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Low-density series expansions for directed percolation: II. The square lattice with a wall

Iwan Jensen

Department of Mathematics and Statistics, University of Melbourne, Parkville, Victoria 3052, Australia

E-mail: I.Jensen@ms.unimelb.edu.au

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Abstract. A new algorithm for the derivation of low-density expansions has been used to greatly extend the series for moments of the pair-connectedness on the directed square lattice near an impenetrable wall. Analysis of the series yields very accurate estimates for the critical point and exponents. In particular, the estimate for the exponent characterizing the average cluster length near the wall, $\tau_1 = 1.000\,14(2)$, appears to exclude the conjecture $\tau_1 = 1$. The critical point and the exponents $\nu_\parallel$ and $\nu_\perp$ have the same values as for the bulk problem.

1. Introduction

Surface critical behaviour in equilibrium systems has received a lot of attention in recent years [1, 2]. Close to a surface, thermodynamic quantities have critical exponents which may depend on the specific boundary conditions and differ from the exponents characterizing the behaviour in the bulk. While relatively little attention has been paid to surface critical behaviour in non-equilibrium systems, it is clear that, as in the bulk case, similar scaling ideas and principles should apply [3].

Directed bond percolation (DP) [4, 5] can be thought of as a purely geometric model in which bonds placed on the edges of a lattice are either present with probability p or absent with probability $q = 1 - p$. Connections are only allowed along a preferred direction given by an orientation of the edges. The behaviour of the model is controlled by the branching probability (or density of bonds) p. When p is smaller than a critical value p_c all clusters of connected bonds remain finite. Above p_c there is a non-zero probability of finding an infinite cluster, and the average cluster size $S(p)$ diverges as $p \to p_c$. In most interpretations the preferred direction is time, and one realization is as a model of an epidemic without immunization. More precisely, the directed square lattice has sites which are the points in the t–x plane with integer coordinates such that $t \geqslant 0$ and $t + x$ is even. There are two edges leading from the site (t, x) which terminate at the sites $(t + 1, x \pm 1)$. A wall will be said to be present if the bonds leading to sites with $x < 0$ are always absent. In a recent paper [6] this model was studied using series expansions. The analysis of the series, which were calculated to order 67, raised the very interesting possibility that the mean cluster length with the initial seed close to the wall has a critical exponent $\tau_1 = 1$. Here, the subscript 1 is used to indicate that the value of the exponent is in the presence of a wall. The value of τ_1 has also been obtained from Monte Carlo simulations [7] and the estimate $\tau_1 = 1.000(5)$ is consistent with the conjecture

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$\tau_1 = 1$. If true this would be quite remarkable since no other (non-trivial) exponents for the DP problem appear to be given by integers or even (simple) rational fractions [8, 9].

In an effort to further investigate this problem I have used a recently devised and very efficient algorithm [10] to greatly extend the low-density series for moments of the pair-connectedness. The series have been derived to order 173, thus more than doubling the number of terms obtained previously. In the following I shall very briefly describe how the series are calculated. The actual algorithm is a simple specialization of the one used for the bulk problem, and details can be found in [10]. The results of the analysis of the series are presented in section 3.

2. Series expansions

In the low-density phase ($p < p_c$) many quantities of interest can be derived from the pair-connectedness $C_{x,t}(p)$, which is the probability that the site x is occupied at time t given that the origin was occupied at $t = 0$. The moments of the pair-connectedness diverge as p approaches the critical point from below:

$$\mu_{n,m}(p) = \sum_{t=0}^{\infty} \sum_{x} x^n t^m C_{x,t}(p) \propto (p_c - p)^{-(\gamma_1 + n\nu_{\perp,1} + m\nu_{\parallel,1})} \qquad p \to p_c^-. \tag{1}$$

