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A calculable model of directed percolation

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Abstract. A new approximate method for studying directed percolation in plane crystals is presented. By applying the method the percolation threshold and some statistical characteristics of the infinite cluster in a plane crystal with a quadratic lattice are found. The results obtained are verified by the Monte Carlo method.

1. Introduction

The rigorous investigation of the percolation process leads to rather difficult mathematical problems. There are some well-known approximate methods of solving these problems, e.g. numerical modelling, series expansions and the renormalization method [1-3]. The percolation threshold was found rigorously only for some specific cases of plane lattices.

Some applied problems, e.g. the motion of a charged particle in a medium under the action of a strong electrical field, or the stochastic process in the lattice which occurs at discrete time intervals, etc., lead to the problems of directed percolation [4]. In this paper we consider the following directed percolation process in a plane crystal with a quadratic lattice. Each site of the crystal is either open or closed for percolation. It is supposed that the percolation through each open site is possible only in three directions, let us say 'up', 'left' and 'right'. The fourth direction, 'down', is forbidden. To simplify the investigation, we suppose that the probability of the given site being open does not depend on the state of other sites (open or closed). The concentrations of open and closed sites are denoted, respectively, by p and q ($q = 1 - p$).

We shall use an approximate model of the process. This model can be treated quite rigorously. It enables one to derive some characteristics of an infinite cluster and leads to the rather unexpected conclusion that, contrary to widely accepted conviction, the transition between the percolation state and the non-percolation one is a phase transition of the first order. It is not inconceivable that this may be erroneous because of the choice of the mathematical model we have made. The comparison by the Monte Carlo method between our model and the classical one shows that the divergence in the data obtained grows as the concentration of open sites approaches the percolation threshold. Nevertheless, the existence of a rather realistic model, in which the phase transition is of first order, seems to be of some interest.

2. The model employed and formulation of the mathematical problem

In order to formulate the difference between the above-mentioned model of directed

percolation and the simplified model actually investigated, we need to introduce some stochastic characteristics of the percolation process.

Let us enumerate the layers of the crystal in a natural way, so that the boundary layer is numbered as one. The set of neighbouring sites in the same layer makes an open group if they all are open, while the two boundary sites are closed. We shall call all open groups in the first layer active. A group in the $(k+1)$ th layer will be called active if in the k th layer at least one of the sites lying immediately under the group belongs to an active group. A set of all the sites belonging to active groups forms a directed cluster, which is the main object of our investigation.

Two active groups in the same layer are considered to be neighbours if between them there are no other active groups. The set of sites between two neighbouring active groups will be called a passive group. The passive (active) group length is defined by the number of sites belonging to it. Let $p_k(s)$ and $q_k(s)$ be the concentrations of active and passive groups of length s in the k th layer. Thus, $p_k(s)$ is the probability for a given site in the k th layer to be the left site of an active group of length s .

The concentrations of active and passive sites in the k th layer are, respectively, equal to

$$C_k = \sum_{s=1}^{\infty} s p_k(s) \quad 1 - C_k = \sum_{s=1}^{\infty} s q_k(s). \quad (1)$$

The percolation is present if the limit $C = \lim_{k \rightarrow \infty} C_k$ is positive, and is absent if it equals zero.

The functions $p_k(s)$ and $q_k(s)$ do not provide a complete statistical description of the k th layer, because knowledge of these functions is insufficient to calculate the probability of encountering the complex consisting of n active groups of lengths s_1, s_2, \dots, s_n with $(n-1)$ passive groups of lengths $\sigma_1, \sigma_2, \dots, \sigma_{n-1}$ between them. A complete statistical description of the first layer can be obtained rather easily. But the problem of finding a complete statistical description for the $(k+1)$ th layer, when such a description for the k th layer is known, leads to an infinite set of linear equations, and the procedure of writing down this set is rather complicated.

