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Distribution of poles in a series expansion of the asymmetric directed-bond percolation probability on the square lattice

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Abstract. We investigate numerically the percolation probability of the asymmetric directedbond percolation on the square lattice with two parameters p and q based on Guttmann and Enting's procedure (1996 *Phys. Rev. Lett.* **76** 344). A series in the form of $\sum_n H_n(q) p^n$ is derived by using the finite transfer-matrix method. The denominator of $H_n(q)$ is directly calculated from the determinant of the transfer matrix and it leads to a proof that poles all lies on the unit circle in the complex q plane. The *solvability* of the bond directed percolation is also discussed.

1. Introduction

The percolation problem (Broadbent and Hammersley 1957) has been associated with a wide variety of critical phenomena. Especially directed percolation (DP) (Durrett 1988, Baxter and Guttmann 1988, Jensen and Guttmann 1995, 1996, Jensen 1996) is a typical statistical model which is nontranslationally invariant and is closely related to stochastic cellular automata (Domany and Kinzel 1984, Kinzel 1985) and interacting particles systems such as the contact process (Harris 1974, Durrett 1988, Konno 1994). Field-theoretical arguments lead to the fact that the DP and Reggeon field theory belong to the same universality class (Grassberger and de la Torre 1979, Cardy and Sugar 1980). It is believed that almost stochastic models with a scalar parameter and a unique absorbing state belong to DP universality class, and so, the DP is a kind of minimal model for the interacting particle system (Janssen 1981, Grassberger 1982, Dickman 1993).

No exact solutions in DP models are found, however, although some critical exponents have been estimated to rather high precision (Jensen and Guttmann 1995, 1996, Jensen 1996). It is well known that critical exponents of many exact solvable statistical models can be represented as simple fractions. In the case of DP, long series expansions obtained by Jensen and Guttmann suggest that the critical exponent of percolation probability of DP is not a simple fraction.

The exact results for the series expansion of DP are very few, but, the following regularities have been found recently. First, the confluent exponent of DP is very close to 1 (Jensen and Guttmann 1995, 1996, Jensen 1996). Secondly, the coefficients of the series are generally given as a finite series of simple combinational numbers (Baxter and Guttmann 1988, Jensen and Guttmann 1995, 1996, Jensen 1996, Bousquet-Mélou 1996,

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Katori et al 1997, Katori and Inui 1997). These results suggest other hidden regularities and exact results.

It is probably quite difficult to determine whether DP is solvable or not. To study the solvability of DP in this paper, we use Guttmann and Enting's proposal for solvability of a statistical mechanical system (Guttmann and Enting 1996, Guttmann 1998, Tsukahara and Inami 1998). They propose a powerful numerical procedure that indicates whether or not a given system is solvable (in the sense of being expressible in terms of *D*-finite functions) and suggests the possibility of application to the DP problem. In this paper, we analyse the series expansion of the asymmetric DP percolation probability by using the finite transfermatrix method (Bidaux and Forgacs 1984, ben-Avraham *et al* 1991) and show several new mathematical properties in the series.

2. Transfer-matrix method and series expansion

Consider a down-pointing triangular region in the square lattice with size k, $V_k = \{(x, y) \in Z^2: x + y = \text{even}, 0 \le y \le k, -y \le x \le y\}$. In particular, we call a subset of sites $\in V_k$ labelled by the same value y = k, 'sites in the *k*th row'. We assume that each bond between a site (x, y) and one site (x - 1, y + 1) (respectively (x + 1, y + 1)) is vacant with probability p (respectively q) and occupied with 1 - p (respectively 1 - q). Let $P^k(p, q)$ be the probability that the origin is connected to at least one site in the *k*th row. The bond percolation probability is defined as $P(p, q) \equiv \lim_{k \to \infty} P^k(p, q)$ and it can be represented as the following polynomial:

$$P(p,q) = \sum_{m,n=0}^{\infty} c_{m,n} p^m q^n = \sum_{n=0}^{\infty} H_n(q) p^n.$$
(2.1)

A short series expansion of the asymmetric bond DP has already been obtained by Katroi *et al* (the list of coefficients is given in Katori *et al* (1997)). In the case of p = q, the series implies the percolation probability of ordinary DP and long series expansions have been given by Jensen and Guttmann (Jensen and Guttmann 1995, 1996, Jensen 1996). The best estimations for critical values and critical exponents of DP are given by these series.

