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Catalan numbers in a series expansion of the directed percolation probability on a square lattice

Norio Inui[†] and Makoto Katori[‡]

 † Department of Mechanical and Intelligent Engineering, Himeji Institute of Technology, 2167, Shosha, Himeji, 671-22, Japan
 ‡ Department of Physics, Faculty of Science and Engineering, Chuo University, Kasuga,

Bunkyo-ku, Tokyo 112, Japan

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Abstract. We regard the bond directed percolation on a square lattice as a discrete-time Markov process of a one-dimensional interacting particle system. The coefficients in series expansion of the probability $P_{n,m}$ of having *m* particles at time n - 1 are studied. We derive the difference equations for the first and the second series of coefficients and prove that these coefficients are expressed using the ballot numbers, whose special cases are known as the Catalan numbers. As a corollary of our results, we prove a part of the conjecture by Baxter and Guttmann that the correction terms are expressed as rational functions of the Catalan numbers. We also give approximations for the percolation probability using the present formula.

1. Introduction and results

Directed percolation (DP) introduced by Broadbent and Hammersley (1957) is a simple probabilistic model of a flow of fluid through a random media. We consider in this paper the bond DP on a square lattice. This model can be regarded as a discrete-time Markov process η_n of interacting particles on a spatio-temporal plane

$$V = \{(x, n) \in \mathbb{Z}^2 : x + n = \text{even}, n = 0, 1, 2, \ldots\}.$$
(1.1)

Let $\mathbb{Z}_e = \{\dots, -4, -2, 0, 2, 4, \dots\}$ and $\mathbb{Z}_o = \{\dots, -3, -1, 1, 3, \dots\}$. Each site *x* in \mathbb{Z}_e and \mathbb{Z}_o takes one of the two states 0 (vacant) and 1 (occupied by particle) and η_n is a set of sites occupied by particles in \mathbb{Z}_e for n = even and in \mathbb{Z}_o for n = odd. Let $\eta_0 = \{0\}$ and the time evolution is given by

$$P(x \in \eta_{n+1}|\eta_n) = f(|\eta_n \cap \{x - 1, x + 1\}|)$$
(1.2)

where $P(\omega_1|\omega_2)$ is the conditional probability of ω_1 given ω_2 and |A| denotes the number of sites included in a set A. Here f is given as a function of a parameter p as

$$f(N) = \begin{cases} 0 & \text{if } N = 0 \\ p & \text{if } N = 1 \\ 1 - (1 - p)^2 & \text{if } N = 2 \end{cases}$$
(1.3)

where $0 \le p \le 1$. Since *f* depends only on the states of a nearest-neighbour pair of sites, this process is a special case of the two-neighbour stochastic cellular automata (Domany and Kinzel 1984, Kinzel 1985). Another definition of η_n is the following. At each bond between (x, n) and (y, n+1) with $y = x \pm 1$ we put an arrow from (x, n) to (y, n+1) independently

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of other bonds with probability p, which denotes that the bond is open in this direction. The bonds without arrows are closed. That is, each bond is open with probability p or closed with probability q = 1 - p. We say 'there is an open path from (x_0, n) to $(x_m, n + m)$ ' for $m \ge 1$, if there is a sequence $(x_0, n), (x_1, n + 1), \ldots, (x_m, n + m)$ of points in V such that for each $0 \le k \le m - 1$ the bond from $(x_k, n + k)$ to $(x_{k+1}, n + k + 1)$ is open and write $(x_0, n) \rightsquigarrow (x_m, n + m)$ for short. The set η_n is defined as

$$\eta_n = \{x : (0,0) \rightsquigarrow (x,n)\}. \tag{1.4}$$

We consider the probability of having *m* particles at time n - 1,

$$P_{n,m} \equiv P(|\eta_{n-1}| = m)$$
(1.5)

for n = 1, 2, ... By definition $P_{1,1} = 1$ and $P_{n,m} = 0$ for m < 0 and for m > n. Let the *light cone* from the origin up to time n - 1: $V_n^0 = \{(x, m) \in \mathbb{Z}^2 : x + m = \text{even}, m = 0, 1, 2, ..., n - 1, -m \le x \le m\}$. Since the total number of bonds in V_n^0 is n(n - 1), $P_{n,m}$ can be expressed by p and q = 1 - p as

$$P_{n,m} = \sum_{i} a_{n,m,i} p^{n(n-1)-i} q^{i}$$
(1.6)

for $0 \le m \le n$, where $a_{n,m,i}$ is the number of bond configurations on V_n^0 such that there are *i* closed bonds and n(n-1) - i open bonds and we have *m* particles at time n-1. In the present paper, we first prove the following lemma.

Lemma 1. For $m \ge 1$,

$$a_{n,m,i} = 0 \qquad \text{if } i + m \leqslant n - 1. \tag{1.7}$$

This lemma implies that (1.6) can be written as

$$P_{n,m} = q^{-2(m-1)} (pq)^{n-1} (pq)^{m-1} p^{(n-1)(n-2)} \sum_{s=0}^{(n-1)(n-2)} a_{n,m}^{(s)} p^{-s} q^s$$
(1.8)

where

$$a_{n,m}^{(s)} \equiv a_{n,m,(n-m)+s}.$$
 (1.9)

Now we can state the main theorem in this paper.

Theorem 2. For $1 \leq m \leq n$

$$a_{n,m}^{(0)} = \frac{2m}{n+m} \begin{pmatrix} 2n-1\\ n+m-1 \end{pmatrix}$$
(1.10)

and

$$a_{n,m}^{(1)} = \{(n-1)^2 - (m-1)\}a_{n,m}^{(0)} - (m+1)a_{n,m+1}^{(0)}.$$
(1.11)

Remark. The number defined by

$$b_{n,m} = \binom{n+m}{m} - \binom{n+m}{m-1} = \frac{n+1-m}{n+1} \binom{n+m}{m}$$
(1.12)

is called a *ballot number* (Riordan 1979). Consider a ballot in which candidate *A* scores α votes and candidate *B* scores β voters with $\alpha > \beta$. The probability that, during the ballot, *A* was always ahead of *B* is given by $b_{\alpha-1,\beta}/{\binom{\alpha+\beta}{\alpha}} = (\alpha-\beta)/(\alpha+\beta)$ (see the Ballot theorem

in Grimmett and Stirzaker (1992) p 77). We find that $a_{n,m}^{(0)} = b_{n+m-1,n-m}$. When n = m, $b_{n,m}$ is called the *Catalan number*,

$$c_n = b_{n,n} = \frac{1}{n+1} \begin{pmatrix} 2n\\ n \end{pmatrix} \tag{1.13}$$

which appears in many kinds of combinatorial problems (Sloane 1973).