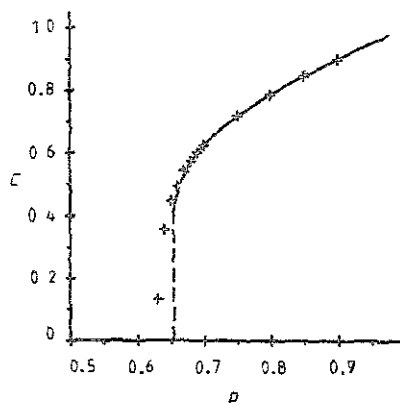


Figure 1. The concentration C of sites belonging to the infinite cluster against the concentration p of open sites: Full curve, the present theory, crosses, the mean concentration values obtained by a 10-fold modelling for each value of p .

To avoid these difficulties, let us consider an approximate model, where there are no correlations between the lengths of neighbouring active and passive groups. We were at first not sure whether such a model would give reasonably good results. To find out how far one may depend on these results, an independent investigation was made using the Monte Carlo method. The Monte Carlo process was repeated 10 times for each value of the parameter p . For $p = 0.63 + 0.01n$ ($n = 0, 1, \dots, 6$) the lattice was chosen to have 2000×2000 sites, for $p = 0.7 + 0.05n$ ($n = 0, 1, 2, 3, 4$) we took the lattice with 1000×1000 sites. The root mean square spread in the concentration C did not exceed 0.02 except for the concentration $p = 0.63$, where the spread is equal to 0.05. The results obtained are shown in figure 1. Thus we got the necessary encouragement to proceed with the investigation of the model.

The percolation problem in the frame of this model may be formulated as a problem of finding the values of $p_k(s)$, $q_k(s)$ ($k, s = 1, 2, \dots$) and their limits $p(s) = \lim p_k(s)$ and $q(s) = \lim q_k(s)$ ($k \rightarrow \infty$).

3. Fundamental relations

The assumption that the lengths of neighbouring active and passive groups do not correlate with each other permits one to evaluate $p_k(s)$ and $q_k(s)$, provided that $p_{k-1}(\sigma)$ and $q_{k-1}(\sigma)$ ($\sigma = 1, 2, \dots$) are known. A similar evaluation is made in the mean field theory in a much simpler case, where the layer state is specified by the concentration of active sites only [4]. No correlations are taken into account in this theory.

The formulae expressing $p_{k+1}(s)$ and $q_{k+1}(s)$ in terms of $p_k(\sigma)$ and $q_k(\sigma)$ ($\sigma = 1, 2, \dots$) are very cumbersome and are not fit for computing. One gets much simpler relations using the generating functions

$$\pi_k[z] \equiv \sum_{s=1}^{\infty} \pi_k(s)z^s \quad \kappa_k[z] \equiv \sum_{s=1}^{\infty} \kappa_k(s)z^s \tag{2}$$

where

$$\pi_k(s) = R_k^{-1} p_k(s) \quad \kappa_k(s) = R_k^{-1} q_k(s) \tag{3}$$

and

$$R_k \equiv \sum_{s=1}^{\infty} p_k(s) = \sum_{s=1}^{\infty} q_k(s). \tag{4}$$

The physical meaning of these quantities is obvious. R_k is the probability for a random site in the k th layer to be the very left site of some active group no matter how long it is. Let U_k be the set of all such sites. Then $\pi_k(s)$ is the probability for a random site from the set U_k to belong to an active group of length s . The conditional probability $\kappa_k(s)$ has a similar meaning.

The recurrence formulae for the generating functions can be written as (see the appendix)

$$q_{k+1}[z] = \frac{R_k}{(1 - \pi_k[qz]\kappa_k[z])} (A_1^2[z]\kappa_k[z] + A_2^2[z]\pi_k[qz] + A_3[z]\pi_k[qz]\kappa_k[z] + A_4[z]) \tag{5}$$

where

$$A_1[z] = \frac{pqz(q+pz)}{(1-qz)(p-z)} \quad (6)$$

$$A_2[z] = p \left(\frac{1}{1-qz} - \kappa_k[p] \frac{p(1-z)}{p-z} \right) \quad (7)$$

