1-1-1989

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Nicholas Pippenger
Harvey Mudd College

SIAM J. DISC. MATH.
Vol. 2, No. 3, pp. 393–401, August 1989

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RANDOM SEQUENTIAL ADSORPTION ON GRAPHS*

NICHOLAS PIPPENGER†

Abstract. This paper analyzes a process whereby the vertices of a graph are considered in a random sequence, and each considered vertex is "occupied" unless it or an adjacent vertex has previously been occupied. The process continues until no more vertices can be occupied, at which point the "jamming limit" has been reached. The case in which the graph is regular (so that every vertex has degree $d \geqq 2$) and has "few short cycles" is treated. In particular, the results apply to infinite regular trees, to finite graphs obtained from them by forming quotient graphs, and to random regular graphs. It is shown that the probability that a vertex is occupied at the jamming limit tends to $(1 - 1/(d-1)^{2/(d-2)})/2$ as the length of the shortest cycle through it tends to ∞. Also treated are graphs that have short cycles but for which every edge is in at most one cycle; in this way approximations are obtained to the occupancy probabilities for two-dimensional triangular, square and hexagonal lattices. Finally, a similar problem is treated in which edges rather than vertices are occupied, and the occupation of an edge prevents the later occupation of edges incident with it. In each case the solution gives the dynamic evolution of the occupancy probabilities, as well as their values at the jamming limit.

Key words. packing, monomers, dimers

AMS(MOS) subject classifications. 60K35, 82A31, 82A68

1. Introduction. We consider the following random process on a graph. A Poisson stream of "molecules" arrives at each vertex of the graph, the streams arriving at different vertices being independent. When a molecule arrives at a vertex, it "occupies" the vertex, unless that vertex or a vertex adjacent to it has previously been occupied. The process continues until no more vertices can be occupied; this situation is called the "jamming limit." We are interested in determining the density of occupied vertices at the jamming limit. More generally, we are interested in the dynamic evolution of the process as time varies from zero (when no vertices are occupied) to ∞ (when the jamming limit is reached). We may take the unit of time to be the mean interarrival time of the Poisson arrival process. Since the various connected components of a graph do not interact in any way during the process, we may assume that the graph is connected.

This process has been studied by chemists and physicists under the name "random sequential adsorption." It is relevant in situations where the reverse process of "desorption" or "evaporation" occurs so slowly that the relaxation time of the system toward equilibrium is long compared with the time of observation. The graphs of interest to chemists and physicists are primarily those modeling polymers and crystal surfaces.

The only graphs for which we know of an exact solution to this problem are those that are essentially "one-dimensional." The simplest of these are those in which each vertex has degree ("coordination number") at most two, in which case the graph must be a path (finite or infinite) or a cycle (finite or infinite). Flory [F] showed that the expected fraction of occupied vertices in a long path or cycle tends to $(1 - e^{-2})/2$ as the length tends to ∞. Further results on one-dimensional cases have been presented by Page [Pa], Downton [D], McQuistan and Lichtman [McQL], and McQuistan [McQ].

In this paper we present a method for solving this problem on regular graphs without many short cycles. Among these are the infinite regular trees ("Bethe lattices"), finite regular graphs obtained from them by forming quotient graphs ("Bethe lattices with periodic boundary conditions"), and random regular graphs (for which the number of cycles of any given length remains bounded as the number of vertices tends to ∞). We show that the probability that a vertex is occupied at the jamming limit tends to

* Received by the editors May 11, 1988; accepted for publication November 29, 1988.

† Department of Computer Science, University of British Columbia, 6356 Agricultural Road, Vancouver, British Columbia, V6T 1W5, Canada, and IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120.

$(1 - 1/(d-1)^{2/(d-2)})/2$ as the length of the shortest cycle through it tends to ∞, where $d > 2$ is the degree. (As $d \to 2$ we have $1/(d-1)^{2/(d-2)} \to e^{-2}$, so, in a sense, this expression is correct for $d = 2$ as well.)

We may also consider a process whereby "dimers" arrive at the edges of a graph, and the occupation of an edge prevents the later occupation of an edge incident (sharing a vertex) with it. (For the case $d = 2$, the two processes are equivalent, but for $d > 2$ they differ.) The method of this paper is applicable to this process as well, and shows that the probability that an edge is occupied at the jamming limit tends to $(1 - 1/(d-1)^{d/(d-2)})/d$ as the length of the shortest cycle through it tends to ∞. (Again the correct value for $d = 2$ emerges as $d \to 2$.)

