Critical packing fraction of rectangular particles on the square lattice

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The random packing of identical and nonoverlapping rectangular particles of size $n\times m$ $(1\leqslant n,m\leqslant 10)$ is studied numerically on the square lattice, and the corresponding packing fractions p_f and percolation probabilities P_∞ are determined. We find that for randomly oriented particles there is a critical packing fraction $p_f^c=0.67\pm0.01$, such that for all particles sizes $n\times m$ for which $p_f<p_f^c$ they do not percolate, i.e., $P_\infty\to 0$ for $L\to\infty$, while when $p_f>p_f^c, P_\infty\to 1$ when $L\to\infty$ and an infinite cluster exists. The value for p_f^c is found to be consistent with the continuum percolation threshold $p_c\cong 0.67$ for overlapping particles in two dimensions.

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Is there any critical behavior underlying the maximum random sequential packing (packing fraction) of particles of different size and shape on a lattice? In order to address this general question we study the particular case of identical, rectangular, and randomly orientated, sequentially and nonoverlappingly packed particles on the square lattice. Concerning more basic quantities such as the packing fraction itself, the special case of square particles has been studied in the past [1]. It was found that for systems consisting of particles of size 2×2 and 3×3 (in units of the lattice constant a), clusters of particles in contact occur that span the whole lattice and percolate in the limit of an infinite system, whereas for particles of size 4×4 and larger, only finite clusters exist. These models are also interesting for understanding particle size effects on the conductivity of mixtures of insulating particles dispersed in a normal ionic conductor [2,3].

In this paper we show that the behavior for square particles can be better appreciated by studying the more general case of rectangular particles of size $n\times m$. We find that there is a critical packing fraction $p_f^c=0.67\pm0.01$ such that for packing fractions $p_f<p_f^c$ only finite clusters exist, while for $p_f>p_f^c$ a percolating cluster of particles in contact occurs. Indeed, in the special cases of square particles one has $p_f\cong0.75$ for size 2×2, $p_f\cong0.68$ for size 3×3, and $p_f\cong0.65$ for size 4×4.

Let us start by briefly mentioning how the packing algorithm is actually implemented. Initially all lattice sites are available for occupation. For a rectangular particle, i.e., for sizes $n\neq m$, we first determine at random the orientation that the particle will take once deposited on the lattice. Thus, on average, the packed rods will be distributed isotropically on the lattice on length scales $\ell\gg a\max\{n,m\}$. Second, a lattice site (denoted as deposition site) is chosen at random, at which the upper-right particle's corner of a new particle can be located. Then, according to the previously determined particle orientation it is checked whether the deposition site, as well as the additional $(n\times m)-1$ lattice sites covered by the particle, are available for occupation. If all $n\times m$ sites are available the particle is deposited, the sites are marked as occupied, and the number of remaining available deposition sites is reduced accordingly. Otherwise, the try is discarded. To speed up the simulations, two flags are associated with each site. One of the flags indicates if or if not it is possible to deposit a horizontally oriented particle with its upper-right corner at the site; the second flag indicates the same for a vertically oriented particle. Each time a particle is deposited on the lattice, the flags in the local surrounding located to the left and above the particle are updated accordingly. The deposition is repeated until there are no more deposition sites available. In this case, the deposition is considered to be completed and the resulting fraction of occupied sites yields the packing fraction p_f $[=p_f(n,m,L)]$. Then, a connectivity analysis is performed to establish whether the particles percolate either horizontally or vertically. This yields the percolation probability P_∞ $[=P_\infty(n,m,L)]$, being just the fraction of configurations in which a percolating (''infinite'') cluster is found within the total number of configurations considered [4].

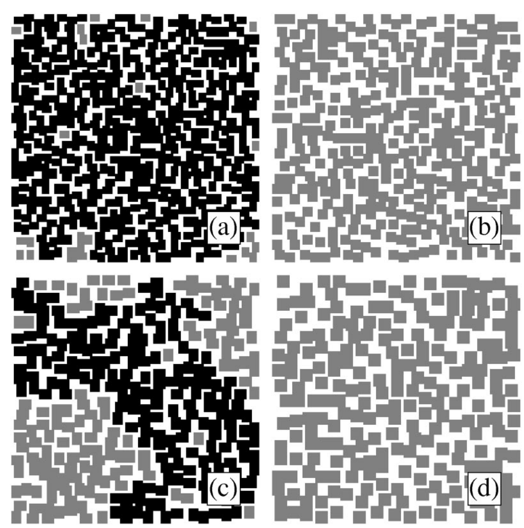

FIG. 1. Illustrations of random packing configurations on the square lattice of linear size $L=100$ for rectangular particles of sizes (a) 3×4 (0.714), (b) 4×4 (0.649), (c) 4×5 (0.684), and (d) 5×5 (0.630). The corresponding asymptotic packing fractions are reported in parentheses. The percolating clusters are shown in black, the remaining finite clusters in gray, and white indicates the unoccupied lattice sites.