$$A_3[z] = p^2 q \left(\frac{2z(q+pz)}{(1-qz)^2(p-z)} + \frac{z}{(1-qz)^2} - \frac{z}{(1-qz)} (\pi'_k[1] - 1) - \frac{p\kappa'_k[p]z(1-z)}{(p-z)} + \frac{\kappa_p[p]z(z(1+p)-2p)}{(p-z)^2} \right) \quad (8)$$

$$A_4[z] = p^2 q \left[\frac{z}{1-qz} (\pi'_k[1] - 1) - \frac{z}{(1-qz)^2} + \frac{p\kappa'_k[p]z(1-z)}{p-z} + \frac{z\kappa_k[p]}{p-z} \left(\frac{2p(1-z)}{1-qz} - \frac{qz}{p-z} \right) \right] \quad (9)$$

and

$$p_{k+1}[z] = \frac{zpq^2}{1-pz} - R_k pq^2 \left(\frac{z\kappa'_k[1]}{1-pz} - \frac{pz^2(1-\kappa_k[pz])}{(1-pz)^2} \right). \quad (10)$$

To these two fundamental relations we shall add the following three equalities.

$$\begin{aligned} \kappa_k[0] &= \pi_k[0] = 0 \\ \kappa_k[1] &= \pi_k[1] = 1 \\ R_k(\pi'_k[1] + \kappa'_k[1]) &= 1. \end{aligned} \quad (11)$$

They immediately follow from the definitions (2)-(4).

4. The step-by-step calculation of stochastic characteristics of the layers

Relations (5) and (10) permit the step-by-step calculation of the characteristics $p_k(s)$ and $q_k(s)$ ($k=2, 3, \dots$; $s=1, 2, \dots$). Indeed, for $k=1$ we obviously have

$$p_1(s) = q^2 p^s \quad q_1(s) = p^2 q^s. \quad (12)$$

For the second step we use the series expansions in powers of z of the fundamental relations and equate the corresponding coefficients. In this way we get relatively simple expressions for $p_k(s)$ and $q_k(s)$, which permit us to make a step-by-step evaluation of $p_k(s)$, $q_k(s)$ ($s=1, 2, \dots$) if the values of $p_{k-1}(\sigma)$, $q_{k-1}(\sigma)$ ($\sigma=1, 2, \dots$) are known. In this manner we evaluated $p_k(s)$, $q_k(s)$ for all $s \leq N$ ($N=100-1000$). The functions $p_k(s)$ and $q_k(s)$ with $s > N$ were approximated by zero. When the concentration of all active sites C_k became constant up to 10^{-6} , the computing process was stopped.

It turned out that the necessary number of steps in this scheme rapidly grew as the concentration p approached the percolation threshold. This prevents one from finding in this way the values of the limiting concentrations $p(s)$ and $q(s)$ when $p - p_c < 0.02$ (p_c being the threshold concentration).

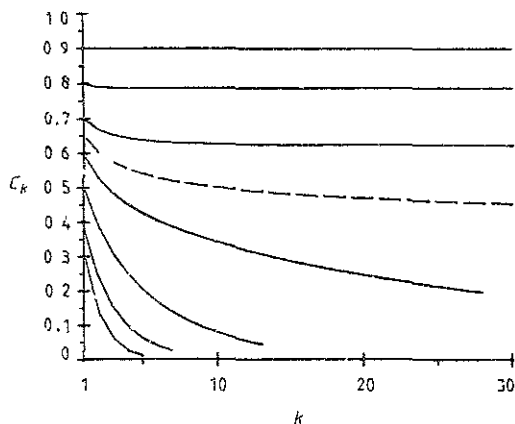


Figure 2. The concentration of active atoms as a function of the number of the layer for some p -values. The broken line shows the theoretical percolation threshold. The concentration $p = C_1$.

The C_k values as functions of the layer number for several concentration p -values are shown in figure 2. It is easily seen that if the difference between the concentration p and the threshold p_c is large enough, then the C_k values reach their limits rather rapidly (in the frame of the approximate model considered, $p_c = 0.65277 \pm 10^{-5}$, as is shown in section 6). However, in the vicinity of threshold it is rather difficult to find these limiting values because of the growing role of the passive groups with large lengths and the slowed down rate of approaching to the corresponding limits.

