Percolation and jamming in random bond deposition

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A model is presented in which on the bonds of a square lattice linear segments (''needles'') of a constant length a are randomly placed. We investigate the dependence of the percolation and jamming thresholds on the length of the needles. The difference from the standard site deposition problem is demonstrated. We show that the system undergoes a transition at $a=6$. When shorter needles are used, the system first becomes percolating before becoming jammed. For longer needles the lattice becomes jammed but there is no percolation. We present evidence that the transition is due to different clustering of the short and long needles. We also determine the Fisher exponent, obtaining the same value as for standard two-dimensional percolation .

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I. INTRODUCTION

Recently there has been much theoretical and experimental interest in random sequential adsorption (RSA) models. In this approach finite objects are randomly deposited, one by one, onto an initially empty substrate (e.g., a lattice or a continuous surface), and are adsorbed if there is no overlapping with previously adsorbed objects. These kinds of models have a wide range of applications in physics, chemistry, biology, etc. for describing processes in which microscopical steps are irreversible.

A large group of RSA problems was motivated by the study of kinetics of some chemical reactions, e.g., simple cyclization reactions (see Ref. [1], in which the RSA approach itself originates), irreversible dissociation from polymer chains [2], and the binding of large ligands to polymer chains [3]. Another area of applicability is the desorption of large molecules like proteins on solid surfaces [4] or macromolecules on biological membranes [5]. Many properties of growth processes in three-dimensional solid state physics [6] are well described by the RSA approach as well. Also some ecological [7] and sociological problems [8] were successfully solved using RSA. For an extensive overview of the field, see Ref. [9].

In the context of RSA the notion of jamming is very important. A system reaches a jamming point if no more objects can be adsorbed due to the lack of available space. The jamming threshold c_j is then defined as a fraction of occupied surface at that moment.

The problem of percolation is an old one [10], but there are still new results and new questions being posed [11,12]. In a standard formulaton on a d-dimensional lattice each site can be occupied with a probability c (or empty with a probability $1-c$). Neighboring occupied sites form a cluster. The cluster is said to be percolating if it reaches two opposite edges of the lattice (e.g., the top and bottom). The lowest concentration of occupied sites for which there is a percolating cluster for an infinite lattice limit is called the percolation threshold c_p [11].

There are many applications of percolation theory, especially in spatially disordered systems, porous media and critical phenomena. For an overview see, e.g., Ref [13].

Apart from the relatively well known case of the RSA of spheres (modelling, e.g., adsorption of spherical molecules [4]) there is an interesting domain of the study of RSA of rectangles or line segments. These models can be used in describing the characteristics of composites or materials made in the process of adsorption of rodlike polymers or conducting needles [14]. In these models (both continuous and discrete) the central point of interest is often the kinetics of the process. However, here we concentrate on the dependence of thresholds on the length ratio a of adsorbed objects (rectangles). As the continuous approach differs in some predictions from the lattice site one [e.g., the jamming threshold $c_j(a)\to 0$ as $a\to\infty$ for the continuous case [15] and $c_j(a)\to c_j^*\neq 0$ for the discrete case [16]], there are also features that distinguish between the site and bond formulation of the discrete (lattice) problem. To the best of our knowledge a needles' adsorption on bonds has never been considered in the literature.

II. MODEL

Here we investigate a system in which linear segments (''needles'') of length a are randomly placed on the bonds of the square lattice. The needles may touch but they cannot cross each other or have a common bond. At each step of the simulation we randomly generate (from uniform distribution) the position and orientation of the needle to be inserted. If there is no possibility of depositing the needle, we discard it and go on to the next step. The essential difference between the site deposition investigated, e.g., in Refs. [16,17] and the present study is that now the two closest parallel needles themselves do not touch— a connecting path is realized only by vertical and horizontal needles touching somewhere on their length. As before [16], we use hard boundary conditions, meaning that no part of any needle may stick out from the lattice. We have verified that allowing for open boundary conditions does not alter the results.

