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EMPTINESS PROBABILITIES IN RANDOM SEQUENTIAL ADSORPTION ON THE BETHE LATTICE

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When gas molecules bind to a surface they may do so in such a way that the adsorption of one molecule inhibits the arrival of others. Two models which have frequently been studied are the "dimer model" and the "blocking model", and rather complete solutions for these are known on the Bethe lattice. In this note the probability that a connected set of sites remains unoccupied is calculated.

Keywords: Interacting particle systems; random sequential adsorption; Bethe lattice.

1. Introduction

The infinite Bethe lattice of coordination number $z = 2, 3, ...$ has each site connected to z nearest neighbor sites with no closed loops of bonds. It is equivalent to the tree T_{z-1}. A k-site cluster is a set of k connected sites. Cadilhe and Privman [?] consider the case in which particles arrive as dimers and give a formula for the probability that a randomly-chosen k-cluster is empty at time t. It is the purpose of this note to show that their result is true for all clusters, to explain why their formula takes the form it does and to calculate the same probability for the blocking model. There is an extensive survey of random sequential adsorption in Evans [?] and a more mathematical account in Penrose and Sudbury [?].

2. The dimer model

Initially all sites of the lattice are empty. At each site there is a random time at which a monomer attempts to occupy the site. If the site is occupied the attempt fails. For each pair of neighboring sites there is a random time at which a dimer attempts to occupy the two sites. If either of them is occupied then the attempt fails. All these random times are identically distributed and independent for each site and each pair

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(even if they have a site in common). Because only the order of arrival is important, there is no problem in taking the random time to have any distribution, although it is most usual to take it as exponential (Penrose and Sudbury [?]take it to be uniform on $(0, 1)$ to simplify their formulae). In their equation (6) Cadilhe and Privman [?] give a recurrence differential equation for $\{P_k(t)\}, k = 1, ..., \infty$, the probabilities that randomly-chosen k-clusters are empty at time t. They then assume an *ansatz* to derive a formula for $P_k(t)$. They do not define a randomly-chosen k-cluster but one assumes, perhaps, that is some kind of average over clusters of different shapes. On a finite lattice it would not be at all obvious how to choose such a cluster and results would depend on the method of selection. Majumdar and Privman [?] give an informal argument as to why the emptiness probabilities should be independent of the shape of the cluster after their equation (2). In this note a more formal treatment of this will be given which will also explain why their *ansatz* works.

If C_k is a k-cluster, define the boundary ∂C_k to be the set of sites which are not in C_k but which have a neighbor in C_k. If the set A is unoccupied at time t, then we write $I_t(A) = 0$. Suppose $y \in \partial C_k$ and x is its neighbor in C_k, then it might seem obvious that, since y is not connected to any site in C_k except through x, any events that affect C_k only affect y by their effect on x, and thus that $P(I_t(y) = 0 | I_t(C_k) = 0) = P(I_t(y) = 0 | I_t(x) = 0)$. This is in fact true, but the argument is not, as the same is not true for the "blocking process".

We shall assume that dimers arrive at constant rate α and monomers at rate $1 - \alpha$. Following Cadilhe and Privman [?] we shall further assume that each site is blocked at time $t = 0$ independently with probability ρ. The treatment will follow Penrose and Sudbury [?], although in that paper $\alpha = 1$ and $\rho = 0$. We shall consider the process on the tree T_k which is equivalent to the Bethe lattice with coordinate number $k + 1$. The rooted tree R_k has a root with k neighbors, but all other sites having $k + 1$ neighbors (it can be obtained from T_k by cutting one bond or edge). We first consider the situation for a site 0 with one neighbor which is the root of R_k. Define

$$\beta(t) = \text{P(no dimer has made a successful arrival at 0 by time t}|\text{no monomer has arrived)}.$$

This implies

$$\text{P(0 is empty at time t)} = e^{-(1-\alpha)t}\beta(1-\rho).$$

There are two ways in which this probability might change in the interval $(t, t+dt)$. First, a monomer attempts to arrive for the first time, and there has been no successful arrival of a dimer up to that time. Secondly, that a dimer attempts to arrive at 0 and that 0 and its neighbor 1 are both empty. Because 1 is attached to k further sites this requires that all k possible dimer arrivals on 1 and its neighbors have been unsuccessful. Given no monomer has arrived at 1 these events are independent. We thus have

$$[e^{-(1-\alpha)t}\beta(1-\rho)]' = -(1-\rho)\beta(1-\alpha)e^{-(1-\alpha)t} - \alpha e^{-\alpha t}[(1-\rho)e^{-(1-\alpha)t}]^2\beta^k,$$

which reduces to

$$\beta' = -\alpha(1-\rho)e^{-t}\beta^k,$$

giving

Lemma 1.

$$\beta = [1+\alpha(k-1)(1-\rho)(1-e^{-t}]^{-1/(k-1)}.$$

We now revert to T_k. In this case for a site to be empty requires that none of the $k+1$ possible dimers with its neighbors have made successful arrivals.

