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Directed bond percolation on a square lattice: I. Analytical results

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Abstract. A rigorous mathematical formulation of directed percolation is given in terms of matrix recursion equations. The Domany–Kinzel limit is rederived in a very simple way. Expansion around this limit yields surprisingly good results for the percolation probabilities already to first order.

1. Introduction

The problem of directed percolation has gained considerable attention recently. It has been shown that Reggeon field theory (Cardy and Sugar 1980), selected problems of epidemiology (Bailey 1975), astronomy (Schulman and Seiden 1982) and chemistry (Schögl 1972) are related to directed percolation. There are many problems, for example in the paint and oil industry, which are treated by using ideas similar to those of directed percolation. According to Obukhov (1980) the upper critical dimensionality for oriented percolation is $d = 5$ and thus it does not belong to the same universality class as non-oriented percolation (for which the corresponding d is 6). In $d = 2$ Monte Carlo calculations (Kertesz and Vicsek 1980), the method of finite size renormalisation group (Domany and Kinzel 1981, Kinzel and Yeomans 1981), series expansions (Blease 1977, Adler *et al* 1981) were used to determine the critical properties in the general case. For some special cases exact analytical results have been obtained (Domany and Kinzel 1981, Wu and Stanley 1982). Unlike for the problem of directed animals (Nadal *et al* 1982), there are no analytical results for directed percolation in the general case.

The aim of the present work is to give a new, mathematically precise formulation of directed percolation, which will then be applied to derive analytical results beyond the existing ones. Since the method can be used straightforwardly for very effective and fast numerical calculations, in a subsequent paper (Bidaux and Forgács 1984) we will present numerical results for directed percolation obtained through this method.

In § 2 directed percolation on a square lattice will be formulated in terms of matrix recursion equations which are exact. In § 3 we derive the so-called Domany–Kinzel limit (Domany and Kinzel 1981). Section 4 contains results of an expansion around this limit, while § 5 is devoted to some concluding remarks. Some details of the calculation are described in the appendix.

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2. Rigorous mathematical formulation

In what follows we concentrate on a square lattice and imagine 'water' (current, disease, etc) flowing from a source only in the direction of arrows in figure 1. Adjacent lattice sites are either connected through pipes (bonds) with probabilities p_1 and p_2 depending on the direction of flow, or are not connected with probabilities $q_1 = 1 - p_1$ and $q_2 = 1 - p_2$. If water can reach a given lattice site we say it is wet and denote it by +, otherwise it is dry and is denoted by −. The questions one may ask are the following. (1) What is the probability that the observer will find water at the nth level, irrespective of the sites where the flow appears? (2) What is the probability that the observer will find water at a *given site* of the nth level? (3) What are the respective limits of the previous probabilities when n goes to infinity and what are the corresponding critical conditions on p_1 and p_2 for these limits to be non-zero?

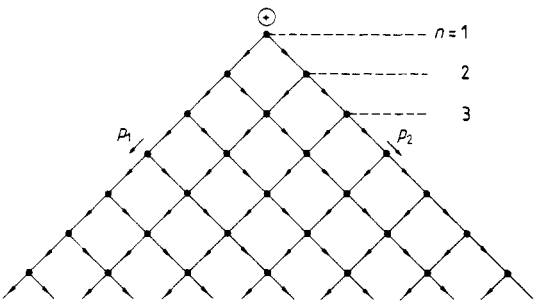

Figure 1. Directed percolation on a square lattice. Arrows indicate the permitted oriented paths for the flow to propagate. Each oriented bond is conducting with probability p_1 in the NE→SW direction, p_2 in the NW→SE direction. The number of sites at each row (level) is used in the text as an index of that row (level). The + sign at the top site indicates that this site is wet.

Inspecting the situation ('dry' or 'wet') of each of the lattice sites at the nth level, we obtain 2^n distinct possible states for this level, which will be classified as follows.

Each state is represented by a sequence of + or − signs of length n, and the kth sign of the sequence (from left to right) represents the situation of the kth site (from left to right in figure 1) for this given state.