The kernel of Guttmann and Enting's proposal is in observing poles of $H_n(q)$ and the shape of the numerator of $H_n(q)$. To study the solvability of DP by Guttman and Enting's proposal, we first have to find the procedure for deriving $H_n(q)$. We stress that we cannot obtain $H_n(q)$ by only extrapolating a finite-series expansion.

Consider a cluster including *s* sites in the *k*th row connected to the origin. If these sites are disconnected from every site in the (k + 1)th row then at least 2*s* bonds between the *k*th row and the (k + 1)th row are vacant. Therefore the order of the probability of a finite cluster which is composed of *s* sites connected to the origin, with respect to *pq* is not less than *s*. It implies that $H_n(q)$ cannot be dependent on the percolation probabilities of clusters including s(> n) sites in some row. In other words, the maximum distance between sites in the same row which are located in the finite cluster contributing to $H_n(q)$ is not greater than *n*. By considering this restriction and translation invariant, we find that $H_n(q)$ is calculated by the finite transfer-matrix method. A configuration of sites in the *k*th row is represented as a list $\{\sigma\}^k = \{\sigma_{-k}, \sigma_{-k+2}, \ldots, \sigma_k\}^k$, where if the site (l, k) is connected (disconnected) to the origin then $\sigma_l = 1(0)$, respectively. We write simply a configuration as an integer $j \equiv \sum_{i=0}^n \sigma_{-n+2i} 2^i$. In order to express the propagation of the percolation in a strip with *n* sites in width, we introduce a transfer matrix $L_n(p, q)$. The transition probability from a configuration *j* to *j'* is given by an element in the *j'*th row, the *j*th column of $L_n(p, q)$ (a detailed definition is given in Bidaux and Forgács (1984) and ben-Avraham *et al* (1991)). For example, the transfer matrix $L_2(p, q)$ for the set of configuration {00, 01, 10, 11} is given by using translation symmetry and equating {10} and {01} as

$$L_2(p,q) = \begin{bmatrix} 1 & pq & p^2q^2 \\ 0 & q(1-p) + (1-q)p & q^2(1-p)p + qp(1-qp) \\ 0 & (1-q)(1-p) & q(1-p)(1-qp) \end{bmatrix}.$$
 (2.2)

We note that the above matrix is not a stochastic matrix, and so, the summation over the column of matrix is not always 1. Using the translation symmetry, we write the set of probability $P_{n,j}^k(p,q)$ of finding the system in the state $j (\leq 2^n)$ within the strip with *n* sites in width as $v_n^k = (P_{n,0}^k(p,q), P_{n,1}^k(p,q), \ldots, P_{n,2^n}^k(p,q))^T$ where T denotes the transpose. Then the propagation of cluster is represented as $v_n^{k+1} = M \cdot v_n^k$ with the initial state $v_n^0 =$ $(0, 1, \ldots, 0, 0)^T$. Let w_n be a vector $((pq)^{s_0}, \ldots, (pq)^{s_j}, \ldots, (pq)^{s_{2^n}})$ defined by s_j = the number of '1' in the state *j*. By introducing \hat{M}_n , \hat{w}_n and \hat{v}_n^0 which are the matrix removed from the first column and the first row from M_n , and the vector removed from the first element from w_n and v_n^0 , respectively, the percolation probability is given by

$$P(p,q) = 1 - \hat{w}_n \sum_{k=0}^{\infty} \hat{M}_n^{(k)}(p,q) \, \hat{v}_n^0 + \mathcal{O}(n+1)$$
(2.3)

where $\mathcal{O}(n+1)$ denotes a polynomial which is a linear combination of $p^i q^j$ (i + j > 2n) and \hat{M}_n^0 is defined as the unit matrix. If the right-hand side of (2.3) converges, it is written as

$$P(p,q) = 1 - \hat{w}_n (I - \hat{M}_n(p,q))^{-1} \hat{v}_n^0 + \mathcal{O}(n+1)$$
(2.4)

where I is the unit matrix and $(I - \hat{M}_n(p, q))^{-1}$ means the inverse of $I - \hat{M}_n(p, q)$. In the case of n = 2, \hat{w}_n is given by $(pq, (pq)^2)$ and P(p, q) is

$$P(p,q) = 1 - \frac{pq(1-q+p)}{(1-q)^2} + \mathcal{O}(3).$$
(2.5)