It would of course be of great interest to obtain corresponding results for the triangular, square, and hexagonal ("honeycomb") lattices in two dimensions. While no exact solutions have been reported, Monte Carlo estimates have been made. Widom [W1], [W2] gives 0.38 ± 0.01 for the occupancy of the hexagonal lattice; Meakin et al. [Me] give 0.36413 ± 0.00001 for the square lattice and 0.23136 ± 0.00001 for the triangular lattice.

In the final section of this paper, we compare these Monte Carlo estimates with exact solutions for lattices that are similar to the two-dimensional ones as regards their degree and their girth (that is, the length of their shortest cycle), yet are sufficiently tree-like to allow the methods of this paper to be applied. The simplest such tree-like lattices are of course the infinite regular trees themselves. For degrees 3, 4, and 6, our results give $\frac{3}{8} = 0.375$, $\frac{1}{3} = 0.3333\cdots$ and $(1 - (\frac{1}{5})^{1/2})/2 = 0.27369\cdots$, respectively. While the first of these falls within the error bars of the available Monte Carlo estimate, the other two are disappointing. We can improve these approximations by taking account of the shortest cycles in the two-dimensional lattices, ignoring longer cycles. When this is done, the result for degree 3 and girth 6 is $0.37649\cdots$; for degree 4 and girth 4, $0.35071\cdots$; and for degree 6 and girth 3, $\frac{2}{9} = 0.2222\cdots$. The last two values match the corresponding Monte Carlo estimates much more closely than those obtained by ignoring all cycles.

2. Random sequential adsorption on graphs. Let $G = (V, E)$ be an undirected graph with vertices V and edges E. Associate with each vertex $v \in V$ a stationary Poisson stream $A(v)$ of independent arrivals, with the streams corresponding to different vertices being independent. We shall assume that each arrival process starts at time zero and that the mean interarrival time for each stream is 1. For the process we are considering, only the first arrival in each stream is important, since only the first molecule to arrive at a vertex has any chance to occupy that vertex. Thus we may turn our attention from $A(v)$ to the *first-arrival time* $t(v)$ for the vertex v. Each first-arrival time has an exponential distribution with density e^{-t} on the interval $[0, \infty]$, with the first-arrival times for different vertices being independent.

If v is a vertex in a finite graph G with n of vertices, then there are just $n!$ possible orders of first arrivals. For each of these, v is either occupied or "vacant" (that is, not occupied) in the jamming limit; thus, the probability that v is occupied in the jamming limit is a rational number with denominator dividing $n!$. If G has an automorphism group that acts transitively on the vertices, then this probability is the same for all vertices, and we may speak without ambiguity of the "occupancy probability in the jamming limit."

If v is a vertex in an infinite graph G, more must be said. Suppose that all vertices in G have degree at most d. Let us say that a sequence $v_0, v_1, \cdots, v_l$ is a "decreasing path" of length l from v_0 to v_l if v_m is adjacent to v_{m-1} and $t(v_m) < t(v_{m-1})$ for $1 \leqq m \leqq l$. Let $D_k^{(v)}$ denote the event "there exists a decreasing path of length k from v."

LEMMA 2.1.

$$\Pr[D_k^{(v)}] \leqq d(d-1)^{k-1}/(k+1)!.$$

Proof. There are at most $d(d-1)^{k-1}$ simple paths of length k from v, and the probability that such a path is decreasing is $1/(k+1)!$ (since each of the $(k+1)!$ possible orders of arrival is equally likely, and exactly one of them is decreasing). □

Let $E_k^{(v)}$ denote the event "there exists a decreasing path of length k from some vertex that is at distance at most k from v."

LEMMA 2.2.

$$\Pr[E_k^{(v)}] \leqq d^2(d-1)^{2k-2}/k!.$$

Proof. There are at most

$$1+d+d(d-1)+\cdots+d(d-1)^{k-1} \leqq (k+1)d(d-1)^{k-1}$$

vertices that are at distance of at most k from v, and for each such vertex w, the probability that there is a decreasing path of length k from w is as given by Lemma 2.1. □