The probabilities of the 2^n different states of the nth level are displayed in a vertical array u_n of 2^n lines in the way shown explicitly for $n = 1, 2, 3$:

$$u_1 = \begin{bmatrix} \Pr(-) \\ \Pr(+) \end{bmatrix}, \qquad u_2 = \begin{bmatrix} \Pr(--) \\ \Pr(-+) \\ \Pr(+-) \\ \Pr(++) \end{bmatrix}, \qquad u_3 = \begin{bmatrix} \Pr(---) \\ \Pr(--+) \\ \Pr(-+-) \\ \Pr(-++) \\ \Pr(+--) \\ \Pr(+-+) \\ \Pr(++-) \\ \Pr(+++) \end{bmatrix} \tag{1}$$

Note the general rule for constructing u_n: the successive probabilities met as u_n is read

from top to bottom refer to states which are classified according to an increasing value of their binary equivalent ($(-)\equiv 0$, $(+)\equiv 1$).

In what follows, we will omit Pr when writing the components of the vectors u_n, and each component will be called configuration as a short name for configuration probability.

Knowing the configurations in the nth row, one can construct the configurations of the $(n+1)$th row using a 'transfer matrix', whose entries are expressed by $p_1(q_1)$ and $p_2(q_2)$. For example in the case $n=1$

$$u_2=\begin{bmatrix}- & -\\ - & +\\ + & -\\ + & +\end{bmatrix}=\begin{bmatrix}1 & q_1q_2\\ 0 & q_1p_2\\ 0 & p_1q_2\\ 0 & p_1p_2\end{bmatrix}[\mp]=\hat{M}_1u_1. \tag{2}$$

where $u_1=[\bar{+}]=\begin{bmatrix}0\\1\end{bmatrix}$ accounts for the wet site of the first row. The sum of the elements of $\hat{M}_1$ in a given column is unity, which means that $\hat{M}_1$ is a Markov matrix. This is of course true for any $\hat{M}_n$ since directed percolation is a Markovian process. As can be seen from (2) the 'transfer matrix' $\hat{M}$ is a rectangular matrix. It is more convenient to work with square matrices and in order to achieve this we use the following trick. We complete figure 1, as shown in figure 2. Now if we have $(n+1)$ lattice sites at the first level

$$u_{n+1}=(M_{n+1})^nu_1 \tag{3}$$

where u_1 and u_{n+1} describe the configurations of the first and $(n+1)$th level respectively, and M_{n+1} is a $2^{(n+1)}\times 2^{(n+1)}$ square matrix connecting the configurations of two subsequent levels. If now we choose u_1 such that all its components are zero except for the one corresponding to $(+---\ldots-)$, which has weight one, then our 'square' problem will be equivalent to the original one. In other words

$$u_1=\begin{bmatrix}\mathbf{0}\\ \mathbf{1}\end{bmatrix} \tag{4a}$$

where

$$\mathbf{0}=\begin{bmatrix}0\\ \cdot\\ \cdot\\ 0\end{bmatrix},\qquad \mathbf{1}=\begin{bmatrix}1\\ 0\\ \cdot\\ 0\end{bmatrix}, \tag{4b}$$

are 2^n component vectors.

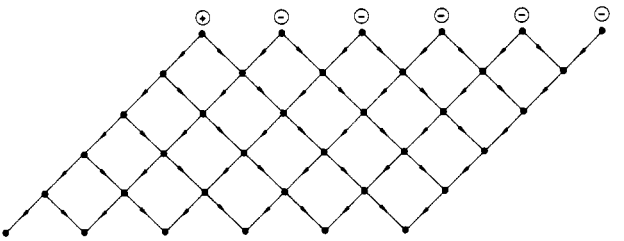

Figure 2. Lattice equivalent to the previous one, using the same convention for oriented bonds. Signs at the top of the first row indicate that the only wet site of that row is at the extreme left. This lattice has been used to derive recursion relations in terms of square matrices.

With the choice (4*a*) the additional lattice sites introduced in figure 2 will always be dry and therefore will not participate in the flow. The first component of u_n (which is denoted by u_{n1}) gives the probability that there is no water at the nth level. The percolation threshold is then defined as

$$\lim_{n\to\infty}(1-u_{n1})=\begin{cases}0 \text{ if } p_2\leqslant f(p_1),\\ \text{some strictly positive probabilistic value if } p_2>f(p_1).\end{cases} \tag{5}$$

Here $p_2=f(p_1)$ determines the critical line along which percolation takes place in the anisotropic case.