5. The limiting concentration values

It is possible to prove the existence of the limits of $R_k, p_k(s), q_k(s), \pi_k(s), \kappa_k(s)$ ($k \rightarrow \infty$) if the percolation is present. The proof is based on the relations (5) and (10). Thus, far enough from the crystal boundary the statistical characteristics of the layers cease to change. It is of interest to calculate the limiting values of these characteristics. However, the evaluation of the limiting concentration values by means of the step-by-step procedure takes too much computer time and becomes practically impossible when the concentration p approaches its threshold value. It is more convenient to make use of the obvious property of the limiting concentrations to be a fixed point under the transformations (5) and (10).

Let us denote the limit of each quantity with an index k by the same symbol but without the index. Then the fundamental relations (5) and (10) yield

$$D[z]\kappa[z]^2 + E[z]\kappa[z] + F[z] = 0 \tag{13}$$

$$\pi[z] = pq^2 \left(\frac{z\pi[1]}{1-pz} + \frac{z^2p}{(1-pz)^2} (1 - \kappa[pz]) \right) \tag{14}$$

where

$$D[z] = \pi[qz]$$

$$E[z] = A_1^2[z] - 1 + A_3[z]\pi[qz]$$

$$F[z] = A_4[z] + A_2^2[z]\pi[qz].$$

From (1i) we get

$$\begin{aligned}\kappa[0] &= \pi[0] = 0 \\ \kappa[1] &= \pi[1] = 1 \\ R(\pi'[1] + \kappa'[1]) &= 1.\end{aligned}\tag{15}$$

In relations (13) and (14) there are three unknown parameters: $\pi'[1]$, $\kappa'[p]$ and $\kappa[p]$. However, there exist two relations between these parameters:

$$\begin{aligned}\pi'[1] &= 1 + 1/p + p\kappa[p]/q \\ \kappa'[p] &= (1+p)(1-\kappa[p])/(p^2q) - 1/p^4.\end{aligned}\tag{16}$$

To obtain the first relation, it is sufficient to put $z=1$ in (14). To derive the second relation, one should differentiate expression (14), put $z=1$ and use the first relation of (16).

Thus, the above-mentioned three parameters depend only on one independent parameter, e.g. $\kappa[p]$. The other two parameters may be easily expressed in terms of $\kappa[p]$.

Relations (13) and (14) permit one to express $\pi(s)$ and $\kappa(s)$ ($s=1, 2, \dots$) in terms of $\kappa[p]$ and $\kappa(\sigma)$ ($\sigma=1, 2, \dots, s-1$). Thus, should $\kappa[p]$ be known, it would be possible to find all the values of $\pi(s)$ and $\kappa(s)$. Actually, the evaluation of $\pi(s)$ and $\kappa(s)$ ($s=1, 2, \dots$) can be made in the following way.

The obvious inequality

$$\sum_{\alpha=1}^s \kappa(\alpha) p^\alpha \leq \kappa[p] \leq \sum_{\alpha=1}^s \kappa(\alpha) p^\alpha + p^{s-1} \left(1 - \sum_{\alpha=1}^s \kappa(\alpha) \right)\tag{17}$$

together with the conditions $\pi(s) \geq 0$, $\kappa(s) \geq 0$ ($s=1, 2, \dots$) permits us to check each trial value of $\kappa[p]$ and thus to calculate it to an arbitrary precision. To make the error less than 10^{-5} , it is sufficient to take the parameter s in inequality (17) in the range $20 \leq s \leq 30$ (for different p -values). This being accomplished, it is easy to find the $\pi(s)$ and $\kappa(s)$ values for as many values of s as is necessary.