Suppose that $t(v)$ is the first-arrival time for v. Then v will be occupied at $t(v)$ unless some vertex v_1 adjacent to v has arrival time $t(v_1) < t(v)$. In the latter case, v_1 will be occupied at $t(v_1)$ unless some vertex v_2 adjacent to v_1 has arrival time $t(v_2) < t(v_1)$. Continuing in this way, we see that whether (and if so, when) the vertex v is occupied depends only on the first-arrival times of vertices on decreasing paths from v. In particular, the occupancy of v is well defined unless there is an infinite decreasing path from v, and the occupancies of all vertices are well defined unless there is an infinite decreasing path from some vertex in G. If there is an infinite decreasing path from some vertex in G, then infinitely many of the events $\{E_k^{(v)}\}_{0 \leqq k < \infty}$ occur. By Lemma 2.2, the expected number of such events that occur is

$$\sum_{0 \leqq k < \infty} \Pr[E_k^{(v)}] \leqq d^2 e^{(d-1)^2}/(d-1)^2.$$

By the Borel-Cantelli Lemma, with probability one, only finitely many of these events occur. Thus, with probability one, the occupancy of every vertex in G is well defined.

Let $G_k^{(v)}$ (the "ball of radius k with center v") denote the subgraph of G induced by the set of vertices at distance of at most k from v. Let $\partial G_k^{(v)}$ (the "sphere of radius k with center v") denote the set of vertices in $G_k^{(v)}$ that are adjacent in G to some vertex not in $G_k^{(v)}$. A vertex in $\partial G_k^{(v)}$ is at distance at most k from v, since it is in $G_k^{(v)}$. If a vertex in $\partial G_k^{(v)}$ were at distance at most $k-1$ from v, then the vertices adjacent to it would be at distance at most $(k-1)+1 = k$ from v, and thus would also be in $G_k^{(v)}$. Thus, $\partial G_k^{(v)}$ comprises just those vertices at distance exactly k from v in G.

Let $t \in [0, \infty]$ be some fixed time. Let $M^{(v)}$ denote the probability that the vertex v is occupied at time t in G, and let $M_k^{(v)}$ denote the probability that the same vertex is occupied at the same time in $G_k^{(v)}$.

LEMMA 2.3.

$$|M^{(v)} - M_k^{(v)}| \leqq d(d-1)^{k-1}/k!.$$

Proof. The occupancy of v in G can differ from the occupancy of v in $G_k^{(v)}$ only if there is a decreasing path from v to some vertex in $\partial G_k^{(v)}$. If there is such a path, its length must be at least k, and thus its initial segment of length k establishes the occurrence of $D_k^{(v)}$. Since the occupancies of v in G and $G_k^{(v)}$ can differ only if $D_k^{(v)}$ occurs, Lemma 2.1 completes the proof. □

In the case of an infinite graph G, Lemma 2.3 shows that the occupancy probability of a vertex is approximated by the occupancy probability of that vertex in a sufficiently large but finite neighborhood of the vertex. In particular, it shows that occupancy probabilities in computable graphs (that is, graphs for which the relation of adjacency is effectively computable) are computable real numbers (in the sense that approximations of prescribed accuracy are effectively computable). Lemma 2.3 is significant even for finite graphs; it shows that long-range correlations are weak, and that graphs that are locally similar have similar occupancy probabilities.

3. Regular graphs with few short cycles. A regular graph without cycles is an infinite regular tree, or "Bethe lattice." By imposing "periodic boundary conditions" on such a lattice, a finite regular graph with large girth is obtained (see Margulis [Ma] and Imrich [I]; the girth grows logarithmically with the number of vertices). In a regular graph with degree d and girth g, balls of radius less than $g/2$ are trees, in which all vertices are either "internal" vertices with degree d or are "leaves" with degree one. We shall determine the occupancy probability for a vertex that is far from the leaves of such a tree; this result will apply to the vertices of regular graphs without short cycles by Lemma 2.3.

A random regular graph with degree d and n vertices (that is, a graph chosen at random with equal probabilities from the set of all such graphs) will probably have some short cycles. A simple calculation shows, however, that the expected number of cycles of length at most k is bounded by a constant depending on k and d, but independent of n. In a large random regular graph, then, most vertices will not lie on any short cycles, and the results of this section will apply to them by Lemma 2.3. Thus, in a random regular graph, the expected fraction of occupied vertices will be the same as in a regular graph without short cycles, although there may be a small number of exceptional vertices with occupancy probabilities much higher or lower than this average.