This result has, at least, two applications to the DP problem, as we explain below. Let

$$P_n \equiv P(|\eta_{n-1}| \neq 0) = \sum_{m=1}^n P_{n,m}$$
(1.14)

which is the *survival probability* of the process at time n - 1. Since this probability is non-increasing in n, it has a limit called the ultimate survival probability or the *percolation probability*

$$P(p) = \lim_{n \to \infty} P_n. \tag{1.15}$$

It is easy to prove that P(p) is a non-decreasing function of p and the critical probability p_c can be uniquely defined as

$$p_{c} = \inf\{p \in [0, 1] : P(p) > 0\}$$

= sup{ $p \in [0, 1] : P(p) = 0$ }. (1.16)

Its value has been estimated so far as

$$0.6298 \leqslant p_{\rm c} \leqslant \frac{2}{3} \tag{1.17}$$

(the lower bound is by Dhar (1982) and the upper bound by Liggett (1995), see also Katori and Tsukahara (1995)). It is expected that P(p) is continuous even at $p = p_c$ and it behaves as $P(p) \sim (p - p_c)^{\beta}$ as $p \rightarrow p_c$ + with a critical exponent β (Baxter and Guttmann 1988). Since neither of the exact value of p_c nor β are known, it is of interest to provide approximations to P(p).

Since

$$P_n - P_{n+1} = P(|\eta_{n-1}| \neq 0 \text{ and } |\eta_n| = 0) = \sum_{m=1}^n P_{n,m} q^{2m}$$
 (1.18)

by definition, we can conclude from (1.8), which is a result of lemma 1, that

$$P_n - P_{n+1} = q^n \sum_{l=1}^{\infty} d_{n,l} q^l$$
(1.19)

with the coefficients $\{d_{n,l}\}$, which can be expressed by $\{a_{n,m}^{(s)}\}$. This implies that if we calculate P_n as a power series of q, going from n to n + 1 leaves the coefficients of $1, q, \ldots, q^n$ unchanged and terms with the coefficients $\{d_{n,l}\}$ give corrections of the order $\mathcal{O}(q^{n+l})$. This property guarantees the convergence of the power series of P_n to a limit $P_{\infty}(q)$ as a formal power series of q and this limit $P_{\infty}(q)$ may be identified with P(q) defined by (1.15). Moreover, if we know the *correction terms* $\{d_{n,l}\}$ for $1 \leq l \leq M$, then we can correctly compute the expansion P_{∞} in q up to the coefficient of q^{n+M} using the coefficients of P_n . Baxter and Guttmann (1988) performed the calculation of P_n up

to n = 29 and gave the following remarkable conjectures. Let c_n be the Catalan number (1.13), then

$$d_{n,1} = c_n$$

$$d_{n,2} = 2c_n - c_{n+1}$$

$$d_{n,3} = -2(n+1)c_n + 2c_{n+1}$$

$$d_{n,4} = 2c_{n-1} + (3n-5)c_n + 5c_{n+1} - 2c_{n+2}$$
....
(1.20)

Inversely, they assumed the validity of these conjectures and extended their expansion of P_{∞} from the 29th coefficient to the 41st coefficient. Recently Jensen and Guttmann (1995) use this technique to extend the series from 41 terms to 54 terms. Such long series expansions are useful to evaluate p_c and β with high precision by the Dlog Padé approximations.

Recently Bousquet-Mélou (1996) generally discussed the relation between the correction terms and the numbers of *compact animals* (Duarte 1990, Delest 1991) of appropriate types and prove the first two equalities of (1.20). On the other hand, since the relation between the correction terms $d_{n,1}$, $d_{n,2}$ and the coefficients $a_{n,1}^{(0)}$, $a_{n,2}^{(1)}$ are easily derived, these equalities are derived as a corollary of theorem 2.

Corollary 3. For
$$n \ge 1$$

 $d_{n,1} = a_{n,1}^{(0)} = c_n$
(1.21)

and

$$d_{n,2} = a_{n,1}^{(1)} + a_{n+1,1}^{(0)} - (n^2 - 2n + 3)a_{n,1}^{(0)}$$

= 2c_n - c_{n+1}. (1.22)

Bousquet-Mélou exactly calculated the first two correction terms not only for the bond DP on the square lattice but also for the site DP on square lattice and the bond DP on the honeycomb lattice. We would, however, like to put emphasis on the fact that concerning the bond DP on the square lattice, our result is more general, since her results can be regarded as a special case with m = 0 in our theorem 2.

Next we explain another application of theorem 2. Let

$$A_{n,m}^{(r)} = \sum_{s=0}^{r} (-1)^{r-s} \left(\frac{(n-1)(n-2) - s}{r-s} \right) a_{n,m}^{(s)}.$$
 (1.23)

Then we have from (1.8)

$$P_{n,m} = \sum_{r=0}^{(n-1)(n-2)} Q_{n,m}^{(r)} q^{-2m+r+2}$$
(1.24)

with

$$Q_{n,m}^{(r)} = (pq)^{n-1} (pq)^{m-1} A_{n,m}^{(r)}.$$
(1.25)

By (1.18) and $P_1 = 1$, the percolation probability (1.15) is given by

$$P(p) = 1 - \sum_{n=1}^{\infty} \sum_{m=1}^{n} P_{n,m} q^{2m}.$$
(1.26)

Using the expression given by (1.23)–(1.25), we have

$$P(p) = 1 - q^2 \sum_{r=0}^{\infty} q^r Q^{(r)}$$
(1.27)

with

$$Q^{(r)} = \sum_{n=n(r)}^{\infty} \sum_{m=1}^{n} Q_{n,m}^{(r)}.$$
(1.28)

Here n(0) = 1 and $n(r) = \lceil (1 + \sqrt{1 + 4r})/2 \rceil + 1$ for $r \ge 1$, where $\lceil N \rceil$ is the least integer not less than N. Let

$$\tilde{P}^{(R)}(p) = 1 - q^2 \sum_{r=0}^{R} q^r Q^{(r)}$$
(1.29)

for R = 0, 1, 2, ... We regard $\tilde{P}^{(R)}(p)$ as the *R*th approximation for the percolation probability. This gives a new systematic way to make approximations and theorem 2 enables us to obtain two approximants.

The paper is organized as follows. In section 2, first we prove lemma 1. Then we derive a set of difference equations for the coefficients $a_{n,m}^{(0)}$ and $a_{n,m}^{(1)}$. These difference equations are linear, in contrast to the equations in the proof by Bousquet-Mélou who derived nonlinear difference equations for $a_{n,1}^{(0)}$ and $a_{n,1}^{(1)}$. We solve the difference equations with appropriate boundary conditions and prove theorem 2 in section 3. Section 4 is devoted to giving approximations $\tilde{P}^{(0)}(p)$ and $\tilde{P}^{(1)}(p)$. There are some interesting future problems related to this work, as discussed in section 5.