By a Taylor expansion near p = 0, we obtain

$$P(p,q) = 1 - \frac{q}{1-q}p + \frac{q}{(1-q)^2}p^2 + \mathcal{O}(p^3).$$
(2.6)

Comparing (2.6) with (2.1), we obtain $H_1(q)$ and $H_2(q)$ as

$$H_1(q) = -\frac{q}{1-q}$$
(2.7)

$$H_2(q) = \frac{q}{(1-q)^2}.$$
(2.8)

Series expansions of these functions, $H_1(q) = -1 - q - q^2 - q^3 - q^4 - \cdots$ and $H_2(q) = -1 - q - 2q^2 - 3q^3 - 4q^4 - \cdots$ are the same as series expansions given by Katori *et al.* For $n \leq 5$, functions $H_n(q)$ obtained in the same way are

$$H_3(q) = -\frac{q(1+q^2)}{(1-q)^3}$$
(2.9)

$$H_4(q) = \frac{q(1+q+3q^2+3q^3+q^4)}{(1-q)^3(1-q^2)}$$
(2.10)

$$H_5(q) = -\frac{q(1+3q+9q^2+20q^3+25q^4+19q^5+10q^6+2q^7)}{(1-q)^2(1-q^2)^3}.$$
 (2.11)

From (2.7) and (2.11), one finds that (i) the numerator and denominator polynomial are of equal degree and (ii) that all poles lie on the unit circle in the complex q plane.

These observations are also found in series expansions of the susceptibility of the Ising model (Guttmann and Enting 1996, Hansel *et al* 1987), self-avoiding polygon (Conway and Guttmann 1996) and so on.

Equation (2.4) determining $H_n(q)$ is simple, however, it is difficult to calculate the inverse matrix for large *n*. Therefore we try to find $H_n(q)$ for $6 \le n \le 8$ satisfying the above observations (i) and (ii) from series expansions up to 51 for each $m \le 8$. The degree of the polynomials is 11, 15, 23 and the denominators of $H_n(q)$ are $(1-q)(1-q^2)^5$, $(1-q^2)^7(1+q+q^2)$ and $(1-q)^8(1+q)^9(1+q+q^2)^3$ for n = 6, 7, 8, respectively. The coefficients of the numerator are summarized in table 1.

Table 1. Coefficients in the numerator of $H_n(q)$. The index *i* denotes the exponent of *q*.

i	n = 6	<i>n</i> = 7	n = 8
0	0	0	0
1	-1	1	-1
2	-5	8	-12
3	-20	44	-90
4	-63	190	-518
5	-135	621	-2354
6	-200	1545	-8564
7	-216	3006	-25407
8	-168	4637	-62506
9	-90	5722	-129237
10	-27	5634	-226653
11	-4	4400	-339384
12		2663	-435452
13		1216	-479 519
14		388	-452640
15		80	-364 981
16		8	-249557
17			-143151
18			-67691
19			-25769
20			-7589
21			-1633
22			-224
23			-13

3. Distribution of poles in the complex plane

In this section, we prove that all poles lie on the unit circle in the complex q plane. We represent each element of v_n^k , $P_{n,j}^k(p,q)$ as the following polynomial of p:

$$P_{n,j}^{k}(p,q) = \sum_{m=0}^{n-s_{j}} C_{j,m}^{k}(q) p^{m}.$$
(3.1)