Let $d \geqq 2$ be a natural number. We shall begin by determining the occupancy probabilities, as a function of time, for certain vertices in certain trees. Let A_0 be a tree containing a single vertex, called its "root." For $k \geqq 1$, if A_{k-1} has been defined, let A_k be the tree obtained from a new vertex, called its "root," together with $d - 1$ disjoint copies of A_{k-1}, where the root of A_k is adjacent to the roots of the copies of A_{k-1}.

Let $Q_k(t)$ denote the probability that the root of A_k is vacant at time t. Clearly, we have $Q_0(t) = 1 - e^{-t}$. The key step of our derivation is the following observation:

$$Q_k(t) = 1 - \int_0^t Q_{k-1}(s)^{d-1} e^{-s}\, ds, \tag{3.1}$$

for $k \geqq 1$. To show (3.1), it suffices to show that the integrand is the rate at which the root is occupied at time s. The rate at which first arrivals occur is e^{-s}. This must be multiplied by the probability that the $d-1$ vertices adjacent to the root are vacant at time s, which is just $Q_{k-1}(s)^{d-1}$. (The vacancies of the $d - 1$ vertices adjacent to the root are not independent, but if the first arrival at the root occurs at time s, then the root is vacant throughout the interval $[0, s)$, and the vacancies of the $d - 1$ vertices adjacent to the root, conditioned on this event, are independent.)

To determine the asymptotics of $Q_k(t)$ as $k \to \infty$, let us consider the fixed point of the transformation $Q_{k-1} \mapsto Q_k$, that is, the solution Q of the integral equation

$$Q(t) = 1 - \int_0^t Q(s)^{d-1} e^{-s}\, ds. \tag{3.2}$$

Differentiation of (3.2) with respect to t yields the differential equation

$$Q'(t) = -Q(t)^{d-1} e^{-t}, \tag{3.3}$$

together with the initial condition $Q(0) = 1$.

The only difficulty in (3.3) comes from the factor e^{-t}, which is the density of first arrivals. This difficulty can be removed by the substitution $t = -\ln(1-\tau)$, $\tau = 1 - e^{-t}$, which "uniformizes" the distribution of τ over the interval $[0, 1]$. Setting

$$P(\tau) = Q(-\ln(1-\tau))$$

for $0 \leqq \tau < 1$, we have

$$P'(\tau) = -P(\tau)^{d-1}, \tag{3.4}$$

together with the initial condition $P(0) = 1$.

Since (3.4) does not involve τ explicitly, it can be solved by quadratures:

$$\tau = -\int_1^{P(\tau)} \frac{dx}{x^{d-1}}$$
$$= \begin{cases} -\ln P(\tau), & \text{if } d=2, \\ -(1-1/P(\tau)^{d-2})/(d-2), & \text{if } d>2, \end{cases}$$

where the lower limit of integration is the initial condition $P(0) = 1$. Thus,

$$P(\tau) = \begin{cases} e^{-\tau}, & \text{if } d=2, \\ 1/((d-2)\tau+1)^{1/(d-2)}, & \text{if } d>2. \end{cases} \tag{3.5}$$

This is the desired solution of the transformed version,

$$P(\tau) = 1 - \int_0^\tau P(\sigma)^{d-1}\, d\sigma, \tag{3.6}$$

of (3.2).

To apply this result, let us now define

$$P_k(\tau) = Q_k(-\ln(1-\tau)),$$

for $k \geqq 0$. Clearly, $P_0(\tau) = 1 - \tau$. From (3.1) it follows that

$$P_k(\tau) = 1 - \int_0^\tau P_{k-1}(\sigma)^{d-1}\, d\sigma, \tag{3.7}$$

for $k \geqq 1$. We shall show that $P_k(\tau) \to P(\tau)$ uniformly in τ as $k \to \infty$.

To this end, let $\Delta_k(\tau) = P_k(\tau) - P(\tau)$. Since $0 \leqq P_0(\tau), P(\tau) \leqq 1$, we have $|\Delta_0(\tau)| \leqq 1$. From (3.6) and (3.7) it follows that

$$\Delta_k(\tau) = \int_0^\tau P(\sigma)^{d-1} - P_{k-1}(\sigma)^{d-1}\, d\sigma$$
$$= -\int_0^\tau \Delta_{k-1}(\sigma)(P(\sigma)^{d-2} + \cdots + P_{k-1}(\sigma)^{d-2}),$$

for $k \geqq 1$. Since $0 \leqq P(\tau), P_{k-1}(\tau) \leqq 1$, we have

$$|\Delta_k(\tau)| \leqq (d-1)\int_0^\tau |\Delta_{k-1}(\sigma)|\, d\sigma.$$

It follows by induction on k that

$$|\Delta_k(\tau)| \leqq (d-1)^k \tau^k / k!. \tag{3.8}$$

Thus $P_k(\tau) \to P(\tau)$ uniformly in τ as $k \to \infty$.