Theorem 1. *In the dimer process on* T_k

$$P(\text{a site is empty at time } t) = e^{-(1-\alpha)t}[1+\alpha(k-1)(1-\rho)(1-e^{-t}]^{-(k+1)/(k-1)}$$

We now consider the emptiness probabilities on clusters by building them up one site at a time. Assume that y is a neighbor of a cluster C. Put $C^+ = C \cup y$. Now break the bond between y and its neighbor in C which we call x. This breaks the graph T_k into two subgraphs T_y and T_x neither of which contains the bond(edge) between x and y. The probability that y remains unoccupied at t when the process is confined to T_y is equal to $(1-\rho)\beta^k e^{-(1-\alpha)t}$. We then have

$$P(I_t(C^+)=0) = (1-\rho)\beta^k e^{-(1-\alpha)t}e^{-\alpha t}P(I_t(C_x)=0),$$

where it is understood that the last probability is for the process on T_x, and that C_x has the same sites as C. We also have that

$$P(I_t(C)=0) = P((I_t(C_x)=0)\beta,$$

since the only difference between the processes comes from the possibility of a dimer arrival between x and y. Combining the last two equations gives

Lemma 2.

$$P(I_t(C^+)=0|I_t(C)=0) = (1-\rho)e^{-t}\beta^{k-1} = (1-\rho)e^{-t}[1+\alpha(k-1)(1-\rho)(1-e^{-t})].$$

The conditional probability above is independent of the size and shape of C. Thus if C has r sites $P(I_t(C)=0) = P(I_t(x)=0)P(I_t(y)=0|I_t(x)=0)^{r-1}$ where y and x are any two neighbors. This result makes clear why the *ansatz* of Cadilhe and Privman [?] works. Combining Theorem 2 and Lemma 3 with this remark gives their equation (11).

Theorem 2. *In a dimer process, if* C *has* r *sites then*

$$P(I_t(C)=0) = (1-\rho)^r e^{(\alpha-r)t}[1+\alpha(k-1)(1-\rho)(1-e^{-t})]^{-(r+2/(k-1))}.$$

Note that Cadilhe and Privman(2004) have $z-2$ for $k-1$ and k instead of r.

3. The annihilating process

Annihilating processes on the tree T_k have been considered in Penrose and Sudbury [?]. We shall refer to the paper as PS. The model can represent the thinning of plants. Initially all sites are occupied. Between each pair of sites occurs a single annihilating event at a random time independently of all other pairs of sites. When such an event occurs one of the two sites (chosen at random) is annihilated (becomes unoccupied). In any finite region the process stops when all sites are either unoccupied or occupied with no occupied neighbors. In this section we follow PS by having the events occurring uniformly on $(0, t)$.

Connections between this process and the dimer process have been noted and the analysis here will follow that of the previous section very closely. Note that the equivalent dimer process has $\alpha = 1, \rho = 0$. We consider a site connected to a single site which is the root of R_k. We define β=P(the site is occupied at time t). Then arguing as before we have

$$\beta' = -\frac{1}{2}\beta^k \Rrightarrow \beta = [1 + (k-1)t/2]^{-1/(k-1)}.$$

We split a cluster C^+ as before and obtain

$$P(I_t(C^+) = 1) = \beta^k(1-t)P((I_t(C_x) = 1), P(I_t(C) = 1) = P((I_t(C_x) = 1)\beta,$$

which implies

$$P(I_t(C^+) = 1|I_t(C) = 1) = (1-t)\beta^{k-1} = \frac{1-t}{1 + (k-1)t/2}.$$

We then have

Theorem 3. *In an annihilating process on the tree T_k, if C has r sites, then*

$$P(I_t(C) = 1) = (1-t)^{r-1}(1 + (k-1)t/2)^{-(r+2/(k-1))}.$$

Note: in this theorem the events occur on $(0, t)$.

4. The blocking process

Blocking processes on the tree T_k have been considered in Penrose and Sudbury [?]. Initially all sites of a graph are unoccupied. At each site there is a random time at which a particle attempts to occupy the site. These times are independent and uniform on $(0, 1)$. The arrival is successful if and only if all neighboring sites are unoccupied. Suppose 0 is the root of the rooted tree T_k^* so that 0 has k neighbors but all other sites have $k+1$ neighbors. Define

$$\beta(t) = P(0 \text{ is unoccupied at time t}).$$

Clearly $\beta(0) = 1$.

PS argues that for x to become occupied in the interval $(t, t + dt)$ requires a particle to arrive in the interval, and for all the neighboring sites to be unoccupied. Since x has been unoccupied up to that time, the neighboring sites can be considered as the roots of independent rooted trees giving

$$\beta' = -\beta(t)^k \Rrightarrow \beta(t) = [1 + (k - 1)t]^{-1/(k-1)}. \tag{12}$$

Note that if we had taken the random times to be exponential then $1 - e^{-t}$ should be substituted for t.