2. Difference equations

In this section we prove lemma 1 and derive the difference equations for $a_{n,m}^{(0)}$ and $a_{n,m}^{(1)}$. Here we regard the bond DP as a discrete-time Markov process η_n as explained in the beginning of section 1, where η_n is a set of sites occupied by a particle at time *n*. If we define a random variable $\eta_n(x)$, for each site *x*, as $\eta_n(x) = 1$ if $x \in \eta_n$ and $\eta_n(x) = 0$ if $x \notin \eta_n$, then a set η_n is identified with a particle configuration $\{\eta_n\}$ which is expressed by a sequence of numbers 0 and 1. The transition matrix ω is defined as $\omega(\xi; \zeta) \equiv P(\eta_n = \xi | \eta_{n-1} = \zeta)$ and the probability $P_{n,m}$, defined by (1.5), is given by the following formula,

$$P_{n,m} = \sum_{\xi} \sum_{\zeta} \delta_{|\xi|,m} \omega(\xi;\zeta) P(\eta_{n-2} = \zeta)$$
(2.1)

where the $\delta_{l,m}$ denotes Kronecker's delta, $|\xi|$ is the number of particles in a configuration ξ and summations are taken over all possible configurations.

Each element of ω can be expressed as

$$\omega(\xi;\zeta) = \sum_{i} c_i(\xi;\zeta) q^i.$$
(2.2)

Let $i_{\min}(\omega(\xi; \zeta)) = \min\{i : c_i(\xi; \zeta) > 0\}$. We find that it depends on $\Delta m = |\xi| - |\zeta|$ and the number of clusters of particles in a configuration ζ , $c(\zeta)$. In other words, this number is defined as

$$c(\zeta)$$
 = the number of sequences {0, 1} in the configuration { ζ }. (2.3)

We show the dependence of $i_{\min}(\omega(\xi; \zeta))$ on $\Delta m = |\xi| - |\zeta|$ and $c(\zeta)$ in table 1. We find that, for each Δm , $i_{\min}(\omega(\xi, \zeta))$ has a minimum value when c = 1 ($\Delta m \leq 0$) and $c = \Delta m$ ($\Delta m > 0$). If we define $i_{\min}(\omega(\Delta m)) = \min\{i_{\min}(\omega(\xi, \zeta)) : |\xi| - |\zeta| = \Delta m\}$ then

$$i_{\min}(\omega(\Delta m)) = \begin{cases} 0 & \Delta m > 0\\ 1 & \Delta m = 0\\ -2\Delta m & \Delta m < 0. \end{cases}$$
(2.4)

Table 1. The dependence of $i_{\min}(\omega(\xi; \zeta))$ on $\Delta m = |\xi| - |\zeta|$ and $c(\zeta)$. The asterisks denote the impossible cases.

| | С | | | | | | |
|------------|---|---|---|--|-----|--|--|
| Δm | 1 | 2 | 3 | | min | | |
| : | | | | | | | |
| 3 | * | * | 0 | | 0 | | |
| 2 | * | 0 | 1 | | 0 | | |
| 1 | 0 | 1 | 2 | | 0 | | |
| 0 | 1 | 2 | 3 | | 1 | | |
| -1 | 2 | 3 | 4 | | 2 | | |
| -2 | 4 | 4 | 5 | | 4 | | |
| -3 | 6 | 6 | 6 | | 6 | | |

Proof of lemma 1. We prove (1.7) by induction with respect to n. When n = 1, the probability $P_{1,m}$ is 1 for m = 1 and 0 for m > 1, so (1.7) is correct for n = 1. For expression (1.6) of $P_{n,m}$, we define

$$i_{\min}(P_{n,m}) = \min\{i : a_{n,m,i} > 0\}.$$
(2.5)

Formula (2.1) gives

$$i_{\min}(P_{n,m}) = \min_{\Delta m} \{i_{\min}(\omega(\Delta m)) + i_{\min}(P_{n-1,m-\Delta m})\}.$$
(2.6)

Now we assume (1.7) is correct for n = k - 1, i.e. $a_{k-1,m,i} = 0$ for $i \le k - m - 2$. This assumption means that $i_{\min}(P_{k-1,m-\Delta m}) > k - (m - \Delta m) - 2$. Therefore (2.4) gives

$$i_{\min}(\omega(\Delta m)) + i_{\min}(P_{k-1,m-\Delta m}) > \begin{cases} k - m + \Delta m - 2 & \Delta m > 0\\ k - m - 1 & \Delta m = 0 \\ k - m - \Delta m - 2 & \Delta m < 0. \end{cases}$$
(2.7)

The $i_{\min}(P_{k,m})$ has minimum value in the following cases:

$$i_{\min}(P_{k,m}) > k - m - 1 \qquad \text{at} \begin{cases} \Delta m = +1 \\ \Delta m = -1 \\ \Delta m = 0. \end{cases}$$

$$(2.8)$$

This means $a_{k,m,i} = 0$ for $i \leq k - m - 1$ and the proof is completed.

Next we derive the difference equations for $a_{n,m}^{(0)}$ and $a_{n,m}^{(1)}$. We list $a_{n,m}^{(s)}$ for n = 1, 2, 3, 4 in table 2. In order to show how these coefficients are determined, we introduce $P_{n,m,c}$ which is a probability of having *m* particles with *c* clusters at time n - 1. By definition $\sum_{c} P_{n,m,c} = P_{n,m}$. In the same way as $P_{n,m}$, it is expressed as

$$P_{n,m,c} = \sum_{i} a_{n,m,c,i} p^{n(n-1)-i} q^{i}$$
(2.9)

with non-negative coefficients $\{a_{n,m,c,i}\}$. We define $a_{n,m,c}^{(s)} \equiv a_{n,m,c,n-m+s}$.

