Optimal Packings of Superdisks and the Role of Symmetry

Y. Jiao,[1] F. H. Stillinger,[2] and S. Torquato[2,3,4,5]

[1]*Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544, USA*
[2]*Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA*
[3]*Program in Applied and Computational Mathematics, Princeton University, Princeton, New Jersey 08544, USA*
[4]*School of Natural Sciences, Institute for Advanced Study, Princeton, New Jersey 08540, USA*
[5]*Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA*
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Almost all studies of the densest particle packings consider convex particles. Here, we provide exact constructions for the densest known two-dimensional packings of superdisks whose shapes are defined by $|x_1|^{2p} + |x_2|^{2p} \le 1$ and thus contain a large family of both convex ($p \ge 0.5$) and concave ($0 < p < 0.5$) particles. Our candidate maximal packing arrangements are achieved by certain families of Bravais lattice packings, and the maximal density is nonanalytic at the "circular-disk" point ($p = 1$) and increases dramatically as p moves away from unity. Moreover, we show that the broken rotational symmetry of superdisks influences the packing characteristics in a nontrivial way.

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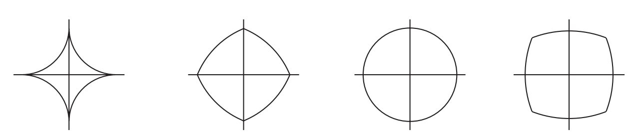
Packing problems, such as how densely a large collection of nonoverlapping particles can fill space, have been of perennial interest to physicists, engineers, and mathematicians [1–8]. A basic property of a packing is the density ϕ, defined as the fraction of space covered by the particles, which is bounded from above by the maximal density $\phi_{\max}$. Dense packings are intimately related to the structure of low-temperature phases of matter, including liquids, glasses, and crystals [1–3] as well as heterogeneous materials [3] and granular media [4]. Finding the maximally dense arrangement of congruent particles located on the sites of a Bravais lattice is one of the basic problems in the geometry of numbers [5,6]. The densest packings in very high Euclidean dimensions are intimately related to the best way of transmitting stored data through a noisy channel [6].

In d-dimensional Euclidean space $\mathbb{R}^d$, packings of congruent spherical particles for $d = 2$ and $d = 3$ provide the few examples of nontiling particles whose maximally dense arrangements can be proved. It is known that the triangular and face-centered cubic lattice packings have the maximal packing density for circular disks ($\phi_{\max} = \pi/\sqrt{12}$) and spheres ($\phi_{\max} = \pi/\sqrt{18}$) [7], respectively. However, very few rigorous results exist for the densest packings of congruent nonspherical particles. For ellipses ($d = 2$), the provably densest packing ($\phi_{\max} = \pi/\sqrt{12}$) is constructed by an affine transformation of the triangular-lattice packing of circular disks [6], which can also be obtained by enclosing each ellipse with a hexagon with minimum area that tessellates the space [9,10]. For ellipsoids ($d = 3$), the densest known packing ($\phi_{\max} \approx 0.77$) is achieved by crystal packings of congruent ellipsoids in which each ellipsoid has contact with 14 others [10]. Recently, Conway and Torquato [11] constructed the densest known packings of regular tetrahedra, and Trovato *et al.* [12] have found dense packings of truncated cones possessing uniaxial symmetry.

Virtually all systematic investigations of the densest particle packings have been carried out for convex objects. In this Letter, we construct the densest known two-dimensional packings of superdisks (defined below) in the plane, which provides a wide class of packings of both convex and concave particles. An analysis of our candidate maximally dense packings reveals that the broken rotational symmetry of superdisks influences the packing characteristics in a nontrivial way that is distinctly different from ellipse (ellipsoid) packings.