It is now not very difficult to show (using induction) that there exists a recursion equation connecting M_{n+1} with M_n, namely

$$M_{n+1}=\begin{bmatrix}M_n & q_1X_n\\ 0 & p_1X_n\end{bmatrix} \tag{5a}$$

where

$$X_{n+1}=\begin{bmatrix}q_2M_n & q_1q_2X_n\\ p_2M_n & (1-q_1q_2)X_n\end{bmatrix}. \tag{5b}$$

In (5*a*, *b*), M_n and X_n are Markovian matrices and the recursion equations preserve this property. The initial values of M_n and X_n are 2×2 matrices which can be obtained by constructing M_2 explicitly and then writing it in the form (5*a*):

$$M_1=\begin{bmatrix}1 & q_1\\ 0 & p_1\end{bmatrix},\qquad X_1=\begin{bmatrix}q_2 & q_1q_2\\ p_2 & (1-q_1q_2)\end{bmatrix}. \tag{6a, b}$$

Equations (5*a*, *b*) with (6*a*, *b*) give a mathematically exact formulation of directed percolation on a square lattice. We have not yet been able to resolve these equations. In what follows a special case and then an expansion around this special case will be discussed.

3. The Domany–Kinzel limit

The Domany–Kinzel limit corresponds to $p_1=1$ ($q_1=0$). In this case the problem essentially reduces to a one-dimensional random walk and can be solved exactly (Domany and Kinzel 1981, Wu and Stanley 1982). We now show how this limit can be treated by using the formalism described in § 2. If $p_1=1$, equations (5*a*, *b*) reduce to

$$M_{n+1}=\begin{bmatrix}M_n & 0\\ 0 & X_n\end{bmatrix},\qquad X_{n+1}=\begin{bmatrix}qM_n & 0\\ pM_n & X_n\end{bmatrix}. \tag{7a, b}$$

Here $p_2=p$, $q_2=q$ have been used. The fact that M becomes block diagonal and X becomes block triangular renders the problem almost trivial. Let us calculate $(M_{n+1})^n u_1$ according to (2), where u_1 is a $2^{(n+1)}$-component vector with the structure given by (4*a*, *b*). Using (7*a*)

$$u_{n+1}=\begin{bmatrix}\mathbf{0}\\ (X_n)^n\mathbf{1}\end{bmatrix}. \tag{8}$$

In order to calculate $(X_k)^k\mathbf{1}$ we again use (7*a*) and (7*b*). By induction one easily finds that

$$[(X_n)^n\mathbf{1}]_i = \begin{cases} \binom{n}{s} q^{n-s}p^s & \text{if } i = 1+2^{n-s}(2^s-1),\ 0 \leqslant s \leqslant n, \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

$\binom{n}{s}q^{n-s}p^s$ then gives the probability that up to (and including) the $(s+1)$th site (counted from the left) all the lattice sites at the $(n+1)$th level are wet, whereas the ones to the right of this site are all dry (note that because of the special limit we are considering, if a given site at the nth level is wet, all the sites left of it are wet). If by $P^{(0)}_{n,s}(p)$ we denote the probability that site $(s+1)$ at the $(n+1)$th level is wet, irrespective of the others, then

$$P^{(0)}_{n,s}(p) = \sum_{l=s}^{n} \binom{n}{l} (1-p)^{n-l}p^l. \tag{10}$$

From (9) one sees that the non-zero components of u_{n+1} form a binomial distribution and (10) means summing part of this distribution. We are interested in the large-n limit, such that $s/n = \alpha$ is finite. In this limit the binomial distribution around its mean (maximum) value np can be approximated by a Gaussian distribution. Since these distributions are normalised to unity we immediately obtain

$$\lim_{n\to\infty} P^{(0)}_{n,s}(p) = \begin{cases} 0 & \text{if } \alpha > p, \\ \frac{1}{2} & \text{if } \alpha = p, \\ 1 & \text{if } \alpha < p. \end{cases} \tag{11}$$

This determines the critical probability (Wu and Stanley 1982) $p_c^{(0)}$ for the Domany–Kinzel case as

$$p_c^{(0)} = \alpha. \tag{12}$$

$p_c^{(0)}$ depends on the position of the site in the last level at which flow is observed. Assuming $(\alpha - p) \ll 1$, for large n one obtains

$$P_{n,s}(p) \sim \mathrm{e}^{-n/\xi} \tag{13}$$

with

$$\xi \sim (\alpha - p)^{-2} \tag{14}$$

which then gives $\nu = 2$ for the critical index of the correlation length.