Consider the transitions from time n - 1 to time n. The state at time n - 1 is assigned by the particle configuration on n sites. The particle configuration at time n depends on this state at time n - 1 and the bond configuration on the 2n bonds connecting the sites at

Table 2. A list of $a_{n,m}^{(s)}$ defined by (1.9) for n = 1, 2, 3, 4. Other coefficients, which are not listed here, are zeros.

| | | | | S | | | |
|--------------|----|----|-----|-----|-----|----|---|
| т | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| n = 1 | | | | | | | |
| 1 | 1 | | | | | | |
| n = 2 | | | | | | | |
| 1 | 2 | | | | | | |
| 2 | 1 | | | | | | |
| <i>n</i> = 3 | | | | | | | |
| 1 | 5 | 12 | 4 | | | | |
| 2 | 4 | 9 | 2 | | | | |
| 3 | 1 | 2 | 0 | | | | |
| n = 4 | | | | | | | |
| 1 | 14 | 98 | 264 | 336 | 208 | 64 | 8 |
| 2 | 14 | 94 | 241 | 280 | 147 | 38 | 4 |
| 3 | 6 | 38 | 90 | 88 | 30 | 4 | 0 |
| 4 | 1 | 6 | 13 | 10 | 1 | 0 | 0 |

time n - 1 and those at time n. Assume that there are m' particles and c' clusters at time n - 1 and m particles at time n and that r bonds are closed and 2n - r bonds are open in the 2n bonds. The number of such configurations is given as

$$f(n, m', c', r, m) = \sum_{i} \sum_{j} 2^{i} {\binom{2c'}{j}} {\binom{m'-c'}{m'+c'-m-j}} {\binom{m'-2c'+j}{i}} \times {\binom{2(n-m')}{r-2(m'+c'-m)+j-i}}$$
(2.10)

where the summations are taken over the following ranges:

$$\max\{0, 2c' - m\} \leq j \leq \min\{2c', m' + c' - m\}$$

$$\max\{0, r - 2(n + c' - m) + j\} \leq i \leq \min\{m - 2c' + j, r - 2(m' + c' - m) + j\}.$$
 (2.11)

The derivation of this formula is as follows. In the light cone V_{n+1}^0 from the origin, each site at time n is connected with one or two sites at time n-1 by bonds. According to the particle configuration at time n-1, the n+1 sites are classified into three sets as $S_k = \{$ sites connected with k occupied sites at time n-1, k = 0, 1, 2. The numbers of such sites are given as $|S_1| = 2c'$ and $|S_2| = m' - c'$. Let a set of bonds connecting sites in S_1 (respectively, S_2) with occupied sites at time n-1 be B_1 (respectively, B_2). The remaining 2(n-m') bonds make a set B_0 . We consider the case that j bonds in B_1 and m' + c' - m - j pairs of nearest-neighbour bonds in B_2 are closed and thus j sites in S_1 and m' + c' - m - j sites in S_2 are vacated. The number of such choices is $\binom{2c'}{j}\binom{m'-c'}{m'+c'-m-j}$. Since we have assumed that r bonds are closed, we have to choose more r - 2(m' + c' - m) + j bonds to be closed. We choose i bonds from the remaining bonds in B_2 and r - 2(m' + c' - m) + j - i bonds from B_0 so that the particle number at time n is fixed to be m. The number of such choices is $2^i \binom{m-2c'+j}{i} \binom{2(n-m')}{r-2(m'+c'-m)+j-i}$. The region of summations (2.11) is decided by the condition so that $x \ge 0$, $y \ge 0$ and $x \ge y$ for each combination $\binom{x}{y}$ in (2.10).

By using (2.10), the coefficient $a_{n+1,m}^{(s)}$ is calculated from $a_{n,m',c'}^{(s')}$ as

$$a_{n+1,m}^{(s)} = \sum_{\Delta m} \sum_{s'} \sum_{c'} f(n, m - \Delta m, c', \Delta i, m) a_{n,m-\Delta m,c'}^{(s')}$$
(2.12)

with $\Delta i = \Delta s - \Delta m + 1(\Delta s = s - s', \Delta m = m - m')$, where the summation is taken over the region satisfying the condition

$$i_{\min}(\omega(\Delta m)) \leqslant \Delta i.$$
 (2.13)

We show the pair $(i_{\min}(\omega(\Delta m)), \Delta i)$ for each Δm and s' in table 3.

Table 3. A list of the pair $(i_{\min}(\omega(\Delta m)), \Delta i)$ as a function of Δm and s'.

| Δm | 0 | 1 | | S | s + 1 | s+2 |
|------------|------------|----------------|---|---------|---------|---------|
| ÷ | : | : | : | : | : | : |
| 2 | (0, s - 1) | (0, s - 2) | | (0, -1) | (0, -2) | (0, -3) |
| 1 | (0, s) | (0, s - 1) | | (0, 0) | (0, -1) | (0, -2) |
| 0 | (1, s + 1) | (1, <i>s</i>) | | (1, 1) | (1,0) | (1, -1) |
| $^{-1}$ | (2, s + 2) | (2, s + 1) | | (2, 2) | (2, 1) | (2, 0) |
| -2 | (4, s + 3) | (4, s + 2) | | (4, 3) | (4, 2) | (4, 1) |
| ÷ | : | | : | : | : | : |

Table 4. A list of the pair $(i_{\min}(\omega(\Delta m)), \Delta i)$ as a function of Δm and s' in the case of s = 0. The asterisks denote those satisfying condition (2.13).

| | 0 | 1 |
|----|------------|---------|
| 2 | (0, -1) | (0, -2) |
| 1 | $(0, 0)^*$ | (0, -1) |
| 0 | $(1, 1)^*$ | (1, 0) |
| -1 | $(2, 2)^*$ | (2, 1) |
| -2 | (4, 3) | (4, 2) |
| | | |

In the case of s = 0, (2.13) allows the combinations $(s', c', \Delta i, \Delta m) = (0, 1, 0, 1)$, (0, 1, 1, 0) and (0, 1, 2, -1) as shown in table 4 and formula (2.10) gives that $f(n, m - \Delta m, c', \Delta i, m) = 1, 2, 1$, respectively. Thus we have

$$a_{n+1,m}^{(0)} = a_{n,m-1,1}^{(0)} + 2a_{n,m,1}^{(0)} + a_{n,m+1,1}^{(0)} \quad \text{for } m \ge 2$$

$$a_{n+1,1}^{(0)} = 2a_{n,1,1}^{(0)} + a_{n,2,1}^{(0)}.$$
(2.14)

We find that condition (2.11) is satisfied in the case s = 0 only when i = 0. This means $a_{n,m,1}^{(0)} = a_{n,m}^{(0)}$ and $a_{n,m,k}^{(0)} = 0$ if $k \neq 1$ for any n and m. Thus we obtain the difference equation for $a_{n,m}^{(0)}$ as

$$a_{n+1,m}^{(0)} = a_{n,m-1}^{(0)} + 2a_{n,m}^{(0)} + a_{n,m+1}^{(0)}$$
(2.15)

with the boundary conditions

$$a_{1,1}^{(0)} = 1$$
 $a_{1,m}^{(0)} = 0 \ (m \ge 2)$ $a_{n,0}^{(0)} = 0 \ (n \ge 0).$ (2.16)

Table 5. A list of $a_{n,m}^{(0)}$ for $1 \le n \le 6$. Blanks denote zeros.