For $k \geqq 1$, let A_k^* be the tree obtained from a new vertex, called its "root," together with d disjoint copies of A_{k-1}, where the root of A_k^* is adjacent to the roots of the copies of A_{k-1}. Let $Q_k^*(t)$ denote the probability that the root of A_k^* is vacant at time t. By an argument analogous to that used to establish (3.1) we have

$$Q_k^* = 1 - \int_0^t Q_{k-1}(s)^d e^{-s}\, ds.$$

Setting

$$P_k^*(\tau) = Q_k^*(-\ln(1-\tau)),$$

we obtain

$$P_k^*(\tau) = 1 - \int_0^\tau P_{k-1}(\sigma)^d\, d\sigma. \tag{3.9}$$

Define

$$P^*(\tau) = 1 - \int_0^\tau P(\sigma)^d\, d\sigma. \tag{3.10}$$

Then we have the following.

LEMMA 3.1.

$$P^*(\tau) = \begin{cases} (1+e^{-2\tau})/2, & \text{if } d=2, \\ (1+1/((d-2)\tau+1)^{2/(d-2)})/2, & \text{if } d>2. \end{cases}$$

Proof. From (3.10) and (3.4) we have

$$\begin{aligned} P^*(\tau) &= 1 - \int_0^\tau P(\sigma)^d\, d\sigma \\ &= 1 + \int_0^\tau P(\sigma)P'(\sigma)\, d\sigma \\ &= 1 + \int_{P(0)}^{P(\tau)} x\, dx \\ &= 1 + \frac{P(\tau)^2 - P(0)^2}{2}. \end{aligned}$$

The lemma follows by substitution of (3.5). □

LEMMA 3.2.

$$|P_k^*(\tau) - P^*(\tau)| \leqq d(d-1)^{k-1}\tau^k/k!.$$

Proof. This follows by an argument analogous to that used to establish (3.8). □

These lemmas give us the limiting value of the vacancy probability for a vertex far from the leaves of a large regular tree. The analysis in this section is summarized by the following theorem.

THEOREM 3.3. *Let v be a vertex in a regular graph G of degree $d \geqq 2$, and suppose that there is no cycle of length at most $2k+1$ through v. Then*

$$|Q^{(v)}(t) - Q^*(t)| \leqq 2d(d-1)^{k-1}/k!,$$

where

$$Q^*(t) = \begin{cases} (1+e^{-2(1-e^{-t})})/2, & \text{if } d=2, \\ (1+1/((d-2)(1-e^{-t})+1)^{2/(d-2)})/2, & \text{if } d>2. \end{cases}$$

Proof. By the hypothesis on v in G, there is an isomorphism between $G_k^{(v)}$ and A_k^* that maps v to the root of A_k^*. Thus $Q_k^{(v)}(t) = Q_k^*(t)$. The theorem then follows from Lemmas 2.3, 3.1, and 3.2. □

We conclude this section with the remark that a similar analysis applies to the process whereby "dimers" arrive at the edges of a graph, and the occupation of an edge prevents the later occupation of an edge incident with it. In this case, the occupancy probability in the jamming limit is $(1 - 1/(d-1)^{d/(d-2)})/d$.

4. Regular graphs with nonoverlapping short cycles. We shall now consider some infinite regular graphs with many short cycles. If all simple cycles have a common length g, are uniformly distributed (in the sense that the same number c of simple cycles pass through each vertex), and are nonoverlapping (in the sense that at most one simple cycle passes through each edge), then the methods of the preceding section can be adapted to determine the occupancy probability. (The differential equations that arise in this way will in general not be solvable in closed form, but can easily be integrated numerically.) By varying the degree d, the girth g, and the parameter c, a variety of exactly solvable lattices can be obtained. Our main interest in these lattices is as "approximations" (in some sense that we shall not make precise) to the two-dimensional triangular, square, and hexagonal lattices. The simplest and crudest such approximations are the infinite regular trees of degree 6, 4, and 3. The result of the preceding section gives occupancy probabilities in the jamming limit of $(1 - (\frac{1}{5})^{1/2})/2 = 0.27639\cdots$, $\frac{1}{3} = 0.33333\cdots$, and $\frac{3}{8} = 0.375$, respectively.

