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On random walks in percolation models

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Abstract. Random walks on percolation clusters of any dimension consisting of both directed and undirected bonds are studied. Results conjectured to be exact and supported by Monte Carlo simulation are deduced for the critical parameters of the problem. It is shown that in the undirected case of the model the probabilities of finding the particle in the sites of a finite cluster have a uniform limit distribution.

1. Introduction

The study of random walks on lattices with a certain distribution of transfer rates between pairs of neighbouring sites has recently arisen as an approach to the problem of classical diffusion in disordered systems (Odagaki and Lax 1981, Webman 1981). In the special case when the transfer rate is zero on a fraction $(1-p)$ of the bonds, the model describes random walks on percolation clusters. This problem was introduced and called 'the ant in the labyrinth' by de Gennes (1976). The main quantity describing the process is the mean squared displacement $\langle R^2(t)\rangle$ as a function of time which was obtained for site (Mitescu *et al* 1978) and bond (Vicsek 1981) percolation problems by Monte Carlo methods and in a closed form for the Bethe lattice (Straley 1980).

Introducing directed bonds into percolation models has currently attracted much interest. Directed percolation was shown to be in a universality class different from the pure percolation (Blease 1977, Kertész and Vicsek 1980, Obukhov 1980) and to have relevance to various physical problems (Grassberger and de la Torre 1979, Cardy and Sugar 1980, Van Lien and Shklovskii 1981). Transport properties such as conductivity (Redner 1982, Harms and Straley 1982) and wetting velocity (Dhar 1982) in random networks consisting of resistor and diode-like elements have also been studied. Besides the above-mentioned important features, directed percolation is of interest because in some special cases it allows analytic treatment. A square lattice directed model with all horizontal bonds occupied was exactly solved by Domany and Kinzel (1981), while Wu and Stanley (1982), treating this kind of model as a random walk problem, obtained an exact solution for an analogously occupied triangular lattice. In addition, an asymptotically exact expression was given by Vicsek *et al* (1982) for the mean distance of random walks on directed clusters of any dimension.

In this paper we study random walks on d-dimensional hypercubic lattices occupied by three types of bonds, allowing transitions (i) in both directions, (ii) only in the positive direction and (iii) only in the negative direction. The corresponding occupation probabilities are p, p_+ and p_-, respectively, while the fraction of the empty (not transmitting) bonds is obviously $p_0 = 1 - p - p_+ - p_-$. Positive directions are defined by the basic vectors $\{e_i\}$ of the Cartesian coordinates associated with the hypercubic lattice. The walk is defined as follows: the particle tries to proceed in a randomly selected direction in each unit of time. Its position is changed if the corresponding transition to a nearest-neighbour site is allowed (the given bond is occupied and has no opposite directionality); in the other case the particle stays in the original site for a further unit time.

A problem similar to this was investigated by Stephen (1981) in the effective medium approximation. Our approach is quite different: we start from a qualitative analysis of the process and obtain results conjectured to be exact. These results are checked by Monte Carlo simulation of random walks on the square lattice. Finally, we investigate the $p_- = p_+ = 0$ case using a limit distribution theorem of Markov chains (see e.g. Rényi 1970).

2. Critical parameters for R^2_∞

In this section the long-time limit of the mean square displacement $\lim_{t\to\infty} \langle R^2(t)\rangle = R^2_\infty$ is investigated as a function of the occupation probabilities p, p_+ and p_-.

Contrary to intuitive expectations, transport ($R^2_\infty \to \infty$) in this model is possible only for rather special choices of these parameters. This behaviour can descriptively be interpreted by investigating the sites from the point of view of whether the particle can proceed from them or not. Obviously, if a site is connected only to occupied bonds directed towards it, the particle once arrived stays in this site forever. Several such combinations of directed bonds can be realised, e.g. on the square lattice the number of configurations consisting of three bonds directed into a site is equal to 4.

In general, the fraction of sites on a d-dimensional simple cubic lattice in which the particle may be blocked is

$$p_t = \sum_{i=1}^{d} \sum_{j=1}^{d} \binom{d}{i}\binom{d}{j} p_+^i p_-^j p_0^{2d-i-j} + \sum_{i=1}^{d} \binom{d}{i} (p_+^i + p_-^i) p_0^{2d-i} \tag{1}$$

where the index t stands for the word trap, denoting the property that a particle can never leave such sites. In (1) we considered that there are $\binom{d}{i}\binom{d}{j}$ configurations consisting of i positively and j negatively directed bonds leading into a site from the $2d$ possible directions, where $\binom{k}{m} = k!/m!(k-m)!$. Besides these traps a cluster of bonds surrounded by bonds all directed into the perimeter sites of this cluster represents a trap of more general kind and is described by higher-order terms appearing in the model.