We investigate two phenomena, percolation and jamming. The percolation threshold is defined as a concentration c_p of needles at which there is an uninterrupted path, following the bonds occupied by the needles, from the top to the bottom of the lattice [11]. The smallest possible length of the needles, $a=1$, corresponds to the standard bond percolation, for which we recover the well-known result $c_p=0.5$ [11]. The

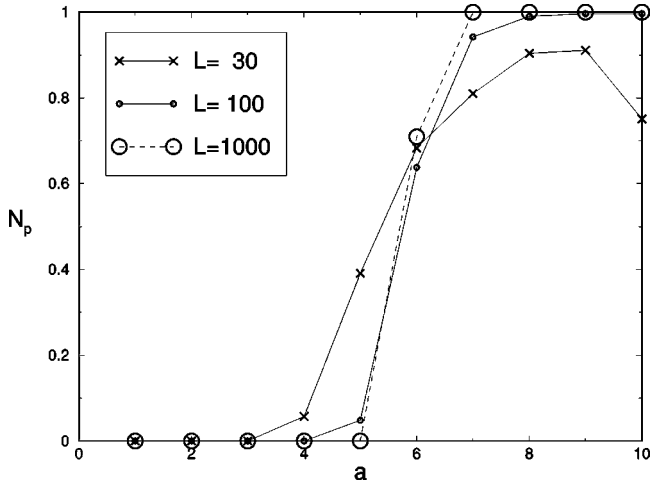

FIG. 1. Probability N_p for the absence of percolation in the system vs needle length $a=1\ldots6$ for lattice sizes $L=30$, 100, and 1000, averaged over 1000 samples.

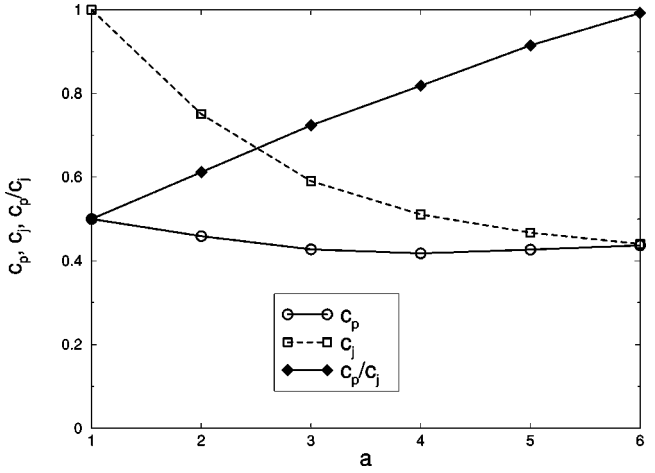

FIG. 2. Thresholds for percolation c_p, jamming c_j, and their ratio c_p/c_j for $a=1\ldots6$. The lattice size is $L=1000$, averaged over 100 samples.

jamming threshold is defined as a concentration c_j of needles, above which it is impossible to add another needle of a given length to the lattice [9].

We shall study, using Monte Carlo simulations, the dependence of the two thresholds and their ratio on the length a of the needles. We shall also compare the results with those obtained for site percolation and jamming [16]. Most of the results were found for a $L=1000$ square lattice (although smaller and larger lattices, $L=30$, 100, 300, and 3000, were also considered) and averaged over 100 independent runs. We have checked that the statistics is not much improved by averaging over 1000 runs.

III. RESULTS

We have found that percolation in the system sets in only for short needles with $a\leqslant a^*=6$. In the case of longer needles no percolating cluster exists for large enough lattices (e.g., out of 1000 samples for $a=7$, only two percolate on a 300×300 lattice, but none on a 1000×1000 lattice). The longer the needles, the higher the chance of absence of percolation (jamming sets in in the system first). This probability is drawn in Fig. 1 against the needle length. The transition from a percolating to a nonpercolating system occurs at a rather narrow range of the needle length. Asymptotically ($L\rightarrow\infty$) we expect a step function. A possible explanation for the existence of a nonpercolating regime is discussed further. This behavior distinguishes between the bond problem and the site one, since in the latter we can always reach percolation threshold for all needle lengths [16]. The absence of percolation was reported earlier in a different context and for the site problem; see, e.g., Ref. [18] in the case of the RSA of squares, or a more general model [19] of RSA of rectangles, both on site square lattices.