A d-dimensional *superball* is a centrally symmetric body in d-dimensional Euclidean space occupying the region $|x_1|^{2p} + |x_2|^{2p} + \cdots + |x_d|^{2p} \le 1$, where x_i ($i = 1, \ldots, d$) are Cartesian coordinates and $p \ge 0$ is the *deformation parameter*, which indicates to what extent the particle shape has deformed from that of a d-dimensional sphere ($p = 1$). In particular, a *superdisk* G is our designation for the two-dimensional case ($d = 2$). When $p = 1$, the superdisk is just a circle. As p continuously increases from 1 to ∞, a family of superdisks with square symmetry is obtained. As p decreases from 1 to 0.5, another family of square-symmetric superdisks is obtained, but with the symmetry axes rotated 45 degrees with respect to that of the first family (see Fig. 1). At the limiting points $p = \infty$ and $p = 0.5$, the superdisk becomes a perfect square. When $p < 0.5$, the superdisk is concave and becomes a *cross* in the limit $p \to 0$.

Here, we construct the densest known packings of both convex and concave superdisks. For convex superdisks, we



(a) p = 0.45 (b) p = 0.75 (c) p = 1.0 (d) p = 2.0

FIG. 1. Superdisks with different deformation parameter p.

demonstrate that the maximal packing density $\phi_{\max}$ significantly increases as p changes from unity, i.e., as one moves off the circle point. For $p \neq 1$, the rotational symmetry of a circular-disk is broken (see Fig. 1), which results in a cusp in $\phi_{\max}$ at $p = 1$; i.e., the initial increase of $\phi_{\max}$ is linear in $|p - 1|$, and thus $\phi_{\max}$ is a nonanalytic function of p at $p = 1$. Note that for ellipse packings, $\phi_{\max}$ is not influenced by the broken rotational symmetry introduced by stretching the optimal circle packing along a particular direction, which maintains six contacts per particle, and thus no improvement over the maximal circle density is possible. For superdisks, one can take advantage of the fourfold rotationally symmetric shape of the particle by arranging them on the sites of certain lattices to obtain a dramatic improvement on the maximal circle packing density. By contrast, one needs to use higher-dimensional counterparts of ellipsoids ($d \geq 3$) in order to improve on $\phi_{\max}$ for spheres [10]. Even for three-dimensional ellipsoids, $\phi_{\max}$ increases smoothly as the aspect ratios of the semiaxes vary from unity and hence has no cusp at the sphere point [13]. Thus, optimal superdisk packings possess packing characteristics that are *distinctly* different from optimal ellipse (or ellipsoid) packings for reasons detailed below.

We use a recently developed event-driven molecular dynamics (MD) packing algorithm to guide us to obtain the analytical construction of the densest packings of *convex* superdisks [15]. The MD simulation technique generalizes the Lubachevsky-Stillinger (LS) sphere-packing algorithm [16] to the case of other centrally symmetric convex bodies (e.g., ellipsoids and superballs). Initially, small superdisks are randomly distributed and randomly oriented in a box (fundamental cell) with periodic boundary conditions and without any overlap. The superdisks are given translational and rotational velocities randomly, and their motion followed as they collide elastically and also expand uniformly, while the fundamental cell deforms to better accommodate the packing. After some time, a jammed state with a diverging collision rate γ is reached and the density reaches a locally maximum value.

Extensive experience with spheres and circular disks has shown that, for reasonably large packings, a sufficiently slow growth rate leads to jammed packings that are very near the densest arrangements, i.e., face-centered-cubic lattice and triangular-lattice, respectively [17,18]. However, to obtain perfect crystalline packings from such simulations, one needs to know the "magic number" of particles to use in a particular simulation box *a priori*, which generally is not possible. We note that in two dimensions, because the densest local packing of circular disks (an equilateral triangle with three circular disks centered at its corners) can tessellate the space, large packings of circular disks are usually nearly completely crystallized; i.e., they contain grains of circular disks on a triangular lattice and dislocations, even when a moderate expansion rate is used. We find from simulations that this is also true for packings of superdisks, which implies that the densest equilibrium state (densest packing) of convex superdisks is consistent with the structure of the densest local clusters that tessellate space. Thus, we should be able to identify the densest packings of superdisks by running the simulations for relatively small packings and experimenting with a wide range of particle numbers in the fundamental cell to find the "magic number."