Next we make use of the assumption that a finite fraction of traps results in a finite expectation of the time to being blocked, hence on the average the particle does not move away arbitrarily far from the origin. This assumption is a consequence of our expectation that—like in analogous models with traps—the probability of a t-step walk decreases exponentially with increasing t. Correspondingly, we arrive at the following conjecture for the exact critical parameters of the problem. There is a very narrow region of the parameter values in which transport is possible: the mean square displacement diverges only if one of the two pairs of relationships

$$\text{(i)} \qquad p \geq p_c \quad \text{and} \quad p_+ = p_- = 0 \tag{2a}$$

or

$$\text{(ii)} \qquad p_0 = 1 - p - p_+ - p_- = 0 \quad \text{and} \quad p_+ p_- = 0 \tag{2b}$$

is obeyed, since from (1) it follows that p_t equals zero only in these two cases, with p_c being the percolation threshold of the isotropic problem. Therefore, adding directed bonds to an already percolating network of undirected bonds stops the transport due to the traps necessarily appearing in the system.

In figure 1, we marked with bold lines those values of the parameters p, p_+ and p_- for which (2*a*) or (2*b*) is valid. Lines $\overline{\mathrm{A}p_c}$, $\overline{\mathrm{AB}}$ and $\overline{\mathrm{AC}}$ are critical in the sense that R_∞^2 diverges with a certain exponent when these parameter values are approached. These critical lines are supposed to be exact, since the only assumption we used in obtaining them was that a finite probability of being trapped leads to a finite mean squared length of the walks. Montroll (1969) showed that at least this is so ($R_\infty^2 < \infty$) in a lattice with $p = 1$ and regularly distributed traps, but we are not aware of any exact proof concerning our particular model. Therefore, we carried out a Monte Carlo simulation of the problem on the square lattice. (Details of the method are described in Vicsek 1981.) It was found that the particle is indeed blocked sooner or later if (2*a*) or (2*b*) is not obeyed.

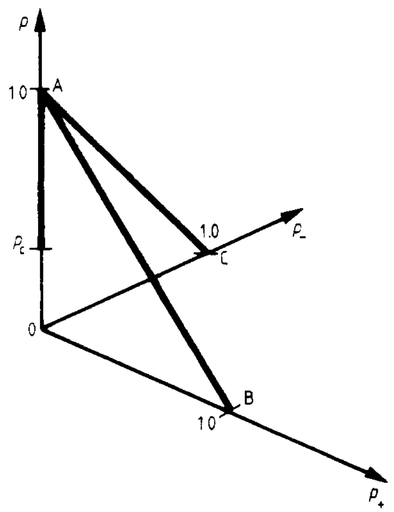

Figure 1. Critical values of the parameters p, p_+ and p_-. The long-time limit of the mean squared displacement becomes singular when the $\overline{\mathrm{A}p_c}$, $\overline{\mathrm{AB}}$ and $\overline{\mathrm{AC}}$ intervals are approached.

In one of our Monte Carlo calculations we approached the $\overline{\mathrm{AB}}$ critical line along the $p = p_+$, $p_- = 0$ line. Dependence of R_∞^2 on the quantity $\Delta p = 1 - p - p_+$ in this case is shown in figure 2. Defining a critical exponent u through $R_\infty^2 \sim (\Delta p)^{-u}$, we get from the slope of this log–log plot $u = 4.3 \pm 0.5$, in good agreement with the value $u = 4$ obtained for the fully directed model (Vicsek *et al* 1982). This fact seems to support the assumption that the directionality is a relevant parameter: introducing directed bonds into an undirected model, we recover the same critical exponent as in the fully directed case. The result $u = 4$ is expected on the basis of (1) as well, since when $(p + p_+) \to 1$ the number of traps decreases quadratically, while R_∞^2 for the directed

