r* relative to the origin which may be written

$$C(\mathbf{x},t) \approx S \boldsymbol{\xi}_{\perp}^{-D} \boldsymbol{\xi}_{\parallel}^{-1} \Phi(\mathbf{x}/\boldsymbol{\xi}_{\perp},t/\boldsymbol{\xi}_{\parallel})$$
(1.1)

where S is the mean cluster size, t is the component of r parallel to the preferred axis and x is the D-dimensional component perpendicular to the preferred axis.

In the random media considered here the fluid flows along the nearest-neighbour bonds of an infinite regular lattice. The passage of the fluid is interrupted by randomly placed dams on the bonds (or sites). If p is the probability that a bond (or site) is not dammed, the percolation probability P(p) is the probability that the region wetted by fluid introduced at the orgin is unbounded. The critical probability  $p_c$  is defined by  $p_c = \sup\{p : P(p) = 0\}$  and it will be assumed that near  $p_c$ 

$$\begin{split} P(p) &\approx (p - p_{c})^{\beta}, \qquad p \to p_{c}^{+}, \\ S &\approx |p_{c} - p|^{-\gamma}, \qquad \xi_{\perp,\parallel} \approx |p_{c} - p|^{-\nu_{\perp,\parallel}}, \qquad p \to p_{c}. \end{split}$$

The equivalence with Reggeon field theory leads to the hyperscaling relation (Cardy and Sugar 1980)

$$\boldsymbol{\beta} = (\boldsymbol{D}\boldsymbol{\nu}_{\perp} + \boldsymbol{\nu}_{\parallel} - \boldsymbol{\gamma})/2. \tag{1.2}$$

The mean number of sites on the preferred axis reached by fluid flowing from the origin  $S_0$  is also singular at  $p_c$  with critical exponent  $\gamma_0$ . Integration of C(0, t) together with the scaling form (1.1) leads to the scaling relation (De'Bell and Essam 1983a, hereafter referred to as I)

$$\gamma_0 = \gamma - D\nu_\perp. \tag{1.3}$$

In I estimates of the exponents for the two-dimensional problems considered were found to be in excellent agreement with the scaling relation (1.2). However, difficulties arising (presumably) from insufficient length of series led to some ambiguity with respect to (1.3). In this paper the low density series for three-dimensional systems are analysed and the critical exponents serve to confirm the common universality class of directed percolation and Reggeon field theory and provide a test of the above scaling relations. The results are summarised in table 2.

### 2. Series expansions and analysis

The simple cubic (sc) and body centred cubic (BCC) lattices are considered and half the number of bonds at each site are directed outwards so as to form the edges of a pyramid with axis in the preferred direction. Low density expansions for S,  $S_0$ , and the second moments

$$\mu_{2x} = \sum_{r} x^{2} C(r)$$
 and  $\mu_{2t} = \sum_{r} t^{2} C(r)$ 

are obtained. The results for the bond problem on the sc lattice and the site problem on the sc and BCC lattices are tabulated in appendix 1. The first eight terms of the mean size series for the sc lattice bond problem have already been given by Blease (1977a).

The sc lattice bond problem series were obtained by using the 'transfer matrix' method of Blease (1977c) to generate the pair connectedness for sites at most six steps from the origin. This gives the series complete as far as  $p^6$ , and the partial contributions to the higher powers were completed up to  $p^{13}$  using the weak subgraph expansion (Dunn *et al* 1975, Blease 1977b). This composite method has been fully described in I (§ 4) and the lattice constants used are given in appendix 2.  $S_0(p)$  is the sum of the pair-connectedness over points on the preferred axis (x = 0). Nevertheless the calculation of contributions to  $S_0(p)$  from graphs with both parallel and non-parallel parts required  $\rho_n(x)$ , the number of *n*-step random walks from 0 to x on the *D*-dimensional projection of the lattice (Blease 1977a, figure 1(d)), and if  $n_1$ ,  $n_2$  and  $n_3$  are the numbers of steps taken parallel to the three bond directions in arriving at x, then

$$\rho_n(\mathbf{x}) = n!/n_1!n_2!n_3!$$
 or 0 (2.1)

depending on whether or not x is reachable in exactly n steps. This condition may be stated in terms of the number of steps N in the shortest path to x as: x is reachable

For the site problem we have used the perimeter method (Domb 1959) together with an animal counting program to generate the series. For the sc lattice we have verified the data by the same method used for the bond problem. This provides an excellent check on the validity of both methods.