Consider the infinite graph obtained by joining triangles so that three triangles meet at every vertex and there are no other simple cycles. This lattice, which corresponds to the choice $d = 6$, $g = 3$, and $c = 3$, may be regarded as the Cayley graph of a free product of three copies of the integers modulo 3; it has the same degree and girth as the triangular lattice, but differs in that every vertex is in three triangles rather than six, and every edge is in one rather than two. The lattice is sufficiently tree-like so that the methods of the preceding section can be adapted to determine the occupancy probability in the jamming limit. The differential equation analogous to (3.4) is

$$P'(\tau) = -P(\tau)^4,$$

with the initial condition $P(0) = 1$. This is the same as for the infinite regular tree with $d = 5$, and the solution is $P(\tau) = 1/(3\tau + 1)^{1/3}$. The occupancy probability in the jamming limit is

$$\int_0^1 P(\tau)^6 \, d\tau = \tfrac{2}{9} = 0.2222\cdots,$$

considerably closer to the Monte Carlo estimate 0.23136 given by Meakin et al. [Me] than the value $0.27639\cdots$ obtained by ignoring all cycles.

Consider now the infinite graph obtained by joining squares so that two squares meet at every vertex and there are no other simple cycles. This lattice, which corresponds to the choice $d = 4$, $g = 4$, and $c = 2$, may be regarded as the Cayley graph of a free product of two copies of the integers modulo 4; it has the same degree and girth as the square lattice, but differs in that every vertex is in two squares rather than four, and every edge is in one rather than two. The differential equation analogous to (3.4) is

$$P'(\tau) = -\frac{2P(\tau)^3 + 1}{3},$$

with the initial condition $P(0) = 1$. Integrating numerically yields $P(1) = 0.43066\cdots$. The occupancy probability in the jamming limit is

$$\begin{aligned}\int_0^1 (-P'(\tau))^2 \, d\tau &= -\int_{P(0)}^{P(1)} \frac{2x^3+1}{3} \, dx \\ &= \frac{3 - P(1)^4 - 2P(1)}{6} \\ &= 0.35071\cdots,\end{aligned}$$

which is considerably closer to the Monte Carlo estimate 0.36413 given by Meakin et al. [Me] than the value $0.33333\cdots$ obtained by ignoring all cycles.

Finally, consider the infinite graph obtained by joining hexagons and edges so that one hexagon and one edge meet at every vertex and there are no other simple cycles. This lattice, which corresponds to the choice $d = 3$, $g = 6$, and $c = 1$, may be regarded as the Cayley graph of a free product of the integers modulo 6 with the integers modulo 2; it has the same degree and girth as L_3, but differs in that every vertex is in one hexagon rather than three, and every edge is in zero or one rather than two. There are now two differential equations analogous to (3.4):

$$P_1'(\tau) = -P_2(\tau)$$

and

$$P_2'(\tau) = -\frac{2P_1(\tau)^5 + 10P_1(\tau)^2 + 3}{15},$$

with the initial conditions $P_1(0) = P_2(0) = 1$. Differentiating the first with respect to τ, substituting the second, multiplying by the integrating factor $2P_1'(\tau)$, and integrating yields

$$P_1'(\tau)^2 = \frac{2P_1(\tau)^6 + 20P_1(\tau)^3 + 18P_1(\tau) + 5}{45},$$

where the constant of integration has been chosen to satisfy the initial condition $P_1'(0) = -P_2(0) = -1$. Taking square roots (the initial condition shows that the negative root must be taken) and integrating numerically yields $P_1(1) = 0.30738\cdots$ and $P_1'(1) = -0.49700\cdots$. The occupancy probability in the jamming limit is

$$\begin{aligned}\int_0^1 (-P_1'(\tau))(-P_2'(\tau)) \, d\tau &= -\int_{P_2(0)}^{P_2(1)} x \, dx \\ &= \frac{1 - P_2(1)^2}{2} \\ &= \frac{1 - P_1'(1)^2}{2} \\ &= 0.37649\cdots.\end{aligned}$$

Both this and the value 0.375 obtained by ignoring all cycles are within the error estimate 0.01 for the Monte Carlo value 0.38 given by Widom [W1].

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