In particular the average cluster size $S(p) = \mu_{0,0}(p) \propto (p_c - p)^{-\gamma}$. Any directed path to a site whose parallel distance from the origin is t contains at least t bonds. From this it follows that if $C_{x,t}$ has been calculated for $t \leqslant t_{\max}$ then one can determine the moments to order $t_{\max}$. The pair-connectedness can be calculated via a transfer-matrix-type algorithm by moving a boundary line through the lattice one row at a time with each row built up one site at a time. The sum over all contributing graphs is calculated as the boundary line is moved through the lattice. At any given stage the boundary line cuts through a number of, say, k sites where each site j is in a state $\sigma_j = 1$ if there is a bond entering the site from the row above, and $\sigma_j = 0$ otherwise. Configurations along the boundary line can thus be represented as binary numbers, and the contribution from each configuration is given by a truncated polynomial in p. Let $S_{a,b} = (\sigma_1, \ldots, \sigma_{j-1}, a, b, \sigma_{j+2}, \ldots, \sigma_k)$ be the configuration of sites along the boundary with $\sigma_j = a$ and $\sigma_{j+1} = b$. As the boundary is moved at position j, the boundary polynomials, BP are updated as follows [10]:

$$\begin{aligned}
BP(S_{1,1}) &= p^2 BP(S_{1,0}) + (p - p^2) BP(S_{1,1}) \\
BP(S_{0,1}) &= pBP(S_{1,0}) - pBP(S_{1,1}) + BP(S_{0,1}) \\
BP(S_{1,0}) &= pBP(S_{1,0}) \\
BP(S_{0,0}) &= BP(S_{0,0}).
\end{aligned}$$

In a calculation to a given order N we need to calculate the contributions for all $t \leqslant N$. For a given $t' < t$ the possible configurations along the boundary line are limited by constraints arising from the facts that graphs have to terminate at level t and have no dangling parts. The 'no dangling parts' restraint is equivalent to demanding that sites with incoming bonds also have outgoing bonds. Therefore, a configuration for which the maximal separation between sites with incoming bonds is r will take at least another r steps before collapsing to a configuration with a single incoming bond. Consequently if $t' + r > t$, that configuration makes no contribution to $C(x, t)$ for any x, and so can be discarded. Furthermore if the minimal order to which a configuration contributes, $N_{\text{cont}} > N$, the configuration can be discarded since it will only contribute at an order exceeding that to which we want to carry out our calculation. In order to calculate N_{cont}, observe that a configuration can be constructed and deconstructed

in this manner. First take $t' - r$ steps, start branching for r steps until the given configuration is produced, then start coalescing branches for another r steps, and then take the remaining $t - t' - r$ steps. It is easy to calculate the minimum order, $N_{\min}$, of the boundary polynomial as the configuration is built up, and from the arguments given above it follows that

$$N_{\text{cont}} = 2N_{\min} + t - 2t'. \tag{2}$$

Further memory savings are obtained by observing that in calculating $C(x, t)$ we know that the graphs have at least t bonds so we need only store $N - t$ coefficients, and when the boundary is moved from one row to the next we discard the lowest-order term in each boundary polynomial.

3. Analysis of the series

The series for moments of the pair-connectedness were analysed using differential approximants (DAs). A comprehensive review of these and other techniques for series analysis may be found in [11]. This allows one to locate the critical point and estimate the associated critical exponents fairly accurately, even in cases where there are additional non-physical singularities. Here it suffices to say that a Kth-order DA to a function f, for which one has derived a series expansion, is formed by matching the coefficients in the polynomials Q_i and P of order N_i and L, respectively, so that the solution to the inhomogeneous differential equation

$$\sum_{i=0}^{K} Q_i(x) \left(x \frac{\mathrm{d}}{\mathrm{d}x} \right)^i \tilde{f}(x) = P(x) \tag{3}$$

agrees with the first series coefficients of f. The equations are readily solved as long as the total number of unknown coefficients in the polynomials is smaller than the order of the series N. The possible singularities of the series appear as the zeros x_i of the polynomial Q_K and the associated critical exponent λ_i is estimated from the indicial equation

$$\lambda_i = K - 1 - \frac{Q_{K-1}(x_i)}{x_i Q'_K(x_i)}.$$

The physical critical point is generally the first singularity on the positive real axis.

3.1. The critical point and exponents

In this section I will give a detailed account of the results of the analysis of the series $S(p)$, $\mu_{1,0}(p)$, $\mu_{2,0}(p)$, $\mu_{0,1}(p)$, and $\mu_{0,2}(p)$. For fixed K and a fixed order, L, of the inhomogeneous polynomial, estimates of the critical point and exponents were obtained by averaging over DAs using at least 150 terms, with the further constraint that the order of the polynomials, Q_j, differ by at most 1. In table 1 I have listed the estimates obtained from second- and third-order DAs for a few values of L. The numbers in parenthesis are error-estimates reflecting the spread among the various approximants. It should be emphasized that these errors are at best indicative of the 'true' error since they do not reflect more systematic errors such as a possible systematic drift in the estimates as the order of the polynomials used to form the approximants is increased. In short, the quoted errors will tend to be too small and give a false sense of how well-converged the estimates really are.