The variation of the percolation threshold c_p with increasing needle length a is shown in Fig. 2 (we consider only $a\leqslant6$, since above this point there is no percolation). The uncertainties of the c_p are below 0.004; therefore, we are convinced that there is a minimum for $a=a_{min}=4$. As there was a similar minimum for the site problem (see Ref. [15]), for longer needles ($a_{min}=13$), we expect the same mechanism to be responsible for both phenomena. For longer needles there is a competition between enlarging the range of connection and the increasing difficulty in restoring connection (for details, see Ref. [16]). For $a\geqslant6$, however, it is so difficult for one needle to become connected to others that percolation does not appear. The difference between sites and bonds here is crucial. In the site problem two close parallel needles can be connected via other parallel needles lying in between them. In a bond problem, however, even the two closest parallel needles remain disconnected unless they both touch the same perpendicular needle. Thus we suppose that for long needles small clusters work as shields, preventing the formation of a connected network of bonds in the system. Another argument supporting our conjecture is found by a direct inspection of snapshots of the needle arrangement, an example of which can be seen in Fig. 3. The state of a system of needles with $a=8$ at the jamming point is shown there.

In order to obtain some more insight into the problem, we have also examined the cluster structure of the system at jamming, when no more needles can be added. As we can see in Fig. 4, there is a clear change in the shape for $a=6$. For small a most of the mass carried by the needles constitutes a large percolating cluster. For long needles more and more mass is accumulated in very small clusters, especially in single isolated needles. That is, 2.5% of the total mass is concentrated in such needles for $a=4$, and 16.5% for $a=7$.

To establish a connection between our model and other percolation critical phenomena we have verified the so called Fisher law [11]. It is generally observed that, for percolation models the cluster size distribution function measured at the percolation point follows a power law

$$n_s(c_p)\propto s^{-\tau},$$

where the Fisher exponent is equal [13] to

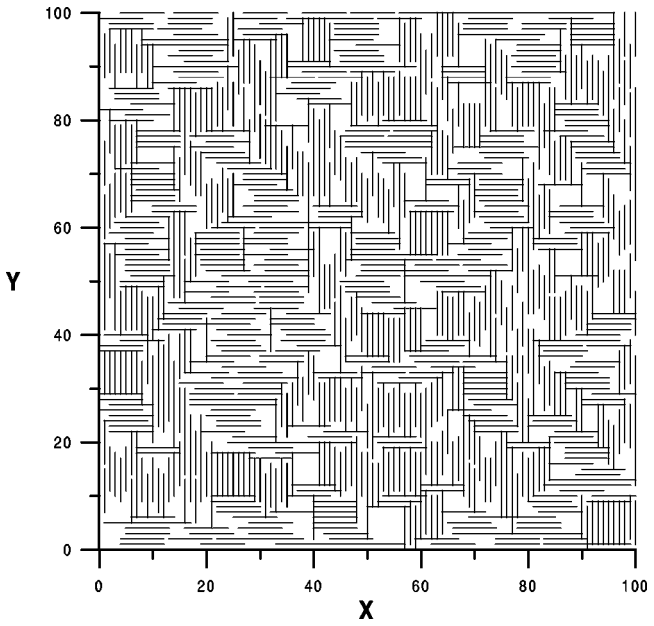

FIG. 3. Snapshot of a spatial distribution of needles at the jamming threshold for $L=100$. The needle length is $a=8$; therefore, no percolation appears.

$$\tau = \frac{187}{91} \approx 2.055,$$

and is a universal quantity throughout many two-dimensional (2D) models. The results of our investigations are presented in Fig. 5, where size distribution functions for clusters at percolation are ploted on a log-log graph for various needle lengths. Averaged over 100 samples on a 1000×1000 lattice, ''experimental'' points follow straight lines with the same slope for all $a=1\ldots6$, determined to be $-\tau=-2.02\pm0.04$. Thus our model ($a>1$) manifests the same characteristic as in standard 2D percolation ($a=1$).