| | | | | 1 | 10 | |
|---|---|----------|-------------------------|---|--|--|
| | | | 1 | 8 | 44 | |
| | | 1 | 6 | 27 | 110 | |
| | 1 | 4 | 14 | 48 | 165 | |
| 1 | 2 | 5 | 14 | 42 | 132 | |
| | - | - | | ~ | | |
| | 1 | 1 1 2 | $1 \\ 1 \\ 1 \\ 2 \\ 5$ | $ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$ | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |

Table 6. A list of the pair $(i_{\min}(\omega(\Delta m)), \Delta i)$ as a function of Δm and s' in the case of s = 1. The asterisks denote those satisfying condition (2.13).

| | 0 | 1 | 2 |
|------------|--------------------------|-----------------------|--------------------|
| 3 | (0, -1) | (0, -2) | (0, -3) |
| 2 1 | $(0, 0)^*$ $(0, 1)^*$ | (0, -1) $(0, 0)^*$ | (0, -2) (0, -1) |
| 0 | (1, 2)* | (1, 1)* | (1, 0) |
| $-1 \\ -2$ | $(2,3)^*$ $(4,4)^*$ | $(2, 2)^*$ (4, 3) | (2, 1) (4, 2) |
| -3 | (6, 5) | (6, 4) | (6, 3) |

Table 7. The combinations which satisfy condition (2.13) in the case of s = 1.

| No | s' | c' | Δi | Δm |
|----|----|----|------------|------------|
| 1 | 0 | 1 | 1 | 1 |
| 2 | 0 | 1 | 2 | 0 |
| 3 | 0 | 1 | 3 | -1 |
| 4 | 0 | 1 | 4 | $^{-2}$ |
| 5 | 0 | 2 | 0 | 2 |
| 6 | 0 | 2 | 1 | 1 |
| 7 | 0 | 2 | 2 | 0 |
| 8 | 0 | 2 | 3 | -1 |
| 9 | 0 | 2 | 4 | $^{-2}$ |
| 10 | 1 | 1 | 0 | 1 |
| 11 | 1 | 1 | 1 | 0 |
| 12 | 1 | 1 | 2 | -1 |

The $a_{n,m}^{(0)}$'s are given in table 5 for small n.

In the case of s = 1, condition (2.11) is satisfied when i = 0 or i = 1. This means $a_{n+1,m}^{(1)} = a_{n+1,m,1}^{(1)} + a_{n+1,m,2}^{(1)}$, and thus we have to derive the equations for $a_{n+1,m,1}^{(1)}$ and $a_{n+1,m,2}^{(1)}$. We have 12 cases which satisfy condition (2.13) (see table 6 and table 7). In table 7, the cases with numbers from 5 to 9 have s' = 0 and c' = 2 and give no contribution, since we have found $a_{n,m,2}^{(0)} = 0$ for any n and m. In the other cases c' = 1.

We consider the transition from the state at time n - 1 with m' particles in n sites and c' = 1 to the state at time n with $m = m' + \Delta m$ particles in n + 1 sites. We have $|S_1| = 2$ and $|S_2| = m' - 1$. Let $|B_i|$ be the number of bonds in the set B_i , i = 0, 1, 2. Then $|B_0| = 2(n - m')$, $|B_1| = 2$ and $|B_2| = 2(m' - 1)$. First we consider the first case in table 7. Since $\Delta i = 1$, we have to choose one bond and make it closed. If we choose this bond from set B_1 , then $\Delta m = 0$. Therefore we should choose it from $B_0 \cup B_2$ to make $\Delta m = 1$ (see figure 1, 1-(i)). The number of such choices is $2n - |B_1| = 2(n - 1)$. In the second case in table 7, we have to choose two bonds and make them closed. There are two ways provided $\Delta m = 0$: (i) choose one bond from B_1 and another bond from $B_0 \cup B_2$, or (ii) choose two successive bonds from B_2 which are connected with the same site at time n (see figure 1, 2-(i) and 2-(ii)), respectively. The numbers of choices are given as 4(n - 1) and m' - 1, respectively. It should be remarked that in case 2-(i), the number of clusters at time n is c = 1, while in case 2-(ii), c = 2.

| 1-(i) | |
|---------|--|
| 2-(i) | $\sim\sim\sim\sim\sim\sim\sim\sim$ |
| 2-(ii) | |
| 3-(i) | $ \land \land$ |
| 3-(ii) | ~~~~ ~~ ~~ ~~ ~~ ~~ ~~ ~~ ~~ ~~ ~~ ~~ ~ |
| 3-(iii) | |
| 4-(i) | |
| 4-(ii) | $\land \lor \lor \land \lor \land \lor$ |

Figure 1. Typical configurations of bonds for each case in table 8.

Table 8 classifies the possible ways to choose appropriate closed bonds and shows c and the numbers of choices (NC) also for the third and fourth cases. The typical bond configurations are illustrated in figure 1.

The contributions from the cases with numbers from 10 to 12 in table 7 can be calculated in the same way as in the case of s = 0.

Combining the above considerations gives the following equations for $a_{n+1,m,1}^{(1)}$ and $a_{n+1,m,2}^{(1)}$ as

$$a_{n+1,m,1}^{(1)} = 2(n-1)a_{n,m-1,1}^{(0)} + 4(n-1)a_{n,m,1}^{(0)} + 2na_{n,m+1,1}^{(0)} + 2a_{n,m+2,1}^{(0)} + (a_{n,m-1,1}^{(1)} + 2a_{n,m,1}^{(1)} + a_{n,m+1,1}^{(1)})$$

$$a_{n+1,m,2}^{(1)} = (m-1)(a_{n,m,1}^{(0)} + 2a_{n,m+1,1}^{(0)} + a_{n,m+2,1}^{(0)}) \quad \text{for } n \ge 1.$$
(2.17)

Using (2.14) and by the fact that $a_{n,m}^{(0)} = a_{n,m,1}^{(0)}$ and $a_{n,m}^{(1)} = a_{n,m,1}^{(1)} + a_{n,m,2}^{(1)}$, we obtain the following difference equations for $a_{n,m}^{(1)}$:

$$a_{n+1,m}^{(1)} = a_{n,m-1}^{(1)} + 2a_{n,m}^{(1)} + a_{n,m+1}^{(1)} + 2(n-1)a_{n,m-1}^{(0)} + (4n-3)a_{n,m}^{(0)} + 2na_{n,m+1}^{(0)} + a_{n,m+2}^{(0)}$$

for $n \ge 2$ and $m \ge 2$ (2.18)

Table 8. Classification of the possible ways to choose appropriate closed bonds for the cases with numbers from 1–4 in table 7. Here c is the number of clusters at time n and NC is the number of choices.