Apart from a few second-order cases with low L-values the estimates are consistent with $p_c = 0.644\,700\,175(35)$. This is in excellent agreement with the more accurate estimate $p_c = 0.644\,700\,185(5)$ obtained from the bulk series [10], and confirms without reasonable doubt the observation made in [6] that the introduction of the wall does not change the value of the critical point. It is worth noting that the estimates from the series $\mu_{0,2}(p)$ are exceptionally

Table 1. Estimates of the location of the critical point and exponents obtained from second- and third-order DAs.

	Second-order DAs		Third-order DAs	
L	p_c	γ_1	p_c	γ_1
0	0.644 700 235(11)	1.820 594(27)	0.644 700 203 4(41)	1.820 541 9(69)
10	0.644 700 232(10)	1.820 582(32)	0.644 700 203 6(24)	1.820 542 5(41)
20	0.644 700 209 3(67)	1.820 551 7(98)	0.644 700 201 2(15)	1.820 538 1(26)
30	0.644 700 209 4(48)	1.820 550 9(68)	0.644 700 202 1(29)	1.820 539 6(50)
40	0.644 700 207 2(20)	1.820 548 6(35)	0.644 700 203 7(27)	1.820 542 6(49)
50	0.644 700 207 1(16)	1.820 549 1(29)	0.644 700 205 7(20)	1.820 546 1(37)
L	p_c	$\gamma_1 + \nu_{\parallel,1}$	p_c	$\gamma_1 + \nu_{\parallel,1}$
0	0.644 700 205 8(13)	3.554 408(22)	0.644 700 196 7(10)	3.554 381 6(24)
10	0.644 700 205 1(22)	3.554 399(13)	0.644 700 196 19(94)	3.554 380 5(21)
20	0.644 700 200 2(33)	3.554 390 3(76)	0.644 700 197 1(17)	3.554 382 6(38)
30	0.644 700 201 4(55)	3.554 392(16)	0.644 700 197 1(19)	3.554 382 7(35)
40	0.644 700 203 1(14)	3.554 398(11)	0.644 700 196 70(80)	3.554 381 5(15)
50	0.644 700 204 7(58)	3.554 403(20)	0.644 700 196 1(29)	3.554 380 9(61)
L	p_c	$\gamma_1 + 2\nu_{\parallel,1}$	p_c	$\gamma_1 + 2\nu_{\parallel,1}$
0	0.644 700 187 44(16)	5.288 203 82(35)	0.644 700 187 40(20)	5.288 203 76(35)
10	0.644 700 187 42(10)	5.288 203 74(23)	0.644 700 187 28(15)	5.288 203 56(26)
20	0.644 700 187 19(40)	5.288 203 32(70)	0.644 700 187 44(46)	5.288 203 89(87)
30	0.644 700 187 61(46)	5.288 204 17(93)	0.644 700 187 52(22)	5.288 204 00(41)
40	0.644 700 187 82(22)	5.288 204 61(41)	0.644 700 187 7(10)	5.288 204 5(23)
50	0.644 700 187 44(61)	5.288 203 9(11)	0.644 700 186 7(20)	5.288 203 2(30)
L	p_c	$\gamma_1 + \nu_{\perp,1}$	p_c	$\gamma_1 + \nu_{\perp,1}$
0	0.644 700 139 8(82)	2.917 206(13)	0.644 700 161(13)	2.917 255(35)
10	0.644 700 139 7(48)	2.917 212(28)	0.644 700 162 8(68)	2.917 257(21)
20	0.644 700 149 8(67)	2.917 206(10)	0.644 700 167 5(18)	2.917 264 0(40)
30	0.644 700 151 3(47)	2.917 227 4(76)	0.644 700 176(11)	2.917 286(29)
40	0.644 700 147 9(27)	2.917 221(19)	0.644 700 170 1(32)	2.917 270 0(76)
50	0.644 700 147 8(51)	2.917 229(13)	0.644 700 173 5(88)	2.917 277(21)
L	p_c	$\gamma_1 + 2\nu_{\perp,1}$	p_c	$\gamma_1 + 2\nu_{\perp,1}$
0	0.644 700 140(10)	4.014 024(20)	0.644 700 157 7(35)	4.014 066(10)
10	0.644 700 140 8(75)	4.014 025(16)	0.644 700 157 5(46)	4.014 060(44)
20	0.644 700 142(11)	4.014 028(21)	0.644 700 161 3(23)	4.014 076 3(75)
30	0.644 700 126(12)	4.014 04(11)	0.644 700 163 6(25)	4.014 081 3(69)
40	0.644 700 140(11)	4.014 025(53)	0.644 700 171 0(68)	4.014 101(20)
50	0.644 700 135 5(65)	4.013 985(41)	0.644 700 149(10)	4.014 049(24)