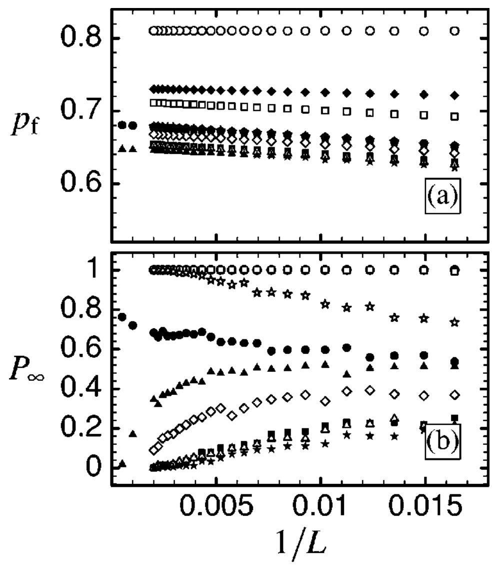

FIG. 2. Plot of (a) packing fractions p_f and (b) percolation probabilities P_∞, for rectangular particles of sizes $4\times m$ versus the inverse of the lattice size L, in the cases $m=1$ (open circles), $m=2$ (full diamonds), $m=3$ (open squares), $m=4$ (full triangles), $m=5$ (open stars), $m=6$ (full circles), $m=7$ (open diamonds), $m=8$ (full squares), $m=9$ (open triangles), and $m=10$ (full stars). Averages are performed over 1000 realizations each.

Additionally, one can either forbid or allow the particles to be partially outside the lattice. In our quantitative analysis we have adopted the first criterion. By allowing the particles to exceed the boundaries of the lattice, we have verified that the asymptotic values obtained for both p_f and P_∞ remain unchanged.

As an illustration, we show in Fig. 1 four typical configurations obtained for the lattice size $L=100$, and particle sizes (a) 3×4, (b) 4×4, (c) 4×5, and (d) 5×5. The black color indicates a percolating cluster, i.e., a cluster of particles in contact that spans the whole system, connecting opposite sides of the lattice. The remaining finite clusters are indicated in light gray color. Surprisingly, a percolating cluster is found in the cases (a) and (c), i.e., for sizes 3×4 and 4×5, whereas as expected only finite clusters exist for 4×4 and 5×5. It is interesting to notice that a small particle anisotropy (here illustrated for the case 3×4 and 4×5) favors percolation. To establish whether this behavior holds asymptotically, in the limit $L\rightarrow\infty$, we have studied larger system sizes, up to $L=2000$, and plotted the percolation probability P_∞ versus $1/L$. When $L\rightarrow\infty$, P_∞ tends either to zero (only finite clusters exist) or it tends to one (an infinite cluster exists).

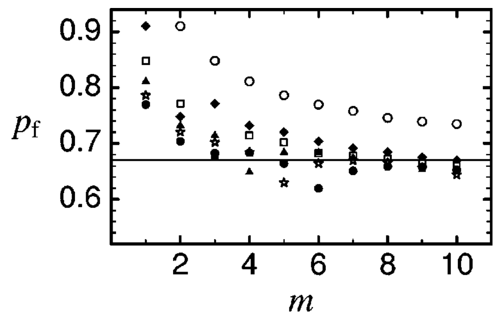

FIG. 3. Plot of the asymptotic packing fractions p_f for rectangular particles of sizes $n\times m$ versus the linear size m, in the cases $n=1$ (open circles), $n=2$ (full diamonds), $n=3$ (open squares), $n=4$ (full triangles), $n=5$ (open stars), and $n=6$ (full circles). The horizontal line indicates the value $p_f^c=0.67$, corresponding to our estimate for the critical value of the packing fraction. Averages are performed over 1000 realizations each.

The small $1/L$ (large L) behavior of P_∞ is evident from the plots shown in Fig. 2, where the packing fractions p_f and percolation probabilities P_∞ are shown as a function of the inverse lattice size $1/L$, for particle sizes $4\times m$ with $1\leqslant m\leqslant 10$. While the packing fraction displays an almost linear dependence on $1/L$, the percolation probability P_∞ shows a less trivial behavior. In some cases, as for $m=4$, 6, and 7, the asymptotic limit (either 0 or 1) is observed only for very large L values, indicating a rather large correlation length in the system, reminiscent of a critical behavior.

TABLE I. Table of the asymptotic packing fractions p_f for rectangular particles of size $n\times m$. The error bars for the present values are estimated to be ± 0.010 in all cases (except for the trivial case 1×1).