| No | | How to choose closed bonds | с | NC |
|----|-------|---|---|--------------------|
| 1 | (i) | One bond from $B_0 \cup B_2$ | 1 | 2(n-1) |
| 2 | (i) | One bond from B_1 and another bond from $B_0 \cup B_2$ | 1 | 4(n-1) |
| | (ii) | Two successive bonds from B_2 connected with the same site at time n | 2 | m'-1 |
| 3 | (i) | Two bonds from B_1 and one bond from $B_0 \cup B_2$ | 1 | 2(n-1) |
| | (ii) | One bond from B_1 and two successive bonds from B_2 connected with the same site at time n , one of which is located next to the first chosen bond | 1 | 2 |
| | (iii) | One bond from B_1 and two successive bonds from B_2 connected with the same site at time <i>n</i> , both of which are not located next to the first chosen bond | 2 | 2(<i>m</i> ′ – 2) |
| 4 | (i) | Two bonds from B_1 and two successive bonds from B_2 connected with the same site at time n , one of which is located next to the first chosen bonds | 1 | 2 |
| | (ii) | Two bonds from B_1 and two successive bonds from B_2 connected with the same site at time <i>n</i> , both of which are not located next to the first chosen bonds | 2 | <i>m′</i> – 3 |

and

$$a_{n+1,1}^{(1)} = 2a_{n,1}^{(1)} + a_{n,2}^{(1)} + 4(n-1)a_{n,1}^{(0)} + 2na_{n,2}^{(0)} + a_{n,3}^{(0)} \qquad \text{for } n \ge 2$$
(2.19)

with the boundary conditions

$$a_{1,m}^{(1)} = a_{2,m}^{(1)} = 0 \ (m \ge 1).$$
 (2.20)

The $a_{n,m}^{(1)}$'s are given in table 9 for small n.

Table 9. A list of $a_{n,m}^{(1)}$ for $1 \le n \le 6$. Blanks denote zeros.

| | 1 | 2 | 3 | 4 | 5 | 6 | п |
|---|---|---|----|----|-----|------|---|
| 1 | | | 12 | 98 | 576 | 2970 | |
| 2 | | | 9 | 94 | 639 | 3630 | |
| 3 | | | 2 | 38 | 346 | 2354 | |
| 4 | | | | 6 | 99 | 918 | |
| 5 | | | | | 12 | 204 | |
| 6 | | | | | | 20 | |
| m | | | | | | | |

3. Solving the difference equations

From now on we write $\alpha_{n,m} \equiv a_{n,m}^{(0)}$ and $\beta_{n,m} \equiv a_{n,m}^{(1)}$ for simplicity, and define

$$\gamma_{n,m} = \beta_{n,m} + \alpha_{n+1,m} - (n^2 - 2n + 3)\alpha_{n,m}.$$
(3.1)

Results (2.15), (2.18) and (2.19) of the previous section give the following linear difference equations,

$$\alpha_{n+1,m+1} = \alpha_{n,m} + 2\alpha_{n,m+1} + \alpha_{n,m+2} \tag{3.2}$$

 $\alpha_{n,n}$

and

$$\gamma_{n+1,m+1} = \gamma_{n,m} + 2\gamma_{n,m+1} + \gamma_{n,m+2} + (\alpha_{n+1,m+2} - \alpha_{n+1,m+1}) - \delta_{m,0}\alpha_{n,1}$$
(3.3)

where $\delta_{m,0} = 1$ if m = 0 and $\delta_{m,0} = 0$ otherwise. Here we will solve these difference equations with the following boundary conditions, respectively,

$$\alpha_{n,m} = 0 \qquad \text{if } n \leqslant 0, \text{ or } m \leqslant 0, \text{ or } m \geqslant n+1 \tag{3.4}$$

(3.5)

$$= 1$$
 for all $n \ge 1$

and

$$\gamma_{n,m} = 0 \qquad \text{if } n \leqslant -1, \text{ or } m \leqslant 0, \text{ or } m \geqslant n+2$$

$$\gamma_{n,n+1} = 1 \qquad \text{for all } n \geqslant 0$$

$$(3.6)$$

We introduce the generating functions

$$\Phi(x, y) = \sum_{n=1}^{\infty} \sum_{m=1}^{n} \alpha_{n,m} x^n y^m$$
(3.8)

and

$$\Psi(x, y) = \sum_{n=0}^{\infty} \sum_{m=1}^{n+1} \gamma_{n,m} x^n y^m.$$
(3.9)

Combining equations (3.2) and (3.3) with conditions (3.4) and (3.6), respectively, gives

$$\Phi(x, y) = \frac{xy(a(x) - y)}{x(y+1)^2 - y}$$
(3.10)

and

$$\Psi(x, y) = \frac{1}{x(y+1)^2 - y} [(y-1)\Phi(x, y) + y(1+xy)a(x) + xyb(x) + y^2(x-1)] \quad (3.11)$$

where

$$a(x) = \sum_{n=1}^{\infty} \alpha_{n,1} x^n \tag{3.12}$$

and

$$b(x) = \sum_{n=0}^{\infty} \gamma_{n,1} x^n.$$
 (3.13)

The functions a(x) and b(x) are determined by conditions (3.5) and (3.7). First we explain how to determine a(x). By definition (3.8) we have

$$\Phi(x, y) = \sum_{m=1}^{\infty} \phi_m(x) y^m$$
(3.14)

with

$$\phi_m(x) = \sum_{n=m}^{\infty} \alpha_{n,m} x^n.$$
(3.15)

Condition (3.5) means that

$$\phi_m(x) = x^m + \mathcal{O}(x^{m+1})$$
(3.16)

for all $m \ge 1$. Expansion of (3.10) as a power series of y gives

$$\phi_{1} = a(x)$$

$$\phi_{2} = -1 - \left(2 - \frac{1}{x}\right)a(x)$$

$$\phi_{3} = \left(2 - \frac{1}{x}\right) + \left(3 - \frac{4}{x} + \frac{1}{x^{2}}\right)a(x)$$
....
(3.17)

Therefore conditions (3.16) for m = 1, 2, 3 determine the function a(x) up to the order x^5 as

$$a(x) = x + 2x^{2} + 5x^{3} + 14x^{4} + 42x^{5} + \mathcal{O}(x^{6}).$$
(3.18)

It should be remarked that the coefficients 1, 2, 5, 14, 42 are the Catalan numbers.