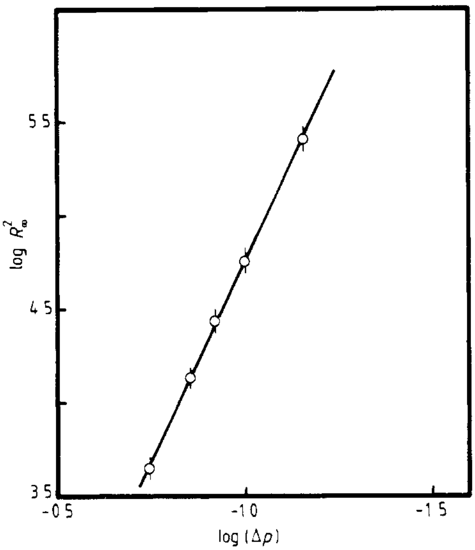

Figure 2. Dependence of the $\lim_{t\to\infty} \langle R^2(t)\rangle = R^2_\infty$ values on $\Delta p = 1 - p - p_+$ for $p_- = 0$. From the slope of this log–log plot we obtain the exponent $u = 4.3 \pm 0.5$.

walks is proportional to the square of the inverse of the trapping probability. In general, $u = 2d$ since the leading term in (1) describing the trap concentration is p_0^d.

The lines of singular behaviour shown in figure 1 are qualitatively different from those obtained by Stephen (1981) from an effective medium approximation (EMA). According to his results, the transport is possible in a relatively wide, three-dimensional region of parameters p, p_+ and p_-. Hence EMA turns out to be an unexpectedly inaccurate approximation for the description of directed walks.

3. Limit distribution for walks on finite undirected clusters

The $p < p_c$, $p_+ = p_- = 0$ limit (undirected walks below the percolation threshold) has further interesting problems to be clarified. In particular, one may put the question: what is the probability q_j of finding the particle in the jth site of a finite cluster after a long time? This problem first arose in Monte Carlo simulations, where results turned out to depend on the definition of the walk (Roussenq 1980, Vicsek 1981).

The random walk defined in the introduction corresponds to an N-state Markov chain (N is the number of sites in the cluster) characterised by the transition matrix $P = \{p_{ij}\}$, where p_{ij} is the probability of the transition from the state i into state j. Obviously, P is symmetrical ($p_{ij} = p_{ji}$) in the $p_+ = p_- = 0$ case and $p_{ij} = 1/z$ if the corresponding bond is occupied, while p_{ii} may take the values $0, 1/z, \ldots, (z-1)/z$, 1, z being the coordination number.

Introducing $p_{ij}^{(n)}$, the n-step transition probability between sites i and j, we can use a limit distribution theorem of Markov (Rényi 1970, Markov 1912). According to this theorem the limit values

$$\lim_{n\to\infty} p_{ij}^{(n)} = q_j \tag{3}$$

exist if there are integers $k > 0$ and $j_0 > 0$ such that the inequalities

$$p_{ij_0}^{(k)} > 0 \qquad (i = 1, 2, \ldots, N) \tag{4}$$

hold. Besides, $\{q_j\}$ is the only solution of the system of equations

$$q_j = \sum_{i=1}^{N} p_{ij} q_i \tag{5}$$

satisfying the condition $\Sigma_{i=1}^{N} q_i = 1$. $\{q_j\}$ is called the limit distribution of the Markov process and q_j is equal to the probability of being in the state j when $t \to \infty$.

Condition (4) is always satisfied if random walks on a finite undirected percolation cluster are considered: from any sites of this cluster all the others can be reached in less than N steps, therefore, the transition probability corresponding to such walks is greater than zero. However, in order to avoid some undesired oscillating effects it is also required that for a given j_0 (4) must hold with the same k for all i. The fulfilment of this condition is provided by the fact that in a finite cluster there must always be at least one site for which $p_{ii} > 0$.

Finally, we make use of the fact that P is symmetrical, therefore, as a consequence of the trivial $\Sigma_{j=1}^{N} p_{ij} = 1$, the relationship

$$\sum_{i=1}^{N} p_{ij} = 1 \tag{6}$$

is valid as well. Let us substitute $\{q_j\} = 1/N$ into the system of equations (5). Because of (6) we obtain an identity and taking into account that (5) has only one solution this is the true distribution we were looking for. Of course, random walk definitions leading to a transition matrix contradicting (6) (e.g. Mitescu *et al* 1978) result in a non-uniform distribution of the q_j values.

4. Conclusions

The problem of random walks on percolation clusters made of directed and undirected bonds has been shown to have similarities with the so-called trap models. The critical parameters of the process have been determined from the condition that the fraction of sites where the particle may be blocked should be equal to zero. These results are in agreement with the Monte Carlo simulations and conjectured to be exact. Finally, it was shown using a theorem on Markov chains that for a properly defined random walk the probabilities of finding the particle in the sites of a finite undirected cluster are distributed uniformly in the $t \to \infty$ limit.

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