$m\backslash n$	1	2	3	4	5	6	7	8	9	10
1	1	0.910	0.848	0.811	0.786	0.770	0.758	0.746	0.739	0.735
2	0.910	0.748	0.771	0.732	0.720	0.704	0.692	0.685	0.675	0.670
3	0.848	0.771	0.679	0.714	0.702	0.683	0.678	0.672	0.664	0.660
4	0.811	0.732	0.714	0.649	0.684	0.683	0.669	0.660	0.658	0.652
5	0.786	0.720	0.702	0.684	0.630	0.664	0.667	0.666	0.657	0.644
6	0.770	0.704	0.683	0.683	0.664	0.620	0.651	0.659	0.658	0.653
7	0.758	0.692	0.678	0.669	0.667	0.651	0.608	0.638	0.650	0.653
8	0.746	0.685	0.672	0.660	0.666	0.659	0.638	0.601	0.631	0.644
9	0.739	0.675	0.664	0.658	0.657	0.658	0.650	0.631	0.600	0.626
10	0.735	0.670	0.660	0.652	0.644	0.653	0.653	0.644	0.626	0.589

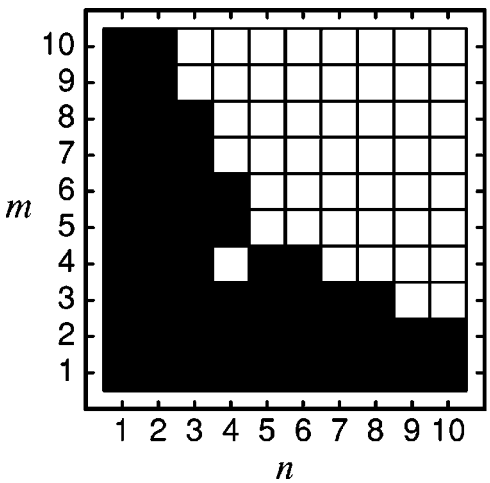

FIG. 4. Phase diagram for the asymptotic packing fractions p_f and percolation probabilities P_∞, for rectangular particles of sizes $n\times m$. White indicates the case $p_f<p_f^c$ and $P_\infty=0$, whereas black indicates the case $p_f>p_f^c$ and $P_\infty=1$.

To make this finding more quantitative and to elucidate whether our system is characterized by a percolation threshold p_f^c, in the sense that an infinite cluster exists when $p_f>p_f^c$ and no percolating cluster occurs when $p_f<p_f^c$, *independently* of both n and m, we have performed extensive simulations for n and m in the range $1\leqslant n$, $m\leqslant 10$. The results for the asymptotic packing fractions p_f, obtained by linear fitting p_f as a function of $1/L$ and taking $1/L\to 0$, for $1\leqslant n\leqslant 10$ and $1\leqslant m\leqslant 6$ are displayed in Fig. 3. The numerical data for p_f for particle sizes $1\leqslant n$, $m\leqslant 10$ are shown in Table I.

For the lattice sizes considered, one generally observes that for any particle size $n\times m$ in the range $1\leqslant n$, $m\leqslant 10$, P_∞ clearly tends to 0 or 1 for large systems. The behavior of P_∞ for a given pair of values (n,m) is found to be strongly related to the respective quantity p_f: In all cases where $p_f<0.67$, we find $P_\infty\to 0$ as $L\to\infty$, while when $p_f\geqslant 0.67$ the limit $P_\infty\to 1$ is obtained for $L\to\infty$. Thus, we estimate the packing fraction threshold to be $p_f^c=0.67\pm 0.01$. The behavior of p_f and P_∞ can be summarized in a ''phase diagram'' as shown in Fig. 4.

To conclude, we have shown that the packing fraction p_f of rectangular particles on a square lattice plays a similar role as the occupation probability p in standard percolation, in the sense that there is a critical packing fraction p_f^c such that for $p_f<p_f^c$ only finite clusters exist, while for $p_f>p_f^c$ a percolating cluster spans the lattice. In contrast to the occupation probability p in standard percolation, however, the quantity p_f cannot be chosen arbitrarily, but is a result of the packing process and has to be determined *a posteriori* for a given shape and particle size. We note that the obtained value $p_f^c=0.67\pm 0.01$ is consistent with the critical concentration for continuum percolation of overlapping objects ($p_c\cong 0.6766$, as obtained for disks [5]) in two dimensions. Our finding of a critical packing fraction for rectangular particles, which does not depend on their size, is supported by the fact that in two dimensions the continuum percolation threshold p_c is believed to be independent of the form of the overlapping (convex) objects considered (cf. [6,7] and references therein). Since the packing fraction itself is a much easier quantity to determine than the percolation probability, our result suggests a simple criterion to establish whether a system of particles of arbitrary (convex) shape will percolate or not. The possibility that the critical value $p_f^c\cong 0.67$, obtained here for rectangular particles on the square lattice, holds also for other particle shapes and lattice types remains to be investigated.

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