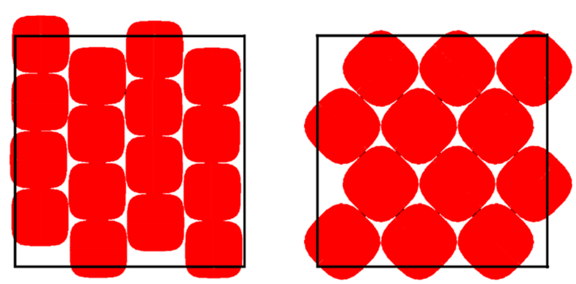
Two types of highly dense lattice packings of convex superdisks emerge from the simulations (see Fig. 2), which are run for a variety of different values of deformation parameter p. Importantly, we do not exclude the possibility of the existence of denser periodic packings with a complex particle basis, although we did not find any such packings from our simulations. Subsequent analytical calculations suggested by these simulation results led us to the following conclusion: there are two families of Bravais lattices Λ_0 and Λ_1, consistent with the symmetry of superdisk G, one of which will give the densest packing of G for different values of deformation parameter p ($0.5 < p < \infty$). In the densest packings, each superdisk has six contacting neighbors. The lattice vectors of Λ_0 and Λ_1 are $\mathbf{e}_1 = 2\mathbf{i}$, $\mathbf{e}_2 = \mathbf{i} + (2^{2p} - 1)^{1/2p}\mathbf{j}$ and $\mathbf{e}_1 = 2^{(1-1/2p)}\mathbf{i} + 2^{(1-1/2p)}\mathbf{j}$, $\mathbf{e}_2 = (2^{-1/2p} - 2^{1/2}s)\mathbf{i} + (2^{-1/2p} + 2^{1/2}s)\mathbf{j}$, respectively, where $\mathbf{i}$, $\mathbf{j}$ are unit vectors along x_1- and x_2-directions, and s is the smallest positive root of the following equation: $|2^{-(1+1/2p)} - 2^{-1/2}s|^{2p} + |2^{-(1+1/2p)} + 2^{-1/2}s|^{2p} = 1$.

The maximal packing density as a function of p (see Fig. 3) is explicitly given by

$$\phi_{\max} = \frac{4}{|\mathbf{e}_1||\mathbf{e}_2|\sin\theta}\int_0^1 (1 - x^{2p})^{1/2p}dx, \qquad (1)$$

where $\theta = \cos^{-1}[\mathbf{e}_1 \cdot \mathbf{e}_2/(|\mathbf{e}_1||\mathbf{e}_2|)]$. When $p \in (1, p^*)$, $\mathbf{e}_i$ ($i = 1, 2$) are the lattice vectors of Λ_0; otherwise, they are the lattice vectors of Λ_1. At $p^* \approx 1.286$, the two distinct lattice packings have the same density, i.e., $\phi^*_{\max} \approx 0.916$. Figure 3 shows that $\phi_{\max}$ increases dramatically as p moves away from the circle point ($p = 1$).

As the deformation parameter p changes from unity, the continuous rotational symmetry of circular disks is broken;



(a) Λ_0-lattice packing (b) Λ_1-lattice packing

FIG. 2 (color online). Two types of lattice packings of superdisks that have the maximal packing density for different deformation parameter p. In the figures (a) and (b), $p = 2.0$ and $p = 1.5$, respectively. In both cases, Λ_1 packing is denser. The boundaries of the simulation box are shown by dark lines.

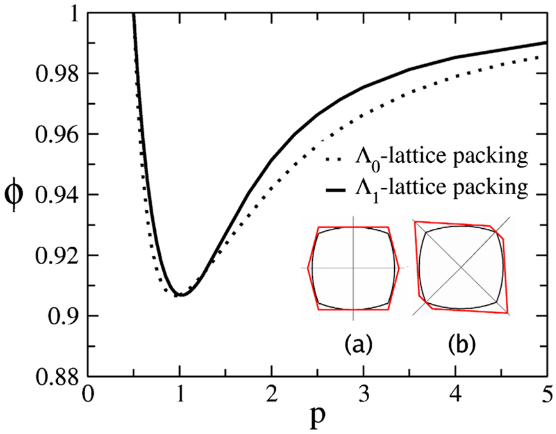


FIG. 3 (color online). Density versus deformation parameter p for the $\Lambda_0$lattice and Λ_1-lattice packings of superdisks. Inserts: The enclosing cells C_0 (a) and C_1 (b) of the superdisks with $p = 2.0$ for Λ_0 lattice and Λ_1 lattice, respectively.