4. Expansion around the Domany–Kinzel limit

The results of § 3 have already been previously obtained (although in a more complicated way) by other authors (Domany and Kinzel 1981, Wu and Stanley 1982), using a different approach. The simplicity of the present formulation allows one also to perform an expansion around the Domany–Kinzel limit without too much difficulty. Let us write $p_1 = 1-\varepsilon$ and treat ε as a small parameter. Writing

$$M_n(\varepsilon) = M_n + \varepsilon m_n, \qquad X_n(\varepsilon) = X_n + \varepsilon x_n, \tag{15a, b}$$

using (5*a*, *b*) one gets

$$m_{n+1}=\begin{bmatrix} m_n & X_n \\ 0 & -X_n+x_n \end{bmatrix}, \qquad x_{n+1}=\begin{bmatrix} qm_n & qX_n \\ pm_n & -qX_n+x_n \end{bmatrix}. \tag{16a, b}$$

Here again $p_2=p$, $q_2=q$. Calculating u_{n+1} according to (2), using (5*a*, *b*) and (16*a*, *b*) up to first order in ε,

$$u_{n+1}(\varepsilon)=\begin{bmatrix} \mathbf{0} \\ (X_n)^n\mathbf{1} \end{bmatrix}+\varepsilon\begin{bmatrix} \sum_{l=1}^{n}(M_n)^{n-l}(X_n)^l\mathbf{1} \\ -n(X_n)^n\mathbf{1}+\sum_{l=0}^{n-1}(X_n)^{n-1-l}x_n(X_n)^l\mathbf{1} \end{bmatrix}. \tag{17}$$

Once the components of u_{n+1} are known, the quantity $P_{n,s}(p)$ defined in § 3 can again be calculated by summing the appropriate elements of u_{n+1}. Some details of the evaluation of sums in (17) and of the calculation of $P_{n,s}(p)$ are given in the appendix. Let us write

$$P_{n,s}(p)=P_{n,s}^{(0)}(p)+\varepsilon P_{n,s}^{(1)}(p)+O(\varepsilon^2). \tag{18}$$

Here $P_{n,s}^{(0)}(p)$ is given by (10). Let us evaluate (18) at $p=p_c(\varepsilon)=p_c^{(0)}+\varepsilon p_c^{(1)}$, where $p_c^{(0)}$ is determined by (12). Using (11) we obtain

$$P_{n,s}(p_c)=\tfrac{1}{2}+\varepsilon\left[p_c^{(1)}\left(\frac{d}{dp}P_{n,s}^{(0)}(p)\right)_{p=\alpha}+P_{n,s}^{(1)}(\alpha)\right]. \tag{19}$$

The derivative of $P_{n,s}^{(0)}$ is easily evaluated from (10):

$$\frac{d}{dp}P_{n,s}^{(0)}(p)|_{p=\alpha=s/n}=n\binom{n-1}{s-1}\alpha^{s-1}(1-\alpha)^{n-s}\xrightarrow[n\gg 1]{}\left(\frac{n}{2\pi\alpha(1-\alpha)}\right)^{1/2}+O\left(\frac{1}{\sqrt{n}}\right). \tag{20}$$

According to (A8) the leading term in $P_{n,s}^{(1)}(\alpha)$ is also proportional to $n^{1/2}$. This means $p_c^{(1)}$ must be chosen such that the $n^{1/2}$ contributions cancel in $P_{n,s}$. This leads to

$$p_c^{(1)}=(1-\alpha)^2. \tag{21}$$

In the isotropic case ($p_1=p_2$) it is plausible that percolation occurs first for $\alpha=s/n=\frac{1}{2}$ (that is, at the central site of the last level). To obtain the approximate value of the percolation probability in this case, we can use $p_c^{(0)}(\alpha=\frac{1}{2})$ and $\varepsilon=1-p_1=\frac{1}{2}$. This leads to (Grassberger 1983)

$$p_c^{(1)}(\alpha=\tfrac{1}{2})=\tfrac{1}{4} \tag{22}$$

and

$$p_c(\text{isotropic})=\tfrac{1}{2}+\tfrac{1}{4}\varepsilon=0.625. \tag{23}$$

(23) compares rather well with the numerical estimates (Kertesz and Vicsek 1980, Kinzel and Yeomans 1981, Adler *et al* 1981). Finally, using the O(1) term in (A8) we get

$$P_{n,s}(p_c)=\tfrac{1}{2}-\varepsilon[(1-\alpha)/\alpha][\tfrac{3}{2}-\tfrac{1}{2}(1-2\alpha)]. \tag{24}$$