Of course, if we obtain ϕ_m for higher *m*'s and impose condition (3.16), we will determine the higher coefficients of the expansion of a(x); however, we explain another method here. Let *X* be the inverse function of a(x); x = X(a), and we consider the following Laurent expansion of 1/X(a) with respect to *a*:

$$\frac{1}{x} = \frac{1}{X(a)} = \sum_{k=-\infty}^{\infty} \delta_k a^k.$$
(3.19)

Since we have already known that $a(x) = x + O(x^2)$, (3.16) is equivalent to the condition

$$\phi_m(a) = a^m + \mathcal{O}(a^{m+1})$$
(3.20)

for all $m \ge 1$. Substituting (3.19) for 1/x in ϕ_2 given by the second equation of (3.17) and imposing (3.20) with m = 2, we have $\delta_k = 0$ for $k \le -2$, $\delta_{-1} = 1$, $\delta_0 = 2$ and $\delta_1 = 1$. The similar procedure for m = 3 concludes $\delta_2 = \delta_3 = 0$. Thus we have $1/x = (1+a)^2/a + \mathcal{O}(a^4)$. As explained in appendix A.1, we can prove that $\delta_k = 0$ for all $k \ge 2$ and we have the result

$$x = \frac{a}{(1+a)^2}.$$
 (3.21)

This gives a quadratic equation for a and we choose the solution which has the expansion in the form (3.18) as

$$a(x) = \frac{1}{2x} \{1 - 2x - \sqrt{1 - 4x}\}.$$
(3.22)

If we assume $x \leq \frac{1}{4}$, we can expand a(x) in x and prove that the coefficients are generally given by the Catalan numbers $\{c_n\}$:

$$a(x) = \sum_{n=1}^{\infty} c_n x^n.$$
 (3.23)

Next we consider b(x) defined by (3.13). First we transform the variable x in (3.11) into a(x) by (3.21). We obtain

$$\Psi = \frac{y}{(1-ay)^2(y-a)} [y(a+1)\{(a^3-a+1)-ay\} - a(1-ay)b(x)].$$
(3.24)

Let

$$\Psi = \sum_{m=1}^{\infty} \psi_m(a) y^m.$$
(3.25)

Then (3.7) is equivalent to the condition

$$\psi_m(a) = a^{m-1} + \mathcal{O}(a^m) \tag{3.26}$$

for all $m \ge 1$. Following a similar argument, we can prove that

$$b = 1 - a^2. (3.27)$$

More details are given in the appendix, A.2.

Now we can completely determine the generating functions as

$$\Phi(x, y) = \frac{a(x)y}{1 - a(x)y}$$
(3.28)

and

$$\Psi(x, y) = -\frac{1+a(x)}{a(x)} + \frac{(1+a(x))^2}{a(x)(1-a(x)y)} - \frac{1+a(x)}{(1-a(x)y)^2}$$
(3.29)

with (3.22). Expanding these functions with respect to y, we find

$$\phi_m(x) = \sum_{n=m}^{\infty} \alpha_{n,m} x^n = a(x)^m$$
(3.30)

and

$$\psi_m(x) = \sum_{n=m-1}^{\infty} \gamma_{n,m} x^n = a(x)^{m-1} - (m-1)a(x)^m - ma(x)^{m+1}$$
(3.31)

for $m \ge 1$. It follows that

$$\gamma_{n,m} = \alpha_{n,m-1} - (m-1)\alpha_{n,m} - m\alpha_{n,m+1}.$$
(3.32)

It is easy to confirm that this is equivalent to the relation (1.11) of theorem 2.

Already we have shown that $\alpha_{n,1} = c_n$ by (3.12) and (3.23). Thus it is easy to prove (1.10) of theorem 2 using equation (3.2) inductively. It is noticed that (1.10) can be concluded from (3.30) with (3.22) directly, if the following identity is available,

$$\sum_{k=m-1}^{n-1} b_{k+m-2,k-m+1} b_{n-k,n-k-1} = b_{n+m-1,n-m}$$
(3.33)

for $1 \leq m \leq n$, where $b_{n,m}$ is the ballot number defined by (1.12). Now the proof of theorem 2 is complete.

4. Approximations

In this section, we follow the procedure given at the end of section 1 and give two approximations $\tilde{P}^{(0)}(p)$ and $\tilde{P}^{(1)}(p)$ for the percolation probability. By definition (1.23), $A_{n,m}^{(0)} = \alpha_{n,m}$ and $A_{n,m}^{(1)} = \beta_{n,m} - (n-1)(n-2)\alpha_{n,m}$. Since $\beta_{n,m} = a_{n,m}^{(1)}$ is given by (1.11) of theorem 2, we have

$$A_{n,m}^{(1)} = (n-m)\alpha_{n,m} - (m+1)\alpha_{n,m+1}.$$
(4.1)

It follows that

$$Q^{(0)} = \sum_{n=1}^{\infty} \sum_{m=1}^{n} (pq)^{n-1} (pq)^{m-1} \alpha_{n,m}$$
(4.2)

and

$$Q^{(1)} = \sum_{n=3}^{\infty} \sum_{m=1}^{n} (pq)^{n-1} (pq)^{m-1} \{ n\alpha_{n,m} - m\alpha_{n,m} - (m+1)\alpha_{n,m+1} \}.$$
 (4.3)

We can find that they are derived from the generating function (3.8) of $\alpha_{n,m}$ and a(x) given by (3.12) as follows:

$$Q^{(0)} = \left[\frac{1}{xy}\Phi(x,y)\right]_{x=y=pq}$$
(4.4)

and

$$Q^{(1)} = \left[\frac{1}{x}\frac{\partial}{\partial x}\Phi(x,y) - \frac{1+x}{x^2}\frac{\partial}{\partial y}\Phi(x,y) + \frac{1}{x^2}a(x)\right]_{x=y=pq}.$$
(4.5)

Using the result (3.28) and the fact a(pq) = (1 - p)/p, we obtain

$$\tilde{P}^{(0)}(p) = 1 - (1-p)^2 \frac{1}{p^3(2-p)}$$
(4.6)

and

$$\tilde{P}^{(1)}(p) = 1 - (1-p)^2 \left[\frac{1}{p^3(2-p)} + \frac{(2p^2 - 3p - 1)(p-1)^3}{p^5(p-2)^2(2p-1)} \right].$$
(4.7)

Define $p_c^{(R)} = \inf\{p \in [0, 1] : \tilde{P}^{(R)} > 0\}$ for $R \ge 0$. We have $p_c^{(0)} = 0.5310...$ and $p_c^{(1)} = 0.6103...$ Both approximants are increasing concave functions of p for $p_c^{(R)} \le p \le 1$ and go to 1 as $p \to 1$. We expect that $p_c^{(R)}$ will monotonically approach the exact critical value as $R \to \infty$, which is numerically estimated as $p_c = 0.6447006 \pm 0.0000010$ by the recent paper of Jensen and Guttmann (1995).