To find the probabilities $p(s) = R\pi(s)$ and $q(s) = R\kappa(s)$, one needs to know the R -value. This can be found by means of the third relation from set (15). To find $\kappa'[1]$, which is involved in this relation, one may use relation (13)

$$\kappa[z] = \frac{-E[z] \pm (z - \xi_0) \sqrt{\chi[z]}}{2D[z]}\tag{18}$$

where $\chi[z] = (z - \xi_0)^2 \bar{\chi}[z]$, $\chi[z] = E[z]^2 - 4D[z]F[z]$, ξ_0 is the zero of the function $\chi[z]$ of second multiplicity. The sign before the radical is determined by the condition $\kappa[0] = 0$. As $E[0] < 0$, the sign in formula (18) is a plus. After differentiating (18) and putting $z=1$ we get a simple expression for $\kappa'[1]$ in terms of $\kappa[p]$ and $\pi[q]$. For these quantities there exist fast converging series (2).

A less sophisticated way of evaluating $\kappa'[1]$ by using the series

$$\kappa'[1] = \sum_{s=1}^{\infty} \kappa(s) s$$

requires a much greater number of $\kappa(s)$ values to be computed, if good accuracy is necessary.

6. The percolation threshold

For the model considered there exists a rather simple algorithm to evaluate the percolation threshold.

By definition (2), the functions $\pi[z]$ and $\kappa[z]$ are analytical in the circle $|z| \leq 1$, and the coefficients of their Maclaurin series are all positive. Therefore the functions $E[z]$, $\chi[z]$ and $D[z]$ are analytical in the circle $|z| \leq r$ ($r = q^{-1} > 1$). Relation (18) shows that the nearest singular point of the function $\kappa[z]$, say z_0 , is the branch point and is simultaneously the zero of odd multiplicity of the function $\chi[z]$. By Pringsheim's theorem, the point z_0 lies on the positive semiaxis of the complex z -plane.

Let the p -value become less than the critical value. Then either z_0 becomes less than unity, or some of the coefficients $\pi(s)$, $\kappa(s)$ become negative. In the last case we shall say that the positivity condition is violated.

Let us consider the first possibility. If the point $z_0 = 1$ is a simple zero of the function $\chi[z]$, then the derivative $\kappa'[1]$ tends to infinity as the concentration p approaches the critical value. In all other cases, it has a finite limit $\kappa'[1]$. What is the physical meaning of these two cases? From equalities (1), (2) and (3) one may deduce the simple relation

$$C = \frac{\pi'[1]}{\kappa'[1] + \pi'[1]}. \quad (19)$$

According to relation (16), the $\pi'[1]$ value is bounded to all $q \geq \varepsilon$ ($\varepsilon > 0$). Therefore, $\kappa'[1] \rightarrow \infty$ means that $C \rightarrow 0$, i.e. the concentration of active sites tends to zero when the parameter p tends to the percolation threshold. If the point $z_0 = 1$ is a non-simple zero of odd multiplicity of the function $\chi[z]$, then the concentration C tends to the positive limit. In the first case, the transition from a percolation regime to a non-percolation one is the second-order phase transition, and in the second case it is of the first order.

In the model considered, the point $z = 1$ is a zero of the function $\chi[z]$ for all values of p . The multiplicity of this zero is no less than two. This excludes the first case, and thus excludes the possibility of the second-order phase transition.

The threshold values of the concentration p may be calculated from the condition that the multiplicity of the point $z = 1$ as zero of the function $\chi[z]$ is no less than three, i.e. from the condition $\chi''[1] = 0$. The algorithm of the previous section permits us to calculate the $\kappa[p]$ values for different values of p and thus to represent $\chi''[1]$ as a function of the parameter p only. The zero of this function lies in the interval $p_c = 0.65277 \pm 10^{-5}$, the uncertainty $\delta p = 10^{-5}$ is due to the uncertainty of the parameter $\kappa[p]$.

The zero of $\chi''[1]$ is the percolation threshold if the positivity condition is fulfilled. This condition has been verified in the process of determining the value of $\kappa[p]$. The violation of the positivity condition pointed to inaccuracy of the trial value of $\kappa[p]$. With each such step the number of positive coefficients $\pi(s)$ and $\kappa(s)$ grew, and it seems that this number can be made as large as one wishes, if the choice of the $\kappa[p]$ value is good enough. This shows that the positivity condition is weaker than the condition $\chi''[1] = 0$. Thus the threshold value is determined by the condition $\chi''[1] = 0$.