By substituting this expression into $v_n^{k+1} = \hat{M}_n \cdot v_n^k$, the coefficient of p^m , $C_{j,m}^{k+1}(q)$ which is a function of q, is given by a combination of some coefficients $C_{j',m'}^k(q)$. Thus the transition of a vector composed of coefficients of $P_{n,j}^k(p,q)$, $c_n^k \equiv (C_{0,1}^k(q), C_{0,2}^k(q), \dots, C_{1,0}^k(q), C_{2,0}^k(q), \dots, C_{2^n,n-s_{2^n}}^k(q))^T$ can be expressed as $c_n^{k+1} = \tilde{M}_n c_n^k$ with $c_n^0 = (1, 0, ..., 0)^T$. An advantage of this expression is that \tilde{M}_n can always be represented as a lower triangular matrix by arranging the order in c_n^k . We decide the order of the element $C_{j,m}^k(q)$ in c_n^k by following two rules: (i) if m < m' then the coefficient $C_{j,m}^k(q)$ is located before $C_{j,m'}^k(q)$; (ii) if m = m' and j < j' then the coefficient $C_{j,m}^k(q)$ is located before $C_{j',m}^k(q)$. We briefly explain the reason why we can transform \tilde{M}_n into a lower triangular matrix. We can divide \tilde{M}_n into blocks in which elements determine the transition of coefficients $C_{j,m}^k(q)$ with the same index m. Because the exponent of p in the transfer matrix M_n is not less than zero, it is impossible to have a transition from the block with m' to the block with m(< m'). If j < j' then the number of '1' or the maximum distance between '1' in the state j is less than those of the state j'. Thus it is impossible to have a transition from the state j' to the state j within the block; that is, the matrix \tilde{M}_n must be a lower triangular matrix. As an example, we show \tilde{M}_2 for $c_2^k = (C_{1,0}^k(q), C_{2,0}^k(q), C_{1,1}^k(q))^T$ which completely determine $H_2(q)$,

$$\tilde{M}_2(q) = \begin{bmatrix} q & 0 & 0\\ 1-q & q & 0\\ 1-2q & q+q^2 & q \end{bmatrix}.$$
(3.2)

To calculate $H_n(q)$ by using the matrix \tilde{M}_n we define a new vector w'_n . We assume that the *i*th element of c_n^k is $C_{j,m}^k(q)$. If $m + s_j = n$ then the *i*th element of w'_n is q^{s_j} and otherwise is zero. We also define a new matrix A_n given by replacing the first row of $I - \tilde{M}_n$ by the vector w'. By applying Cramers' rules and Laplace's theorem to (2.4), $H_n(q)$ is simply expressed as

$$H_{n}(q) = \frac{|A_{n}|}{|I - \tilde{M}_{n}|}$$
(3.3)

where $|A_n|$ denotes the determinant of the matrix A_n . From (3.3) we find that the poles of $H_n(q)$ are zero points of $|I - \tilde{M}_n|$. Because $I - \tilde{M}_n$ is the lower triangular matrix, the determinant $|I - \tilde{M}_n|$ is given by the product of diagonal elements. For example, the determinants of $|I - \tilde{M}_n|$ for n = 2, 3, 4 are given by $(1 - q)^3$, $(1 - q)^6(1 - q^2)^2$ and $(1 - q)^{10}(1 - q^2)^{10}$, respectively. Each diagonal element of \tilde{M}_n represents the transition between the same configuration and it is generally expressed as q^{α} where α is the number of a pair $\{1, 0\}$ in the configuration, for example, the α with respect to a configuration $j = 19 = \{1, 0, 0, 1, 1, 0, \ldots\}$ is 2. Consequently, we can generally express $|I - M_n|$ in the following form:

$$|I - \tilde{M}_n| = \prod_{j=1}^{\lceil n/2 \rceil} (1 - q^j)^{\kappa_{n,j}}$$
(3.4)

where $\lceil N \rceil$ denotes the smallest integer not less than N. From (3.4) we conclude that all poles lie on the unit circle in the complex q plane.

We determine $\kappa_{n,j}$ as a function of *n* and *j*. Let $a_{n,i,j}$ be the number of configurations satisfying the following conditions: (i) the number of sites is n + 1 (n > 1); (ii) the first site is occupied; (iii) the (n + 1)th site is vacant; (iv) *i* sites are connected to the origin; (v) the number of the pair {0, 1} is *j* in n + 1 sites; (vi) the *n*th site is vacant. By replacing the 'vacant' into 'occupied' in the condition (vi), we define a valuable $b_{n,i,j}$. These variables are connected to $\kappa_{n,j}$ by the following equation:

$$\kappa_{n,j} = \sum_{i=1}^{n} (n+1-i)(a_{n,i,j} + b_{n,i,j}).$$
(3.5)

