Coordination models of random sequential adsorption in one and two dimensions

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Coordination models of random sequential adsorption are studied numerically in one and two dimensions. In one dimension k-mers are deposited and in two dimensions squares of side m. The jamming coverage is examined as a function of coordination number and of k and m in one and two dimensions, respectively.

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INTRODUCTION

Random sequential adsorption (RSA) is the irreversible process by which particles are deposited on a discrete or continuous surface. At each time step a random position is chosen and a particle is deposited in that position if it does not overlap with any of the particles which have been placed previously. This means that not all positions are available for deposition and that after a certain amount of time the surface becomes full, with no further deposition possible.

A number of numerical studies have been performed on RSA models in two dimensions. On the lattice the coverage has been examined for different shapes [1,2] and for squares of different sizes [3,4]. In the continuum there are more possibilities; needlelike objects have been considered [5] as well as finite-sized shapes [6,7]. In one dimension most problems have been solved analytically [8–12]. The placing of an object on a line divides the line into two independent systems which can be treated separately. It is this property, which obviously does not exist for two-dimensional lattices, which has made analytic progress possible. Other theoretical approaches have attempted to bridge the gap between one- and two-dimensional problems by introducing a set of hierarchial rate-filling equations [13,14] or by examining the problem on a Bethe lattice [15].

Recently a generalization of the RSA process has been introduced for lattice deposition — that of coordination models [16]. In this process deposition may only take place if all the particles, including the placed particle, have less than c touching neighbors. Of course the deposited particle must not overlap any previously placed particle, as in the original RSA models. The coordination number can take any value from 0 to 2 in one dimension and from 0 to 6 in two dimensions. The upper limit on c is determined by the largest possible number of neighbors for an object on a lattice. In two dimensions, when $c = 0$ the objects are not allowed to touch one another; when $c = 6$ a placed object can touch any number of neighbors and the process is just that of RSA. Similarly, in one dimension, the $c = 0$ model allows no contact between k-mers, $c = 1$ allows a k-mer to touch one of its neighbors, and $c = 2$ is just the basic RSA model.

Coordination models have been studied in one, two, and three dimensions for objects of size 1 [16]. No numerical work has considered the dependence of these models on the size of the deposited particle and no progress has been made analytically on the one-dimensional models. The property of a deposited object dividing the lattice into two independent parts does not hold for these models, so an analytical approach similar to that taken for the RSA models is not possible.

In this paper the coverage in the jamming limit is determined in two dimensions as a function of both coordination number and of the length of the sides of the deposited squares, m. A nontrivial dependence is found: when $c = 4$, 5, and 6 the coverage falls with increasing m; for lower values of c the coverage increases with m. In one dimension a similar property is observed: for $c = 0$ the coverage rises with the k-mer length k; for $c = 1$ and 2 it decreases.

NUMERICAL RESULTS AND DISCUSSION

The coverage in the jamming limit for a one-dimensional lattice $\theta(k)$ is given as a function of k in Table I. The results were obtained from a periodic lattice

TABLE I. The coverage of k-mers on a one-dimensional lattice in the jamming limit as a function of k and coordination number c.

k	$\theta(k)$		
	$c = 0$	$c = 1$	$c = 2$
2	0.5492	0.6781	0.8645
3	0.6028	0.7042	0.8237
4	0.6337	0.7165	0.8039
5	0.6538	0.7236	0.7924
6	0.6679	0.7282	0.7847
7	0.6782	0.7313	0.7791
8	0.6865	0.7333	0.7751
9	0.6928	0.7352	0.7720
10	0.6978	0.7365	0.7694
20	0.7224	0.7421	0.7584
30	0.7305	0.7441	0.7544
40	0.7350	0.7447	0.7528
50	0.7368	0.7475	0.7518
100	0.7414	0.7476	0.7498
1000	0.7470	0.7476	0.7478
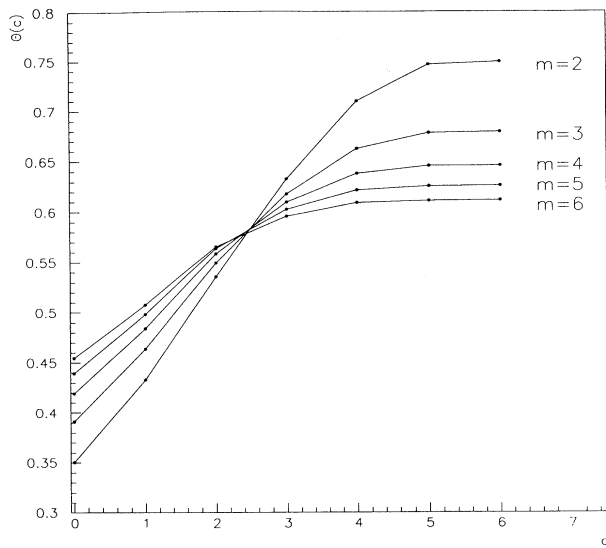
FIG. 1. Jamming coverage vs coordination number (two dimensions).