7. Conclusion

The method of solving the directed percolation problem presented in this paper shows good agreement with Monte Carlo calculations, except for a small region near the percolation threshold. No essential difficulties seem to appear in applying the method to other directed percolation problems in plane crystals.

This paper contains an algorithm for step-by-step calculation of the concentrations $p_k(s)$ and $q_k(s)$ in each layer. There are also algorithms for evaluation of the limiting concentrations $p(s)$ and $q(s)$, and also of the percolation threshold

It is shown that in the frame of the approximate model considered the transition through the percolation threshold is a phase transition of the first order. However, we cannot be sure that this is the property of the real plane crystal and not a mere consequence of the approximation we have made to construct the model considered. The comparison with the data obtained by the Monte Carlo method shows (figure 1) that if in real crystals the discontinuity of concentrations does exist, it is smaller than that obtained above

It may be noted that a more complicated case, where correlation exists in the positions of open and closed sites, can be investigated along the same lines if the sites in question are neighbours and belong to the same layer.

Acknowledgment

The authors thank Professor A S Bakaj for attracting their attention to percolation problems.

Appendix

Here we give our method of reasoning that has led to relations (5) and (10).

Let us take a random set M of s sites in the $(k+1)$ th layer and calculate the probability of its being a passive group.

We denote the two extreme sites of M by \bar{A}_- and \bar{A}_+ (\bar{A}_- being the left site). The two sites in the k th layer lying immediately under \bar{A}_- and \bar{A}_+ are designated as sites A_- and A_+ . We denote the left neighbour of the site A_- by B_- , and the right neighbour of A_+ by B_+ . Let M_- be a group (active or passive) containing the site B_- , and M_+ a group containing the site B_+ . Taking into account that the groups M_- and M_+ may be active or passive and may or may not be identical, we get six different cases. For our purpose, it is sufficient to treat only one of these cases. We choose the case where the group M_- is active and the group M_+ is passive. Let m be the number of groups lying between M_- and M_+ , and l_1, l_2, \dots, l_m be the lengths of these groups. In the case considered, the possible values of m are even non-negative numbers (including zero).

Let α_- (β_-) be the number of the sites belonging to the set M and lying to the left (right) of the site B_- , let α_+ (β_+) be the number of the sites of the set M_+ lying to the right (left) of the site B_+ . The set of numbers

$$\{\alpha_-, \beta_-, \alpha_+, \beta_+, m, l_1, l_2, \dots, l_m\} \quad (\text{A1})$$

gives a complete description of the relevant part of the k th layer. The probability to

meet just the configuration (A1) in the k th layer is equal to

$$R_k \pi_k(\alpha_- + 1 + \beta_-) \varkappa_k(l_1) \pi_k(l_2) \dots \pi_k(l_m) \varkappa_k(\beta_+ + 1 + \alpha_+).$$

The set M is a passive group if and only if the following five conditions are fulfilled:

(i) All sites of M lying above active groups are closed. The probability of this event is equal to $q^{\beta_- + l_2 + \dots + l_m}$.

(ii) The left neighbour of the site \bar{A}_- belongs to an active group. The probability of this event is p .

(iii) The right neighbour of the site \bar{A}_+ belongs to an active group. The respective probability is equal to $p^{\alpha_+ + 2}$.

(iv) The site \bar{A}_- must be closed. The probability of this event is equal to

$$w_- = \begin{cases} 1 & \text{if } \beta_- > 0 \\ q & \text{if } \beta_- = 0 \end{cases}$$

provided the first condition is fulfilled.

(v) The site \bar{A}_+ must be closed. The corresponding probability is equal to

$$w_+ = \begin{cases} 1 & \text{if } \beta_+ = 0, \text{ or } s = 1 \\ q & \text{if } \beta_+ > 0 \end{cases}$$

provided conditions (i) and (iv) are fulfilled.