i.e., superdisks only possess fourfold rotational symmetry. The broken symmetry of superdisks affects the maximal packing density $\phi_{\max}(p)$ in a nontrivial way. There are two discontinuities of the derivative $\phi'_{\max}(p)$: at $p = 1$ and $p = p^*$ (see Fig. 3). Thus, as p changes from 1, $\phi_{\max}$ will increase in a cusplike manner. By expanding $\phi_{\max}(p)$ around $p = 1$, we get

$$\phi_{\max} = \phi_0[1 + a_-(p - 1) + \mathcal{O}((p - 1)^2)] \quad (2)$$

for $p \le 1$ and

$$\phi_{\max} = \phi_0[1 + a_+(p - 1) + \mathcal{O}((p - 1)^2)] \quad (3)$$

for $p \ge 1$, where $\phi_0 = \pi/\sqrt{12}$ is the density of triangular-lattice packing of circular disks; $a_- = (1/3) \times \ln 2 + (1/\sqrt{3}) \ln(2 + \sqrt{3}) - 1 = -0.0086\ldots$ and $a_+ = (2/3) \ln 2 + (1/2) \ln 3 - 1 = 0.0114\ldots$ are the derivatives of $\phi_{\max}$ [Eq. (1)] at $p = 1$ as p approaches from left and right, respectively. The initial increase in $\phi_{\max}$ is linear in $|p - 1|$; i.e., $\phi_{\max}$ is nonanalytic at $p = 1$, which we have noted is not true for either optimal ellipse or ellipsoid packings as one moves off the circle or sphere points, respectively [13]. The fourfold symmetry of a superdisk results in a value of $\phi_{\max}$ that is always above that for the optimal circle packing for any convex shape $p \neq 1$, which is to be contrasted to optimal ellipse packings that have the same maximal density of circles for any aspect ratio.

The other discontinuity at $p = p^*$ corresponds to a jumplike change of the packing structure. In particular, as p increases from 1 (the Λ_0 and Λ_1 lattices coincide at $p = 1$), the packing lattice continuously deforms from the triangular lattice to the Λ_0 lattice till $p = p^*$, where the packing lattice "jumps" from the Λ_0 lattice to the Λ_1 lattice and then proceeds to deform continuously. This is because the superdisk fits the "enclosing cell" (defined below) of the Λ_1 lattice better when p exceeds p^*. Note that superdisks with $p = p^*$ have a twofold degenerate crystalline ground state; i.e., the Λ_0-lattice and Λ_1-lattice packings of these particles have the same density.

Analysis of the packing structure is necessary to understand the aforementioned effects of broken symmetry. We define the *enclosing cell C* of a superdisk to be the polygon whose edges are common tangent lines of the superdisk and its contacting neighbors (see the inserts of Fig. 3). For a particular lattice packing, the enclosing cells for all superdisks are the same and tessellate space. As p varies, the enclosing cell for a particular lattice also deforms continuously, i.e., from a regular hexagon to a square as p increases from 1 to ∞, respectively.

For fixed p, the denser lattice packing is the one with the smaller enclosing cell. The two cells C_0 and C_1 (associated with the Λ_0 and Λ_1 lattices, respectively) accommodate the curvature around the boundary point $(2^{-1/2p}, 2^{-1/2p})$ and its images, and $(1, 0)$ and its images better, to give a higher local density. When p is slightly larger than 1, the curvature around point $(2^{-1/2p}, 2^{-1/2p})$ and its images is dominant, and the denser packing is given by Λ_0 lattice. As p increases, the curvature around point $(1, 0)$ and its images becomes dominant; thus, the denser packing jumps to Λ_1 lattice. For $0.5 \le p \le 1$, the curvature around point $(1, 0)$ is always dominant, and so the Λ_1 lattice gives the denser packing.

Now, we generalize the analysis above to the case of concave superdisks $(0 < p < 0.5)$ [cf. Figure 1(a)]. To construct such candidate maximally dense packings, we attempt to minimize exclusion-volume effects. For each concave superdisk, we consider the convex enclosing box that has the smallest area among all convex boxes that contain the particle, which is a square in this case. First, we construct the densest packing of the convex enclosing boxes, i.e., stacks of square chains. Then, we allow these square chains to overlap as much as possible without violating the interparticle impenetrability constraints.