close to the bulk estimate. Note also that there is a small but systematic change in the p_c estimates from the remaining series as one goes from second- to third-order approximants, with the latter being closer to the bulk estimate. From this table one can obtain the following estimates for the critical exponents:

$$\gamma_1 = 1.820\,544(15)$$
$$\gamma_1 + \nu_{\parallel,1} = 3.554\,385(25)$$

$$\gamma_1 + 2\nu_{\parallel,1} = 5.288\,204(4)$$
$$\gamma_1 + \nu_{\perp,1} = 2.917\,25(4)$$
$$\gamma_1 + 2\nu_{\perp,1} = 4.014\,06(5).$$

Note that since these estimates take into account the differences between the second- and third-order approximants, and the variation with L, the errors are likely to be conservative. In particular they are typically an order of magnitude larger than the 'errors' on any specific estimate in table 1. From the exponent estimates we find that $\nu_{\parallel,1} = 1.733\,820(12)$ and $\nu_{\perp,1} = 1.0968(1)$. The corresponding estimates for the bulk problem are $\nu_{\parallel} = 1.733\,847(6)$ and $\nu_{\perp} = 1.096\,854(4)$, which confirms that $\nu_{\parallel,1} = \nu_{\parallel}$ and $\nu_{\perp,1} = \nu_{\perp}$ as postulated in [6]. It is evident from table 1 that the series $\mu_{1,0}(p)$ and $\mu_{2,0}(p)$ appear to be the worst converged. I therefore also analysed the series $\mu_{2,0}(p)/\mu_{1,0}(p) \propto (p_c - p)^{-\nu_{\perp}}$ and found this to yield the much more accurate estimates $p_c = 0.644\,700\,185(8)$ and $\nu_{\perp} = 1.096\,85(1)$, which do not require further comment.

Due to the high degree of internal consistency of the estimates from the bulk series one would tend to believe quite firmly in their accuracy and correctness and one can then use them to try and obtain more accurate estimates for the exponents for the problem with a wall. In figure 1 I have plotted the estimates for the critical exponents versus the estimates for p_c. By extrapolating the p_c estimates until they lie in the interval given by the bulk estimate $p_c = 0.644\,700\,185(5)$, one obtains the following 'biased' estimates for the exponents for the wall problem

$$\begin{aligned}
&\gamma_1 = 1.820\,51(1)\\
&\gamma_1 + \nu_{\parallel,1} = 3.554\,36(1)\\
&\gamma_1 + 2\nu_{\parallel,1} = 5.288\,202(6)\\
&\gamma_1 + \nu_{\perp,1} = 2.917\,305(15)\\
&\gamma_1 + 2\nu_{\perp,1} = 4.014\,14(1).
\end{aligned} \tag{4}$$

These estimates have a very high degree of consistency and I therefore take $\gamma_1 = 1.820\,51(1)$ as the final estimate. Again, the errors are likely to be conservative since they reflect the variation of the exponents over the entire interval of the bulk estimate of p_c.