In the isotropic case the exact solution should give $P_{n,s}(p_c)=0$. We can estimate p_c (isotropic) again. This time, using $\alpha=\frac{1}{2}$, we find the value of ε for which $P_{n,s}(p_c)=0$. This leads to

$$0=\tfrac{1}{2}-\tfrac{3}{2}\varepsilon \tag{25}$$

and finally $\varepsilon = 1 - p_c = \frac{1}{3}$, which gives

$$p_c(\text{isotropic}) = \tfrac{2}{3} = 0.667. \tag{26}$$

(26) again compares surprisingly well with numerical estimates.

It is interesting to note that the mean of (23) and (26) gives 0.646 for p_c which is almost the same as the best numerical estimates (Blease 1977, Dhar and Barma 1981, Kinzel and Yeomans 1981, Dhar 1982).

5. Conclusions

The method described in the present work gives a systematic expansion of critical probabilities for directed percolation on any lattice. The calculation of higher-order terms in ε is straightforward, though it becomes rather tedious. It is not inconceivable that equations (5*a*, *b*) can be solved exactly. Similar equations are valid in higher dimensions. We hope to solve the completely anisotropic case in $d = 3$ (free flow in a plane). It is quite possible that the method can be used for other problems.

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Appendix

The RHS of (17) is evaluated by using the recursion equations for M_n and X_n. A straightforward calculation gives

$$(M_n)^{n-l}(X_n)^l \mathbf{1}|_{i=1+2^{n-s}(2^s-1)} = \begin{cases} q^l & \text{if } s = 0, \\ \displaystyle\sum_{k=1}^{s} \binom{n-l-k}{s-k}\binom{l+k-1}{k} q^{n-s}p^s & \text{if } 1 \leqslant s \leqslant n-l, \\ \displaystyle\binom{n}{s} q^{n-s}p^s & \text{if } n-l+1 \leqslant s \leqslant n. \end{cases} \tag{A1}$$

The components with i different from the above LHS form are zero. The sum on the RHS of (A1) can be easily evaluated by using

$$\binom{n+p-1}{p} = C^p_{n+p-1} = K^p_n \tag{A2}$$

where the generating function of the K^p_n is defined by

$$\sum_{m=0}^{\infty} K^m_n x^m = (1-x)^{-m}. \tag{A3}$$

In terms of K_n^p

$$A_s = \sum_{k=1}^{s} \binom{n-l-k}{s-k}\binom{l+k-1}{k} = \sum_{k=1}^{s} K_{n-l-s+1}^{s-k} K_l^k. \tag{A4}$$

One can immediately see that the RHS of (A4) is related to the coefficient of the x^s term in the power series of $(1-x)^{-(n-l-s+1)}$. Finally

$$A_s = \binom{n}{s} - \binom{n-l}{s} \tag{A5}$$

and

$$\sum_{l=1}^{n} (M_n)^{n-l}(X_n)^l \mathbf{1}|_{i=1+2^{n-s}(2^s-1)} = \begin{cases} q\dfrac{1-q^n}{1-q} & \text{if } s=0, \\ s\binom{n+1}{s+1} q^{n-s}p^s & \text{if } 1 \leqslant s \leqslant n. \end{cases} \tag{A6}$$

The calculation of the other sum in (17), though again straightforward, is more tedious. All the sums appearing in the course of the calculation can be expressed by means of K_n^p. In the large-n limit the expressions simplify considerably and one obtains

$$P_{n,s}^{(1)}(p) = \sum_{k=s-1}^{n} q^{n-k}p^k\left[-\binom{n}{s+1} + \frac{q}{p}(\alpha-2-s)\binom{n}{s}\right] + O\left(\frac{1}{\sqrt{n}}\right). \tag{A7}$$

The sum in (A7) in the large-n limit can be evaluated using Stirling's formula and the saddle point method. One gets

$$P_{n,s}^{(1)}(p) = -\frac{n^{1/2}}{(2\pi)^{1/2}} q\left(\frac{q}{p}\right)^{1/2} - \frac{q}{p}[\tfrac{3}{2} + \tfrac{1}{2}(p-q)]. \tag{A8}$$

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