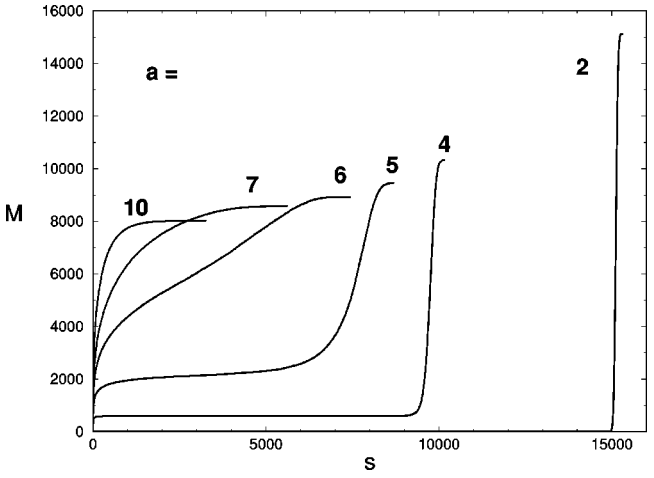

FIG. 4. Plot of $M(s)$, the number of unit bonds in clusters not larger than s vs s, measured at the jamming point. The lattice size is $L=100$, averaged over 10 000 samples. The needle lengths are $a=2$, 4, 5, 6, 7, and 10.

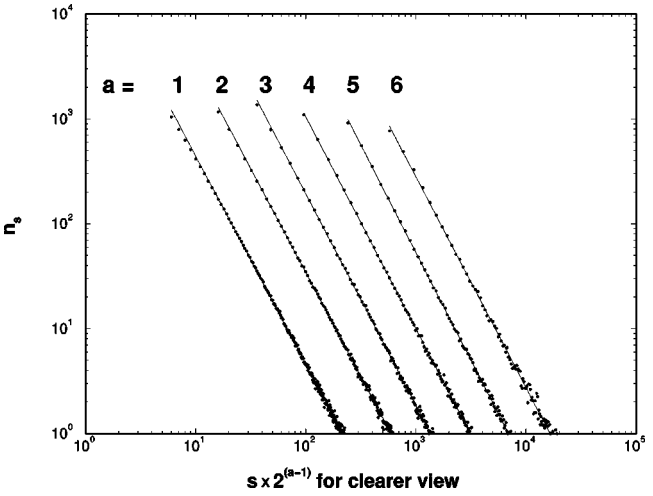

FIG. 5. Cluster size distribution functions n_s for $a=1\ldots6$ at the percolation point, averaged over 100 samples; $L=1000$. Data sets for each a are separated by a factor of 2 for clarity.

Let us now analyze the jamming threshold c_j as a function of the needle length a. It appears that points conform to the following formula with very high accuracy (see Fig. 6):

$$c_j(a) - c_j^* \propto a^{\Delta},$$

where $c_j^*=0.3350\pm0.0025$ and $\Delta=-1.05\pm0.10$ (uncertainties are obtained from graph analysis for various trial values of c_j^* and Δ). The same kind of dependence was found for the site RSA of needles [16], but with $c_j^*(\text{sites})=0.66\pm0.01$. Let us compare the jammed state for both lattices (bonds and sites), especially for very long needles. In both cases needles tend to form domains of parallel alignement, the interdomain space being relatively empty. In domains for sites almost all sites are occupied, but for bonds about 50% of bonds are perpendicular to the needles and are empty. This explains the relation $c_j^*(\text{sites})=2c_j^*(\text{bonds})$.