In order to check the validity of the conjecture $\tau_1 = 1$ one has to rely on scaling relations to express τ_1 in terms of γ_1 and the bulk exponents γ, $\nu_{\parallel}$ and $\nu_{\perp}$. First we note that [6]

$$\tau_1 = \nu_{\parallel} - \beta_1 \tag{5}$$

where β_1 is the exponent characterizing the decay of the percolation probability. Next we use a hyper-scaling relation derived for the case with the seed close to the wall [12]

$$\nu_{\parallel} + d\nu_{\perp} = \beta + \beta_1 + \gamma_1 \tag{6}$$

where $d + 1$ is the dimension of the lattice. This is a simple generalization of the usual bulk hyper-scaling relation

$$\nu_{\parallel} + d\nu_{\perp} = 2\beta + \gamma. \tag{7}$$

By combining all of these relations one finds

$$\tau_1 = \gamma_1 - (\gamma + d\nu_{\perp} - \nu_{\parallel})/2. \tag{8}$$

In [10] it was estimated that $\gamma = 2.277\,730(5)$ and by inserting the previously stated estimates for the remaining exponents one gets the estimate $\tau_1 = 1.000\,14(2)$. So this would clearly rule out the possibility that $\tau_1 = 1$, though it is tantalizingly close.

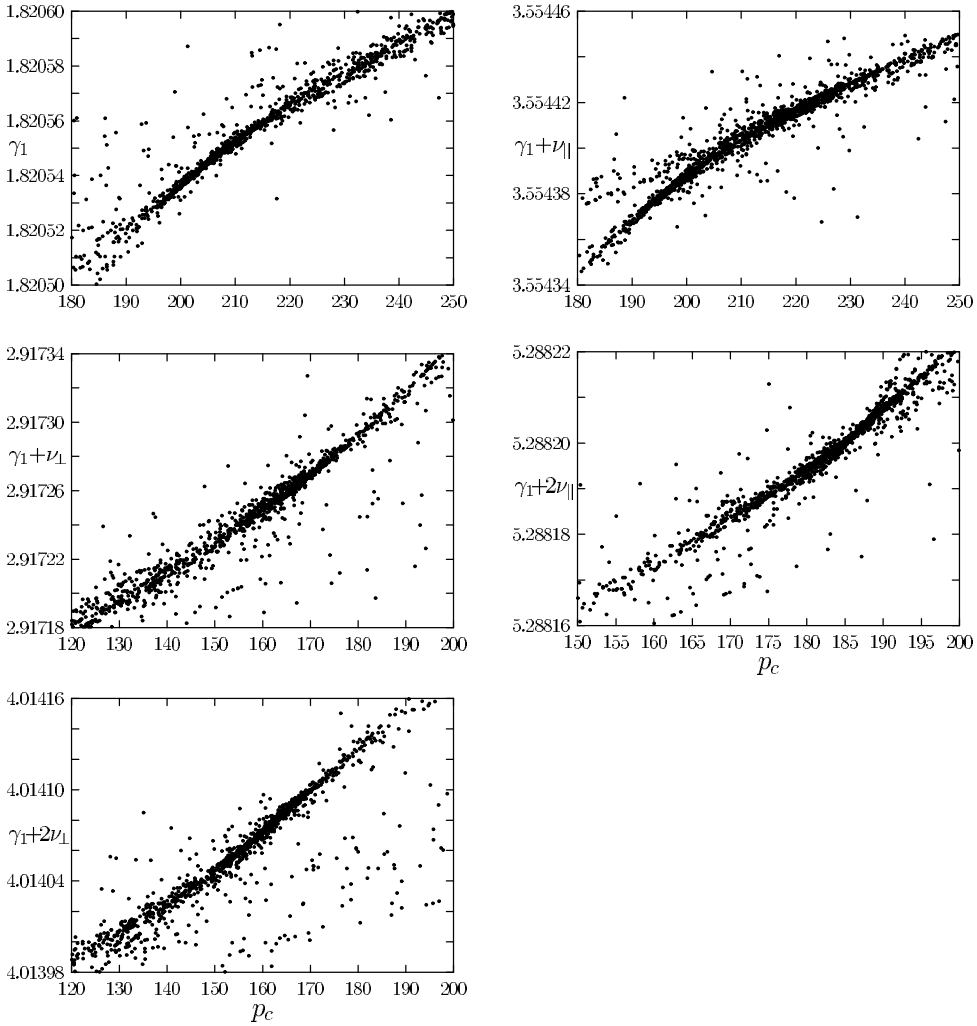

Figure 1. Estimates of the critical exponents obtained from third-order differential approximants versus estimates of the critical point. Numbers along the x-axis are all preceded by 0.644 700. Shown are (from left to right and top to bottom) estimates from the series $S(p)$, $\mu_{0,1}(p)$, $\mu_{1,0}(p)$, $\mu_{0,2}(p)$, and $\mu_{2,0}(p)$.