The series were analysed by forming the usual Dlog Padé approximants. The results for the mean size series are shown in table 1, and first estimates of  $p_c$  based on the apparent convergence of the higher-order approximants are summarised in table 2. The result for the sc bond problem represents a refinement of the value  $p_c = 0.383 \pm 0.003$  given by Blease (1977a). Table 2 also contains estimates of the exponents  $\gamma$ ,  $\nu_{\parallel}$ ,  $\nu_{\perp}$  and  $\nu_0 = (\gamma - \gamma_0)/D$  which were obtained from standard poleresidue plots of the Dlog approximants to S,  $\mu_{2i}/S$ ,  $\mu_{2x}/S$  and  $S/S_0$  respectively. Sample plots are shown in figures 1 and 2. The plots show the usual correlation between residue and pole position, and the estimates in table 2 represent a linear approximation to these data near the central estimates of  $p_c$ .

### 3. Comparison with universality and scaling predictions

When the uncertainty in the critical points is taken into account, the data of table 2 are consistent with all three percolation models being in the same universality class. The most consistent estimates of  $p_c$  are for the sc bond problem, and the exponent estimates for the sc site problem are uniformly lower than those for the other two problems which are in good agreement with one another. Also from table 1(b) it can be seen that all the approximants obtained from the last three terms of the series are either defective or have interfering non-physical poles. Experience with similar series shows that this normally heralds a change in the estimated critical point. In obtaining our final estimates we therefore adjust the critical probability of the sc site problem upwards to 0.434. This value is quite consistent with the pole-residue plots for the other exponents. The slowness of convergence may be caused by an apparent non-physical singularity at p = -0.32 with index of divergence 0.22. Our final estimates of the universal exponent values are

$$p_{c}(sc bond) = 0.382 \pm 0.001,$$
  $p_{c}(sc site) = 0.434 \pm 0.004,$   
 $p_{c}(Bcc site) = 0.344 \pm 0.004,$   
 $\gamma = 1.57 \pm 0.04,$   $\nu_{\parallel} = 1.28 \pm 0.03,$   $\nu_{\perp} = 0.73 \pm 0.02.$ 

In table 2 we also quote the values of  $\nu_{\parallel}$  and  $\nu_{\perp}$  obtained by Brower *et al* (1978) for a lattice model in the same universality class as Reggeon field theory. The excellent agreement with our final values for these exponents confirms the common universality class of the two models (Cardy and Sugar 1980).

The data in table 2 may be used to compute the right-hand side of the scaling relation (1.2), and taking into account the systematic variation of exponent with critical point we obtain the overall estimate

$$(D\nu_{\perp} + \nu_{\parallel} - \gamma)/2 = 0.59 \pm 0.02.$$

Previous direct estimates of the left-hand side are  $\beta = 0.60 \pm 0.05$  for the bond problem (Blease 1977a) and the overall estimate  $\beta = 0.59 \pm 0.02$  for bond and site problems (De'Bell and Essam 1983b) in good agreement with (1.2).

#### Table 1. Poles and residues of the Dlog Padé approximants to the mean size.

(a) Simple cubic bond proble	em
------------------------------	----

	N/N = 2	, ,	N/N - 1		N/N		N/N+1		N/N+2	,	
N	p <sub>c</sub>	γ	p <sub>c</sub>	γ	<i>p</i> <sub>c</sub>	γ	P <sub>c</sub>	γ	<i>p</i> <sub>c</sub>	γ	
3	0.3485	2.920	0.3735	1.381	0.3853	1.672	0.3837	1.619	0.3823	1.577	
4	0.3789	1.482	0.3808	1.530	0.3823	1.575	0.3822	1.573	0.3823†	1.577†	
5		_	0.3822	1.573	0.3823†	1.575+	0.3808	1.511	0.3818	1.559	
6	0.3814	1.543	0.3818	1.556	0.3818	1.558					
7	0.3818	1.558									
( <i>b</i> ) Si	mple cubi	c site prot	olem								
3	0.4839	5.098	0.4322	1.501	0.4305	1.472	0.4316	1.494	0.4318†	1.499†	
1	0.4307	1.476	0.4312	1.486	0.4293+	1.454†	0.4142‡	1.504‡	0.4328†	1.516†	
5	0.4302+	1.468†	0.6722‡	0.8384	0.4299†	1.462†					
6	0.4308+	1.477†									
(c) <b>B</b>	ody centre	d cubic si	te problem								
3	0.3511	4.847	0.3257	1.217	0.3337†	1.359†	0.3427	1.540	0.3462	1.639	
4	0.3366	1.422		_	0. <b>3449</b>	1.593					
5	0.3483	1.702									

<sup>†</sup> Defective approximant. <sup>‡</sup> Interfering non-physical pole. — No real positive pole.