Suppose we have two neighboring sites x, y on T_k, then we may cut the bond (edge) between them to form two disjoint graphs which we shall call $T_k(x/y)$ and $T_k(y/x)$ where $x \in T_k(x/y), y \in T_k(y/x)$ and, except for the missing edge $T_k = T_k(x/y) \bigcup T_k(y/x)$. If $x, y \in C_r$ then this cut similarly splits C_r so that $C_r = C_r(x/y) \bigcup C_r(y/x)$. Define $I_t(C_r(x/y)) = 0$ to be the event that $C_r(x/y)$ is unoccupied at time t when the blocking process is confined to $T_k(x/y)$. We show

Lemma 3.

$$P(I_t(C_r) = 0) = P(I_t(C_r(x/y)) = 0)P(I_t(C_r(y/x)) = 0),$$

where the l.h.s. is for the process on T_k.

Proof. With the blocking process on T_k, if the status of C_r changes in the interval $t, t+dt$ then either it changes at a site of $C_r(x/y)$ or of $C_r(y/x)$ with the probability of both events being $o(dt)$. If at a site of $C_r(x/y)$ then it requires that $I_t(C_r(y/x)) = 0$, in which case $C_r(x/y)$ cannot have been blocked by a site of $C_r(y/x)$ and its evolution on T_k can be coupled to its evolution on $T_k(x/y)$. Thus

$$\frac{d}{dt}P(I_t(C_r) = 0) = \frac{d}{dt}P(I_t(C_r(x/y)) = 0)P(I_t(C_r(y/x)) = 0)$$
$$+P(I_t(C_r(x/y)) = 0)\frac{d}{dt}P(I_t(C_r(y/x)) = 0).$$

from which the result follows. □

For any $x \in C_r$ we can consider cutting all its bonds with other sites in C_r. If there are m such bonds then it has split T_k into $m + 1$ disjoint sets one of which is x. By Lemma 3 the probability that C_r is unoccupied is then the product of the probabilities that each of the $m + 1$ sets is unoccupied, each on its appropriate subset of T_k. In particular the contribution of x is that of a site with $k + 1 - m$ edges, each leading to the root of a copy of the rooted tree T_k^*. Define $\beta_{k+1-m}(t)$ to be the probability such a site is occupied at time t. We then have

$$\beta'_{k+1-m} = -\beta^{k+1-m} = \beta'\beta^{1-m} \Rrightarrow \beta_{k+1-m} = \frac{m - 1 - \beta^{2-m}}{m - 2}, 2 < m < k + 1.$$

using equation (1). For $m = 1$ we have $\beta_k = \beta$, for $m = 2, \beta_{k-1} = 1 + ln\beta$, and for $m = k + 1$, $\beta_0 = 1 - t$. Define $\beta^*_m = \beta_{k+1-m}$.

Theorem 4. *In a blocking process on T_k, let C_r be a connected r-set consisting of sites $x_1, ...x_r$ with each x_i having m_i edges connecting x_i to sites in C_r. Then*

$$P(C_r \textit{is unoccupied at time } t) = \prod_{x_i \in C_r} \beta^*_{m_i}$$

$\beta^*_{k+1} = 1 - t$, $\beta^*_m = \frac{m-1-\beta^{2-m}}{m-2}, 2 < m < k+1$, $\beta^*_2 = 1 + ln\beta$, *and* $\beta^*_1 = \beta$.

The following figure shows how the probability of emptiness declines with time for two types of connected set. A set is called Star if it consists of all sites within a certain distance from a particular site. On T_3 there are 5 sites within distance 1 and 17 within distance 2. A set is called Line if all the sites are connected to 2 other sites in the set, except for the end sites which are connected to 1 each. Rather surprisingly there is very little difference in the probabilities of emptiness between the two shapes. This is because $(\beta^*_2)^3$ is very close to $\beta^*_4(\beta^*_1)^2$ in the range $(0, 1)$ which seems to be a coincidence.

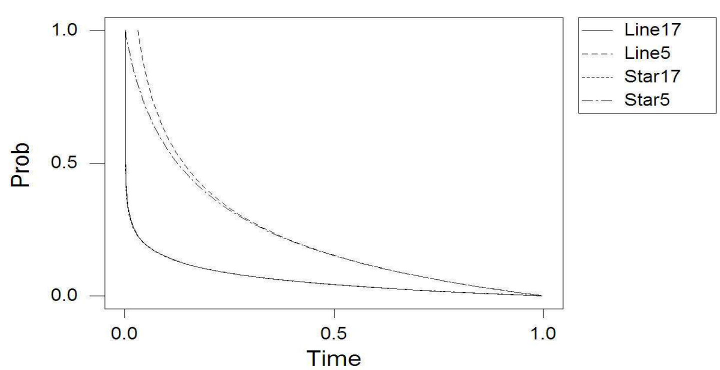

Fig. 1. Emptiness probabilities for two different shapes

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