3.2. Non-physical singularities

The series have a radius of convergence smaller than p_c due to singularities in the complex p-plane closer to the origin than the physical critical point. Since all the coefficients in the expansion are real, complex singularities always come in conjugate pairs. The analysis indicates that the series have quite a large number of non-physical singularities, namely a singularity on the negative real axis and three conjugate pairs in the complex plane. The singularity on the negative real axis at $p_- = -0.516\,66(1)$ and two of the conjugate pairs at $p_1 = 0.010\,05(10) \pm 0.474\,95(15)$i and $p_2 = -0.2255(10) \pm 0.4395(10)$i are also present in the bulk series, while the third conjugate pair at $p_3 = 0.225(5) \pm 0.420(5)$i is unique to the wall problem. At the singularity p_- the exponent estimates are 0.533(3), $-0.463(4)$,

$-1.443(3)$, $0.23(5)$, and $-0.10(3)$, obtained from the series for S, $\mu_{0,1}$, $\mu_{0,2}$, $\mu_{1,0}$, and $\mu_{2,0}$, respectively. The corresponding exponent estimates at the conjugate pair of singularities p_1 are $4.0(1)$, $2.98(5)$, $2.00(5)$, $4.0(3)$, and $4.0(5)$. No meaningful estimates could be obtained for the exponents at p_2 and p_3.

4. Conclusion

In this paper I have reported on the derivation and analysis of low-density series for moments of the pair-connectedness on the directed square lattice with the origin close to an impenetrable wall. The series for bond percolation was extended to order 173 as compared with order 67 obtained in previous work [6]. Analysis of the series led to very accurate estimates for the critical parameters and clearly showed that the critical point p_c and the exponents $\nu_\parallel$ and $\nu_\perp$ have the same values as in the bulk. However, the exponent for the average cluster size differs from the bulk case and has the value $\gamma_1 = 1.820\,51(1)$.

Using the scaling relations an estimate, $\tau_1 = 1.000\,14(2)$, was obtained for the exponent characterizing the average cluster length. This rules out the possibility that $\tau_1 = 1$. This conclusion, however, hinges crucially on having accurate estimates for four exponents and they would not require much altering to get an estimate consistent with $\tau_1 = 1$. On the other hand, so far no one has been able to give theoretical arguments to support $\tau_1 = 1$. Since other exponents for this problem appear not even to be given by (simple) rational fractions, the weight of evidence would at present clearly not favour the conjecture $\tau_1 = 1$. A more direct confirmation of this, say from an extended series for the average cluster length, would clearly be desirable.

E-mail or WWW retrieval of series

The series can be obtained via e-mail by sending a request to I.Jensen@ms.unimelb.edu.au or via the world wide web on the URL http://www.ms.unimelb.edu.au/∼iwan/ by following the instructions.

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References

[1] Binder K 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic)
[2] Diehl H W 1986 *Phase Transitions and Critical Phenomena* vol 10, ed C Domb and J L Lebowitz (New York: Academic)
[3] Lauritsen K B, Fröjdh P and Howard M 1998 *Phys. Rev. Lett.* **81** 2104
[4] Deutsher G, Zallen R and Adler J (ed) 1983 *Percolation Structures and Processes (Ann. Israel Phys. Soc. vol 5)* (Bristol: Adam Hilger)
[5] Stauffer D and Aharony A 1992 *Introduction to Percolation Theory* 2nd edn (London: Taylor and Francis)
[6] Essam J W, Guttmann A J, Jensen I and TanlaKishani D 1996 *J. Phys. A: Math. Gen.* **29** 1619
[7] Lauritsen K B, Sneppen K, Markošová M and Jensen M H 1997 *Physica* **247** 1

[8] Jensen I and Guttmann A J 1995 *J. Phys. A: Math. Gen.* **28** 4813
[9] Jensen I 1996 *J. Phys. A: Math. Gen.* **29** 7013
[10] Jensen I 1999 *J. Phys. A: Math. Gen.* **29** 5233
[11] Guttmann A J 1989 *Phase Transitions and Critical Phenomena* vol 13, ed C Domb and J L Lebowitz (New York: Academic)
[12] Fröjdh P, Howard M and Lauritsen K B 1998 *J. Phys. A: Math. Gen.* **31** 2311