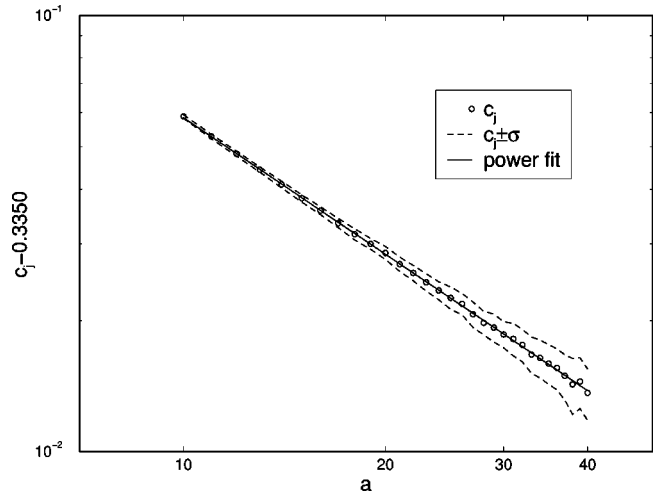

FIG. 6. Power law approach of the $a=\infty$ limit for the jamming threshold. Lattice $L=1000$, averaged over 100 samples, $a=10\ldots40$. A mean standard deviation σ (dotted lines) is also shown.

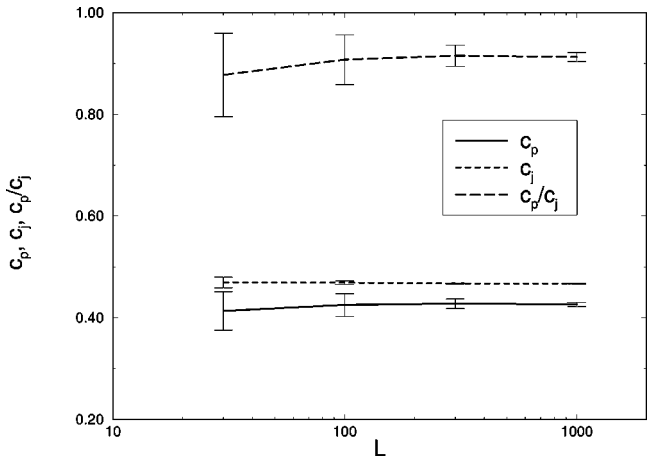

FIG. 7. Convergence analysis. The values of the thresholds c_p, c_j, and c_p/c_j are plotted with error bars against the lattice size L. Here $a=5$, and averaging is over 100 samples.

It should be noted that there were estimates for c_j^*(sites) only (also see Ref. [17]). The dependence of c_j on a is quite different for continuous models of RSA of rectangles (see, e.g., Ref. [15] or [20]): $c_j(a) \propto a^{\Delta}$ with $\Delta=-0.2$ [20] or $\Delta=-0.26$ [15], the threshold tending to zero as $a\to\infty$.

Having determined c_p and c_j we can look at their ratio c_p/c_j carrying some information about the structure of the system (see Fig. 2). One can easily see that c_p/c_j is almost linear with a. Finally, we analyzed the convergence of the thresholds as L tends to infinity. It appears that for $L/a>15$ the values of c_p and c_j do not vary much with increasing L (keeping a constant) while the mean standard deviation σ drops significantly. Thus it is safe to cosider the values of the thresholds obtained for $L=1000$ as the asymptotic (exact) ones—see Fig. 7.

IV. CONCLUSIONS

We have investigated the random deposition of linear segments on the bonds of a square lattice. As in the case investigated earlier [16], we have found a minimum in the percolation threshold dependence on the length of the deposited objects. We believe that the same mechanism is responsible for both results. Unlike the site case, here, for needles longer than $a=6$, the system cannot reach the percolation threshold, since it becomes jammed first. The ratio of the two thresholds shows (till $a=6$) a linear behavior. For the Fisher exponent we obtained the same value as for the standard ($a=1$) 2D percolation problem, which suggests the same universality class.

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