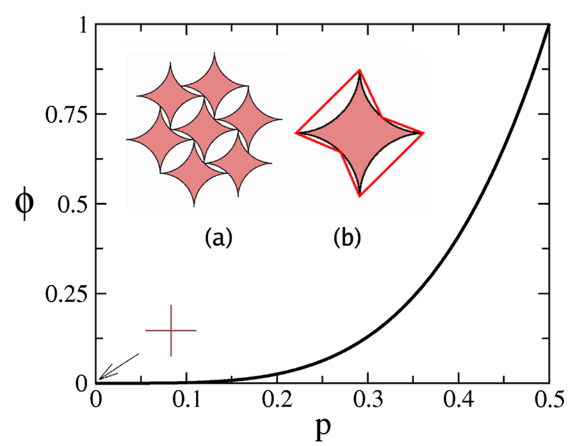


FIG. 4 (color online). Density versus deformation parameter p of the constructed lattice packings of concave superdisks. Inserts: (a) The packing arrangement for the case $p = 0.45$ and (b) the corresponding enclosing cell for a particle. In the limit $p \to 0$, a superdisk becomes a "cross."

This also maximizes the number of contact neighbors for every concave superdisk. In this way, we can construct a family of dense lattice packings of concave superdisks in which each particle has an hour-glass-like concave enclosing box [see the insert (b) of Fig. 4] and six contacting neighbors. The constructed lattice packings of concave superdisks have the symmetry of the Λ_1-lattice packings of convex superdisks and the lattice vectors are $\mathbf{e}_1 = (2^{-1/2p} + 1)\mathbf{i} + 2^{-1/2p}\mathbf{j}$, $\mathbf{e}_2 = 2^{-1/2p}\mathbf{i} + (2^{-1/2p} + 1)\mathbf{j}$.

As p decreases from 0.5, the concave particle shrinks, and the lattice for the optimal packing deforms continuously; in the limit $p \to 0$, the superdisks become "crosses" with vanishing area and packing density. However, the *number density* of the lattice packing we constructed is *twice* that of the square-lattice packing of crosses, whose enclosing box is a square. The packing density of our concave superdisk packings [given by Eq. (1)] is shown in Fig. 4 [19]. Our results for $\phi_{\max}$ exhibit another discontinuity in the derivative at $p = 0.5$ [20]. We emphasize that we cannot rule out the existence of denser periodic packings of such concave particles.

In summary, we have found exact constructions for the densest known packings of both convex and concave superdisks ($0 < p < \infty$), which are achieved by one of two families of lattice packings, i.e., Λ_0-lattice and Λ_1-lattice packings. The result for convex superdisks is consistent with a famous conjecture by Minkowski in geometry of numbers [5,21]. We also showed that the increase of maximal packing density is initially linear in $|p - 1|$; $\phi_{\max}(p)$ has a cusp at $p = 1$ and has another discontinuity in its derivative $\phi'_{\max}(p)$ at $p = p^*$, which are effects of the broken symmetry of superdisks. These features of the superdisk system make it distinctly different from optimal ellipse packings. Interestingly, the result that $\phi_{\max}$ appreciably increases as p varies from unity is also consistent with the dramatic improvement on the lower bound on $\phi_{\max}$ of superballs relative to that for spheres in arbitrarily high dimensions found by Elkies, Odlyzko, and Rush [22]. The optimal Bravais lattice packings of the superdisk for a particular value of p are also the corresponding densest crystal phase states of superdisks in equilibrium. Therefore, our findings provide a starting point to quantify the entire crystal phase behavior of superdisk systems and their nonequilibrium packing characteristics, which should deepen our understanding of the statistical thermodynamics of nonspherical hard particles. Such superdisks can be experimentally mass produced using current lithography techniques.

In future work, we will study both ordered and disordered packings of superballs and superellipsoids in three dimensions, focusing on their "jamming" characteristics [23,24] and the effect of broken symmetry. We expect that increasing the dimensionality of the particle will imbue the optimal packings of "superballs" or "superellipsoids" with structural characteristics that are richer than their two-dimensional counterparts.

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