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It is easy to obtain the different equation for $a_{n,i,j}$ and $b_{n,i,j}$,

$$a_{n,i,j} = a_{n-1,i,j} + b_{n-1,i,j}$$
(3.6)

$$b_{n,i,j} = a_{n-1,i-1,j-1} + b_{n-1,i-1,j}.$$
(3.7)

We introduce the generating functions defined as

$$\Phi(x, y, z) = \sum_{n=2}^{\infty} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_{n,i,j} x^n y^i z^j \qquad \Psi(x, y, z) = \sum_{n=2}^{\infty} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} b_{n,i,j} x^n y^i z^j.$$
(3.8)

Setting $a_2(1, 1) = 1$ and $b_2(2, 1) = 1$ as initial conditions, one can, after some algebra, obtain $\Phi(x, y, z)$ and $\Psi(x, y, z)$ as

$$\Phi(x, y, z) = \frac{x^2 y z}{1 - (1 + y)x + (1 - z)yx^2}$$
(3.9)

$$\Psi(x, y, z) = \frac{(1 - (1 - z)x)x^2y^2z}{1 - (1 + y)x + (1 - z)yx^2}.$$
(3.10)

By combining $\Phi(x, y, z)$ and $\Psi(x, y, z)$ with y = 1, we have the generating function $\Theta(x, z)$ for $\kappa_{n,j}$ as

$$\Theta(x,z) = \frac{(3+2(z-3)x-4(z-1)x^2-(z-1)^2x^3)x^2z}{(-1+2x+(z-1)x^2)^2}.$$
(3.11)

Finally, we expand $\Theta(x, z)$ and obtain $\kappa_{n,j}$ for $n > 1, i \ge 1$ and $j \ge 1$ as

$$\kappa_{n,j} = j \binom{n+1}{2j}.$$
(3.12)

Setting n = 1 in (3.12), we obtain $\kappa_{1,1} = 1$ and 0 if j > 0. Thus $\kappa_{n,j}$ also gives the correct values in the case of n = 1 (see equation (2.7)). We note that the shape of the denominator is found, however, equation (3.4) includes the common factor to the numerator $|A_n|$ in (3.3).

4. Conclusion and discussion

We derived the series expansion of the asymmetric directed percolation probability and proved that all poles of the denominator in the series lie on the unit circle in the complex q plane. Comparing the numerator with the denominator of the series, we cannot find simple constructions in the numerator. This suggests that although we know the form of the denominator, the inversion relation and symmetry relation would be insufficient to implicitly yield the solution. Strictly speaking, we cannot conclude that the bond DP belongs to an unsolvable class according to Guttmann and Enting's criterion, because, we cannot prove that poles become dense on the unit circle as n gets large. It seems to be correct for DP, however its proof remains as an interesting future problem. Finally, we add some comments about the properties of $H_n(q)$ and the transfer matrix. Using the cofactor expansion for the first column of the numerator in (3.3), we see that each is a Hessenberg matrix. Eigenvalues of the Hessenberg matrix with size n are obtained by an effective algorithm which requires about n^2 arithmetic operators (Johnson and Riess 1981, Lancaster and Tismenetsky 1985). The percolation probability P(p, q) is invariant under the exchange of p with q. Thus, the following relations are established:

$$\frac{1}{m!} \frac{d^m H_n(q)}{dq^m} \bigg|_{q=0} = \frac{1}{n!} \frac{d^n H_m(q)}{dq^n} \bigg|_{q=0}.$$
(4.1)

Since the characteristic polynomial of \tilde{M}_n , $f_{\tilde{M}_n}(q)$ is given by

$$f_{\tilde{M}_n}(x) = \prod_{i=1}^{\lceil n/2 \rceil} (x - q^i)^{\kappa_{n,i}}$$
(4.2)

the function defined as $g_n^k(q) = w_n' \tilde{M}_n^k c_n^0$ satisfies

$$\sum_{i=0}^{(n+1)2^{n-2}} \xi(q) g_n^i(q) = 0$$
(4.3)

where $\xi(q)$ is the coefficient of x^i in $f_{\tilde{M}_n}(q)$ (Lancaster and Tismenetsky 1985). By using (4.3), $g_n^k(q)$ is determined recursively. Thus we can observe the dependence of P(p,q) on the row number from (2.3).

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