FIG. 3. $\ln|\theta(k)-\theta(\infty)|$ vs $\ln k$ (one dimension).

of 100 000 sites, averaging over 100 realizations with 100 attempted placements per site. The results are exact to three decimal places and the values for $c=2$ agree with those published previously [17].

The numerical results for two dimensions were obtained from simulations performed on a 200×200 periodic lattice and averaged over 400 runs for $m=2,3,4,5,$ and 6. The values at $c=6$ are broadly in agreement with those of Model A in [3].

For two dimensions the jamming coverage is given as a function of coordination number in Fig. 1. The values from the table have been plotted and joined with straight lines. For an average coordination of about 2.4, the coverage is ≈ 0.58, independent of the size of the deposited
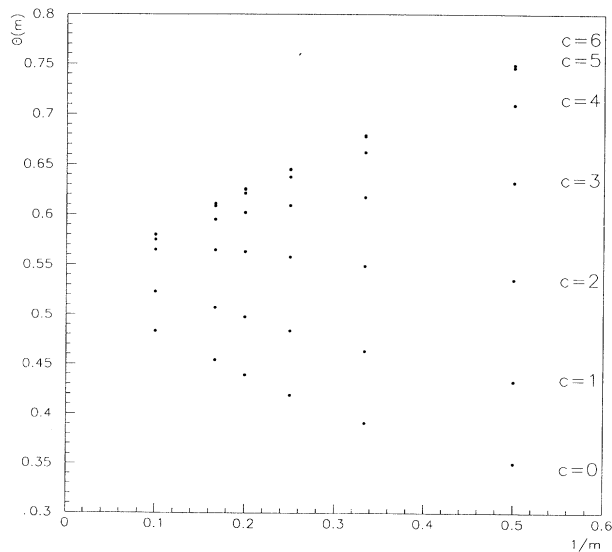
squares. This is the point where the curves intersect. As m gets larger the curves become more horizontal so that as $m \to \infty$ the line becomes horizontal with a coverage, independent of coordination number, of about 0.58. Figure 2 is a plot of coverage vs $1/m$. As m goes to infinity the curves appear to straighten, although statistical uncertainty and the relatively small values of m means that no definite conclusion can be reached about the large-m behavior. The coverage at $m=\infty$, which will be the same for all values of c, appears to be about 0.54. This is a little lower than the value suggested by Fig. 1. The coverage in this limit has been discussed by other authors; values range from 0.554 [18] to 0.564 [3].

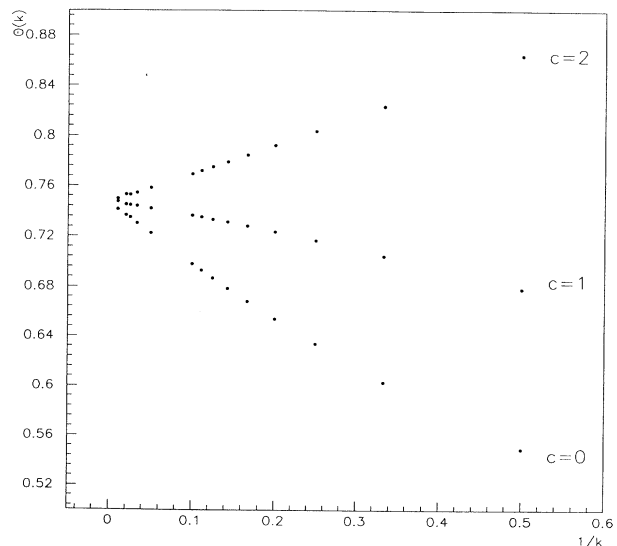In Fig. 3 a plot of $\ln|\theta(k)-\theta(\infty)|$ vs $\ln k$ is given. As

FIG. 2. Jamming coverage vs $1/m$ (two dimensions).

FIG. 4. Jamming coverage vs $1/k$ (one dimension).

can be seen, all three curves have about the same slope: -0.95, -0.97, and -1.00 for $c = 0$, 1, and 2, respectively. The plot was made by taking the value of $\theta(\infty)$ as 0.7476.

In Fig. 4 a graph of $\theta(k)$ vs $1/k$ is given. The curves for $c = 0$, 1, and 2 all approach a straight line as $k \rightarrow \infty$. The coverage in the limit $k \rightarrow \infty$ tends to 0.7476, in agreement with that given for the random sequential adsorption of k-mers onto a one-dimensional lattice [17].

CONCLUSIONS

The deposition of k-mers and squares has been studied for coordination models in one and two dimensions as a function of the size of the deposited object. As k is in-

creased in one dimension, the coverage approached the $k = \infty$ limit like $1/k$ for all values of c. The coverage in this limit is about 0.7476, in agreement with previously published results.

In two dimensions the $m = \infty$ coverage is ≈ 0.56, independent of coordination number. This is also the value of the coverage for deposition processes with an average coordination of $c \approx 2.4$, irrespective of the size of the squares being deposited. As m gets larger the dependence of the coverage in the jamming limit on the coordination number becomes weaker and weaker.

In both one and two dimensions the coverage as a function of shape size approaches the coverage for an infinite shape from below for low values of c and from above for high values.

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