	p <sub>c</sub>	γ	$\nu_{\parallel}$	ν.	$\nu_0$
sc bond problem	$0.382 \pm 0.001$	$1.565 \pm 0.003$ + $37\Delta p_{c}$	$1.279 \pm 0.003$ + $25\Delta p_{c}$	$0.719 \pm 0.003$ + $14\Delta p_{c}$	$0.625 \pm 0.005$ + 11 $\Delta p_c$
SC site problem	0.4315 <b>●</b> 0.0015 <sup>+</sup>	$1.494 \pm 0.001$ + 22 $\Delta p_{c}$	$1.245 \pm 0.010$ + 15 $\Delta p_{c}$	$0.695 \pm 0.001$ + 25 $\Delta p_{c}$	$0.605 \pm 0.003$ + 20 $\Delta p_{c}$
BCC site problem	$0.344 \pm 0.004$	$1.570 \pm 0.004$ + 28 $\Delta p_{c}$	$1.279 \pm 0.002$ + 32.5 $\Delta p_{c}$	$0.745 \pm 0.005$ + $10\Delta p_{c}$	$0.640 \pm 0.003$ + $14\Delta p_{o}$
BCC bond problem§	$0.288 \pm 0.004$	$1.59 \pm 0.002 + 36\Delta p_c$	F C		- · <u>-</u> r t
Overall exponent estimates		$1.57 \pm 0.04$	$1.28\pm0.03$	$0.73 \pm 0.02$	$0.63 \pm 0.02$
Reggeon theory‡			$1.271\pm0.007$	$0.737 \pm 0.012$	

Table 2. Summary of critical probabilities and exponents.

<sup>+</sup> If the central estimate of  $p_c$  is adjusted to 0.434 (see text) the central exponent estimates would be  $\gamma = 1.54$ ,  $\nu_{\parallel} = 1.28$ ,  $\nu_{\perp} = 0.72$ ,  $\nu_0 = 0.62$ .

‡ Brower et al (1978).

§ From the series of Blease (1977a).

 $\Delta p_c$  represents the deviation from the central estimate of  $p_c$ .



**Figure 1.** Pole-residue plot of the Dlog  $S/S_0$  (O) and  $\mu_{2x}/S$  ( $\bullet$ ) series for the body centred cubic site problem.



Figure 2. Pole-residue plot of the Dlog  $\mu_{2i}/S$  series for the body centred cubic site problem.

If the scaling relation (1.3) is valid the value of  $\nu_0$  in table 2 should be equal to  $\nu_{\perp}$ . Our results clearly cannot be said to confirm this relation. In fact, for all three problems considered, the pole-residue plots based on  $S/S_0$  and  $\mu_{2x}/S$  form two distinct curves which do not intersect in the vicinity of the estimated  $p_c$  (see figure 1 for example). Thus agreement with scaling cannot be obtained by a small change in the estimates of  $p_c$ . A direct estimate of  $\gamma_0$  based on the Dlog approximants to  $S_0$  for the sc bond problem gives  $0.298 + 5\Delta p_c \pm 0.005$ , and combining this with the  $\gamma$  estimate gives  $\nu_0 = 0.634 + 16\Delta p_c \pm 0.005$  which shows the internal consistency Padé approximant technique. We believe that the source of the discrepancy lies in the

nature of the  $S_0$  series. The dominant contribution to the early terms comes from walks which terminate at a point on the *t* axis. On the sc lattice such walks must have a length which is divisible by three, and the terms of  $S_0$  therefore form three separate subsequences. This means that the number of available terms is effectively reduced by a factor of three. Similarly the required walks on the BCC lattice must be of even length with the consequent regular oscillation which may be seen in the data of appendix 1. The periodic structure of the series is reflected in the pole distribution of the Padé approximants. For the sc bond problem the Dlog approximants for both  $S_0$  and  $S/S_0$  have a dominant complex pole pair at  $-0.19\pm0.31i$ , whereas the BCC approximants have a pole on the negative real axis which is closer to the origin than  $p_c$ . From this point of view many of the available terms are wasted in representing dominant non-physical singularities. The convergence to the required critical exponent will therefore be slow and a considerable extension of the series would probably be required to resolve this problem.

# 4. Summary

Low density series expansions for the sc bond and site problems and the BCC site problem have been obtained. The earlier estimate (Blease 1977a) of  $p_c$  for the sc bond problem has been refined and first estimates of  $p_c$  for the site problems have been given.

Our estimates for the critical exponents confirm the universality of directed percolation and Reggeon field theory and are in excellent agreement with the hyperscaling relation (1.2). The scaling relation (1.3) is not satisfied by the present estimates for d = 3. However, for reasons given above the number of presently available series coefficients may be insufficient to give reliable estimates of  $\nu_0$ .