Using Kronecker's symbol

$$\delta_{nm} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$$

we may represent the probabilities w_- and w_+ in the form

$$w_- = 1 - p\delta_{0\beta_-}$$

$$w_+ = 1 - p(1 - \delta_{0\beta_+})(1 - \delta_{1s}) = 1 - p(1 - \delta_{0\beta_+}) + p\delta_{1s}(1 - \delta_{0\beta_+})$$

Now we can write down the contribution $w(s)$ of all configurations of the considered type to the probability $q_{k+1}(s)$:

$$w(s) = \sum_{\alpha_-, \alpha_+ = 0}^{\infty} \sum_{\substack{m, \beta_-, \beta_+, \\ l_1, l_2, \dots, l_m}} R_k \pi_k(\alpha_- + 1 + \beta_-) \varkappa_k(l_1) \pi_k(l_2) \dots \pi_k(l_m) \varkappa_k(\beta_+ + 1 + \alpha_+) \times q^{\beta_- + l_2 + \dots + l_m} p^{\alpha_+ + 2} (1 - p\delta_{0\beta_-}) [1 - p(1 - \delta_{0\beta_+})(1 - \delta_{1s})] \quad (A2)$$

(the inner sum is extended to the region: $m = 0, 2, 4, \dots$; $\beta_-, \beta_+ = 0, 1, \dots$; $l_1, l_2, \dots, l_m = 1, 2, \dots$; $\beta_- + \beta_+ + l_1 + l_2 + \dots + l_m = s$).

Now the calculation of the generating function $w[z] \equiv \sum_{s=1}^{\infty} z^s w(s)$ is a rather straightforward operation because of the evident sum rule

$$\sum_{s=0}^{\infty} \sum_{\beta_-, \beta_+, l_1, \dots, l_m} = \sum_{\beta_-, \beta_+ = 0}^{\infty} \sum_{m=0}^{\infty} \sum_{l_1, \dots, l_m=1}^{\infty}$$

(m is even). To use this rule, we extend formally the relation (A2) to the value $s = 0$,

$$w(0) = R_k q \sum_{\alpha_- = 0}^{\infty} \pi_k(\alpha_- + 1) \sum_{\alpha_+ = 0}^{\infty} \varkappa_k(\alpha_+ + 1) p^{\alpha_+ + 2} = R_k p^2 q \varkappa_k[p]$$

and write

$$w[z] = \sum_{s=1}^{\infty} z^s w(s) = -w(0) + \sum_{s=0}^{\infty} z^s w(s)$$

or

$$\begin{aligned}
 w[z] = & -w(0) + R_k p^4 z \sum_{\alpha_-, \alpha_+ = 0}^{\infty} p^{\alpha_+} \sum_{\beta_- + \beta_+ = 1} \pi_k(\alpha_- + 1 + \beta_-) \varkappa_k(\beta_+ + 1 + \alpha_+) q^{\beta_-} \\
 & \times (1 - p\delta_{0\beta_-})(1 - \delta_{0\beta_+}) + R_k p^3 \\
 & \times \left(\sum_{\alpha_-, \beta_- = 0}^{\infty} \pi_k(\alpha_- + 1 + \beta_-) (qz)^{\beta_-} (1 - p\delta_{0\beta_-}) \right) \\
 & \times \left(\sum_{\alpha_+, \beta_+ = 0}^{\infty} p^{\alpha_+} \varkappa_k(\beta_+ + 1 + \alpha_+) z^{\beta_+} (q + p\delta_{0\beta_+}) \right) \\
 & \times \sum_{m=0,2,4,}^{\infty} \left(\sum_{l_1, l_3, \dots, l_{m-1}=1}^{\infty} z^{l_1 + l_3 + \dots + l_{m-1}} \varkappa_k(l_1) \varkappa_k(l_3) \dots \varkappa_k(l_{m-1}) \right) \\
 & \times \left(\sum_{l_2, l_4, \dots, l_m=1}^{\infty} (zq)^{l_2 + l_4 + \dots + l_m} \pi_k(l_2) \pi_k(l_4) \dots \pi_k(l_m) \right)
 \end{aligned}$$