For general $R \ge 0$, we see

$$P^{(R)}(p) - P(p) = \mathcal{O}(q^{n(R+1)+R+3})$$
(4.8)

where $n(r) = \lceil (1 + \sqrt{1 + 4r})/2 \rceil + 1$. The formula for $A_{n,m}^{(s)}$ for $s \ge 2$, similar to (4.1), is required when giving higher approximations.

5. Future problems

We have presented some rigorous results concerning the coefficients in a series expansion of the percolation probability for the bond directed percolation on a square lattice. As a generalization of the fact that the Catalan number plays an important role in extending the series expansion of the percolation probability, we have shown that the ballot numbers are very useful in expressing the coefficients $a_{n,m}^{(s)}$ in a series expansion of $P_{n,m}$. In the present paper we have proved that $a_{n,m}^{(0)}$ and $a_{n,m}^{(1)}$ are expressed as linear combinations of the ballot numbers. Moreover, we can prove that $a_{n,m}^{(2)}$ is also expressed using the ballot number $a_{n,m}^{(0)}$ as

$$a_{n,m}^{(2)} = f(n,m)a_{n,m}^{(0)} - (m+2)(m+1)^2 a_{n,m+1}^{(0)} + \frac{1}{2}m(m+3)a_{n,m+2}^{(0)} + 2a_{n-1,m-1}^{(0)} + 2a_{n-1,m+1}^{(0)} + \delta_{m,1}a_{n-1,m+1}^{(0)}$$

with

$$f(n,m) = \frac{1}{2}n^4 - 2n^3 - \frac{4m^2 - 3m + 2}{2m}n^2 + \frac{2m^3 + 9m^2 + 3m + 3}{m}n$$
$$-(m^3 + \frac{9}{2}m^2 + \frac{15}{2}m + 2) \qquad \text{for } n \ge 2 \text{ and } m \ge 1$$
(5.1)

and

$$a_{n\,m}^{(2)} = 0$$
 for $n \leq 1$ and $m \geq 1$

where $\delta_{m,1}=1$ if m = 1 and $\delta_{m,1} = 0$ otherwise. Since the derivation of this result is long, we will report it elsewhere.

Baxter and Guttmann (1988) and Jensen and Guttmann (1995) conjectured that the correction terms $d_{n,l}$ are expressed as rational functions of the Catalan number for any l as (1.20). In this paper we have proved their conjectures for $d_{n,1}$ and $d_{n,2}$, and the above result (5.1) gives the third one $d_{n,3} = -2(n+1)c_n + 2c_{n+1}$. Although the proof of the conjectures for higher l remains an open problem, our results reported in this paper suggest a generalized conjecture: the coefficients $a_{n,m}^{(s)}$ in a series expansion of $P_{n,m}$ are generally expressed using the ballot numbers. It is a future problem to prove this generalized conjecture and use it to produce a more convincing series expansion for $P_{n,m}$.

Our method can be applied to the site directed percolation (SDP). We found that the first correction term $d_{n,1}$ for the SDP is given by the following difference equations,

$$a_{n+1,m} = \sum_{k=m-1}^{n} (k-m+2)a_{n,k}$$
(5.2)

with $a_{1,1} = 1$, $a_{1,m} = 0$ ($m \ge 2$) and $a_{n,0} = 0$ ($n \ge 0$), and

$$d_{n,1} = \sum_{m=1}^{n} a_{n,m}.$$
(5.3)

For small n, $\{d_{n,1}\}$ are 1, 3, 12, 55, 273.... Onody and Neves (1992) conjectured that $d_{n,1} = (3n)!/\{n!(2n + 1)!\}$ and it was proved by Bousquet-Mélou (1996) by studying directed animals. Another proof will be given by solving these difference equations.

We have found good properties of coefficients in series expansion, some of which were used in this paper. It is an interesting problem to estimate the upper and lower bounds for coefficients using these regularities.

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Appendix

A.1. Proof of (3.21)

Let

Φ

$$\frac{1}{x} = \frac{(1+a)^2}{a} + \Omega(a)$$
(A.1)

with $\Omega(a) = \mathcal{O}(a^4)$. Then (3.10) becomes

av

$$(x, y) = \frac{1}{1 - ay\{1 + (\Omega(a)/a)/(1 - y/a)\}}$$
$$= \sum_{m=1}^{\infty} \left[a^m + \sum_{l=1}^{m-1} \Omega(a)^l \sum_{n=l}^{m-1} \binom{n}{l} \binom{l+m-n-2}{l-1} a^{-m-l+2(n+1)} \right] y^m. \quad (A.2)$$

We see that

$$b_m = a^m \qquad \text{for } 1 \leqslant m \leqslant 3 \tag{A.3}$$

and

$$\phi_m = a^m + \frac{\Omega(a)}{a^{m-3}} + (\text{higher-order terms of } a) \qquad \text{for } m \ge 4.$$
 (A.4)

Condition (3.20) can be satisfied for all *m*, if and only if $\Omega(a) = 0$.

A.2. Proof of (3.27)

Expansion of (3.24) in y gives

q

$$\psi_{1} = b$$

$$\psi_{2} = -a^{3} - a^{2} + a - \frac{1}{a} + b\left(a + \frac{1}{a}\right)$$

$$\psi_{3} = -2a^{4} - 2a^{3} + a^{2} - \frac{1}{a^{2}} + b\left(a^{2} + 1 + \frac{1}{a^{2}}\right).$$
(A.5)

Let $b = \sum_{k=-\infty}^{\infty} \epsilon_k a^k$. If we put condition (3.26) for m = 1, 2, 3, we have $\epsilon_k = 0$ for $k \leq -1$, $\epsilon_0 = 1$, $\epsilon_1 = 0$, $\epsilon_2 = -1$, $\epsilon_3 = 0$ and $\epsilon_4 = 0$, that is

$$b = 1 - a^2 + \omega(a) \tag{A.6}$$

with $\omega(a) = \mathcal{O}(a^5)$. Substituting (A.6) for b in (3.24) gives

$$\Psi = -\frac{1+a}{a} + \frac{(1+a)^2}{a(1-ay)} - \frac{1+a}{(1-ay)^2} - \frac{ay}{(1-ay)(y-a)}\omega(a)$$
$$= \sum_{m=0}^{\infty} \left[a^{m-1} - (m-1)a^m - ma^{m+1} + 1_{\{m \ge 1\}} \frac{\omega(a)}{a^{m-1}} \sum_{s=0}^{m-1} a^{2s} \right] y^m \quad (A.7)$$

where $1_{\{m \ge 1\}} = 1$ if $m \ge 1$ and $1_{\{m \ge 1\}} = 0$ otherwise. Therefore condition (3.26) can be satisfied for all $m \ge 1$, if and only if $\omega(a) \equiv 0$.

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