## Appendix 1. Coefficients of $p^m$ for low density percolation series on some threedimensional lattices

$3\mu_{2x}$	$3\mu_{2i}$	So	S	m
0	0	1	1	0
6	3	0	3	1
36	36	0	9	2
162	243	6	27	3
642	1 284	0	78	4
2 3 5 8	5 913	-6	225	5
8 2 2 6	24 813	81	633	6
27 666	97 731	6	1 785	7
90 324	366 003	-168	4 944	8
288 636	1 321 338	1 388	13 742	9
904 506	4 619 748	-180	37 686	10
2 795 238	15 770 943	-4746	103 767	11
8 518 212	52 644 681	27 572	282 425	12
25 708 278	172 831 605	-624	772 719	13

(a) Simple cubic bond problem

m	s	<b>S</b> <sub>0</sub>	3μ <sub>21</sub>	3µ2x
0	1	1	0	0
1	3	0	3	6
2	9	0	36	36
3	24	6	231	156
4	63	-6	1 1 3 4	576
5	159	-3	4 752	1 944
6	402	96	18 054	6 1 5 6
7	988	-182	63 693	18 648
8	2 4 5 4	18	213 738	54 660
9	5 922	1 773	686 052	155 970
10	14 556	-5 058	2 138 160	436 416
11	34 641	3 108	6 460 848	1 197 954

(b) Simple cubic site problem

(c) Body centred cubic site problem

m	S	<b>S</b> 0	$3\mu_{2i}$	$3\mu_{2x}$
0	1	1	0	0
1	4	0	4	4
2	16	4	64	32
3	54	-6	536	184
4	180	40	3 392	880
5	579	-97	18 240	3 812
6	1 860	496	88 640	15 456
7	5 778	-1682	398 892	59 796
8	18 230	7 670	1 705 472	223 328
9	55 324	- 28 932	6 957 544	810 592

### Appendix 2. Directed lattice constant data for the simple cubic lattice

Here we record the data used in obtaining the bond problem series on the sc lattice. It was also used to check all but the last term for the site problem. The two rooted graphs G which are labelled a to w are drawn in Blease (1977b) except for w which is drawn in I. The body of the table gives the number of ways the directed unlabelled graph may be embedded on the lattice with one root on the origin and the other on site  $\mathbf{r} = (n_1, n_2, n_3)$ . It is convenient to define new coordinates which reflect the symmetry of the problem by

$$\sigma = n_1 + n_2 + n_3, \qquad X = n_1 - n_2, \qquad Y = n_2 - n_3,$$

in terms of which

$$t^2 = \sigma^2/3$$
 and  $|x|^2 = 2(X^2 + XY + Y^2)/3$ .

Only representative points with  $n_1 \ge n_2 \ge n_3$  (or X,  $Y \ge 0$ ) are listed in the table and the contributions from each graph are summed over equivalent points. v and e are the numbers of vertices and edges in G respectively and W(G) is the total number of embeddings used in calculating the mean size.

G	v	e	σ	W(G)	$\frac{3x^2/2}{X, Y}$	0 0, 0	1 1, 0	4 2, 0	9 3, 0	1 0, 1,	3 1, 1	7 2, 1	13 3, 1	21 4, 1	4 0, 2	7 1, 2	12 2, 2	9 0, 3
a	4	4	2	3						3								
b	6	6	3	15		9					6							
с	6	7	3	12		6					6							
d	7	8	4	9			6								3			
е	8	8	4	<b>9</b> 0			75					6			9			
f	7	8	3	12		12												
g	8	9	4	120			96					12			12			
h	10	10	5	594				147		405			6			36		
i	9	10	5	<b>9</b> 0				12		66						12		
Í	7	9	3	6		6												
k	8	9	3	2		2												
1	8	10	4	24			18					6						
т	9	10	4	54			48								6			
n	9	10	4	72			72											
0	8	10	4	24			18								6			
р	9	10	4	84			78								6			
q	10	11	5	720				204		456			12			48		
r	12	12	6	4161		1176			243		2616			6			60	60
\$	10	12	6	27		6					18							3
t	11	12	6	225		87			6		120						6	6
и	11	12	6	540		150			12		348						12	18
v	9	11	5	72				12		48						12		
w	10	11	5	300				78		198			6			18		

### References

Blease J 1977a J. Phys. C: Solid State Phys. 10 917-24 — 1977b J. Phys. C: Solid State Phys. 10 925-36 — 1977c J. Phys. C: Solid State Phys. 10 3461-76 Broadbent S R and Hammersley J M 1957 Proc. Camb. Phil. Soc. 53 629-41 Brower R, Furman M A and Moshe M 1978 Phys. Lett. 76B 213-9 Cardy J L and Sugar R L 1980 J. Phys. A: Math. Gen. 10 1917-26 De'Bell K and Essam J W 1983a J. Phys. A: Math. Gen. 16 385-404 — 1983b J. Phys. A: Math. Gen. 16 3145-7 Domb C 1959 Nature 184 509-12 Dunn A G, Essam J W and Ritchie D S 1975 J. Phys. C: Solid State Phys. 8 4219-35 Kinzel W and Yeomans J M 1981 J. Phys. A: Math. Gen. 14 L285-90 Obukhov S P 1980 Physica 101A 145-55