The sum over l_2, \dots, l_m is equal to $\{\pi_k[qz]\}^{m/2}$, the sum over l_1, \dots, l_{m-1} is equal to $\{\varkappa_k[z]\}^{m/2}$. After summing over m we get

$$\frac{1}{1 - \varkappa_k[z] \pi_k[qz]}$$

The remaining three sums are readily found:

$$\begin{aligned}
 & \sum_{\alpha_-, \alpha_+ = 0}^{\infty} p^{\alpha_+} \sum_{\beta_- + \beta_+ = 1} \pi_k(\alpha_- + 1 + \beta_-) \varkappa_k(\beta_+ + 1 + \alpha_+) q^{\beta_-} (1 - p\delta_{0\beta_-})(1 - \delta_{0\beta_+}) \\
 & = q \sum_{\alpha_-, \alpha_+ = 0}^{\infty} p^{\alpha_+} \pi_k(\alpha_- + 1) \varkappa_k(\alpha_+ + 2) = q(\varkappa_k[p] - \varkappa_k(1)p) / p^2
 \end{aligned}$$

$$\begin{aligned}
 & \sum_{\alpha_-, \beta_- = 0}^{\infty} \pi_k(\alpha_- + 1 + \beta_-) (qz)^{\beta_-} (1 - p\delta_{0\beta_-}) \\
 & = \sum_{\alpha_-, \beta_- = 0}^{\infty} \pi_k(\alpha_- + 1 + \beta_-) (qz)^{\beta_-} - p \sum_{\alpha_- = 0}^{\infty} \pi_k(\alpha_- + 1) \\
 & = \sum_{\gamma=1}^{\infty} \pi_k(\gamma) \sum_{\beta=0}^{\gamma-1} (qz)^{\beta} - p = \sum_{\gamma=1}^{\infty} \pi_k(\gamma) \frac{1 - (qz)^{\gamma}}{1 - qz} - p = \frac{1 - \pi_k[qz]}{1 - qz} - p
 \end{aligned}$$

and similarly

$$\sum_{\alpha_+, \beta_+ = 0}^{\infty} p^{\alpha_+} \varkappa_k(\beta_+ + 1 + \alpha_+) z^{\beta_+} (q + p\delta_{0\beta_+}) = q \frac{\varkappa_k[z] - \varkappa_k[p]}{z - p} + \varkappa_k[p].$$

Thus, for the contribution $w[z]$ we get the following expression.

$$\begin{aligned}
 w[z] = & R_k p^2 \left[-q\varkappa_k[p] + qz(\varkappa_k[p] - p\varkappa_k(1)) + p \left(\frac{1 - \pi_k[qz]}{1 - qz} - p \right) \right. \\
 & \left. \times \left(q \frac{\varkappa_k[z] - \varkappa_k[p]}{z - p} + \varkappa_k[p] \right) \frac{1}{1 - \varkappa_k[z] \pi_k[qz]} \right].
 \end{aligned}$$

In the same way one can consider each of the remaining five cases and thus get relation (5).

The derivation of the second fundamental relation (10) does not take much time. Indeed, the necessary and sufficient set of conditions for the set M in the $(k+1)$ th layer to be active is the following:

(i) All sites, belonging to \bar{M} , are open and border on two closed sites. The probability of this event is $p^3 q^2$.

(ii) In the k th layer there is no passive group containing all sites lying under the set M . The probability of this event is

$$1 - R_k \sum_{\alpha_-, \alpha_+ = 0}^{\infty} \kappa_k(\alpha_- + \alpha_+ + s)$$

Thus

$$p_{k+1}(s) = q^2 p^3 \left(1 - R_k \sum_{\alpha_-, \alpha_+ = 0}^{\infty} \kappa_k(\alpha_- + \alpha_+ + s) \right).$$

This relation readily leads to the second fundamental equation.

References

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