

Dense Packings of Superdisks and the Role of Symmetry

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Abstract

We construct the densest known two-dimensional packings of superdisks in the plane whose shapes are defined by $|x|^{2p} + |y|^{2p} \leq 1$, which contains both convex-shaped particles ($p \geq 0.5$, with the circular-disk case $p = 1$) and concave-shaped particles ($0 < p < 0.5$). The packings of the convex cases with $p \geq 1$ generated by a recently developed event-driven molecular dynamics (MD) simulation algorithm [Donev, Torquato and Stillinger, J. Comput. Phys. **202** (2005) 737] suggest exact constructions of the densest known packings. We find that the packing density (covering fraction of the particles) ϕ increases dramatically as the particle shape moves away from the "circular-disk" point ($p = 1$). In particular, we find that the maximal packing densities of superdisks for certain $p \neq 1$ are achieved by one of the two families of Bravais lattice packings, which provides additional numerical evidence for Minkowski's conjecture concerning the critical determinant of the region occupied by a superdisk. Moreover, our analysis on the generated packings reveals that the broken rotational symmetry of superdisks influences the packing characteristics in a non-trivial way. We also propose an analytical method to construct dense packings of concave superdisks based on our observations of the structural properties of packings of convex superdisks.

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Packing problems, such as how densely given solid objects can fill d -dimensional Euclidean space \mathbb{R}^d , have been a source of fascination to mathematicians and scientists for centuries, and continue to intrigue them today. A basic characteristic of a packing (a large collection of nonoverlapping particles) is the packing density ϕ , defined as the fraction of space covered by the particles. Estimation of the maximal packing density (the maximal fraction of space covered by the particles) ϕ_{max} of a given nonoverlapping body arranged on the sites of a Bravais lattice (i.e., a Bravais lattice packing) is one of the basic problems in the geometry of numbers [1, 2]. Dense packings of nonoverlapping (hard) particles have served as useful models to understand the structure of a variety of many-particle systems, such as liquids, glasses, crystals, heterogeneous materials and granular media [3, 4, 5, 6]. Packing problems in dimensions higher than three are intimately related to the best way of transmitting stored data through a noisy channel [2].

A problem of great interest is the determination of the densest arrangement(s) of such particles and the associated density ϕ_{max} . Packings of congruent circular disks in two dimensions and spheres in three dimensions have been intensively studied. It has been proved that the triangular lattice and face-centered cubic lattice have the maximal packing density for circular disks ($\phi_{max} \approx 0.91$) and spheres ($\phi_{max} \approx 0.74$) [7], respectively. Some progress has been made to identify good candidates for the densest packings when the particles have a size distribution [5], but primarily in two dimensions [8, 9, 10]. However, very few results are known for the densest packings of nonspherical particles. For ellipses ($d = 2$), the densest packing is constructed by an affine transformation of the triangular-lattice packing of circular disks ($\phi_{max} \approx 0.91$) [2], which can also be obtained by enclosing each ellipse with a hexagon with minimum area that tessellates the space [11, 12]. For ellipsoids ($d = 3$), the maximal known packing density ($\phi_{max} \approx 0.77$) is achieved by crystal packings of congruent ellipsoids in which each ellipsoid has contact with 14 others [12]. Recently, Conway and Torquato [13] constructed the densest known packings of regular tetrahedra. Little is known about the densest packings of other nonspherical particles, such as “superballs”, as we will explain below.

A particle is centrally symmetric if it has a center P that bisects every chord through P connecting two boundary points of the particle. A particle is convex if the entire line segment connecting two points of the particle also belongs to the particle. A d -dimensional *superball* is a centrally symmetric convex body in d -dimensional Euclidean space occupying

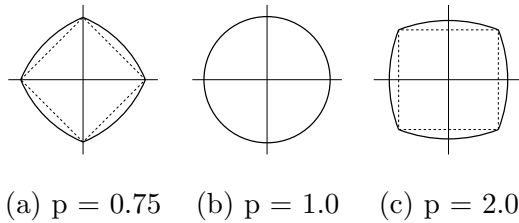


FIG. 1: Superdisks with different deformation parameter p .

the region

$$|x_1|^{2p} + |x_2|^{2p} + \cdots + |x_d|^{2p} \leq 1, \quad (1)$$

where x_i ($i = 1, \dots, d$) are Cartesian coordinates and $p \geq 0.5$ is the *deformation parameter*, which indicates to what extent the shape of the particle has deformed from an d -dimensional sphere. In particular, a *superdisk* G is defined by

$$|x|^{2p} + |y|^{2p} \leq 1, \quad (2)$$

where (x, y) are Cartesian coordinates. When $p = 1$, the superdisk is just a circular disk. As p continuously increases from 1 to ∞ , one can get a family of superdisks with square symmetry; as p decreases from 1 to 0.5, one can get another family of superdisks still possessing square symmetry, but the symmetry axes rotate 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 becomes concave. In the following, we simply refer to convex superdisks as “superdisks” for convenience; and all concave superdisks are explicitly referred to as “concave superdisks” to avoid confusion.

The study of packings of superdisks dates back to Minkowski [14], who formulated the problem in the language of the geometry of numbers. Thus, it is necessary for us to briefly introduce some basic definitions and notions in the geometry of numbers (for a general discussion of this subject, see [1]). A Bravais lattice Λ in \mathbb{R}^d is a subgroup consisting of the integer linear combinations of the vectors that constitute a basis for \mathbb{R}^d . Henceforth, we will simply refer to “Bravais lattice” as “lattice” for convenience. A lattice packing of identical centrally symmetric particles is one in which the centers of such nonoverlapping particles are located at the lattice points of Λ . In a two-dimensional lattice packing of superdisks,

the space \mathfrak{R}^2 can be geometrically divided into identical regions F called fundamental cells, each of which contains the center of just one superdisk. An admissible lattice of a region is the one that has no lattice points in the region except for the origin. The critical lattice of a region is the admissible lattice whose fundamental cell has the smallest volume. Minkowski [14] conjectured that there are two families of G -admissible lattices Λ_0 and Λ_1 , consistent with the symmetry of superdisk G , one of which will be the critical lattice Λ_c of G for different values of deformation parameter p ($0 < p < \infty$), i.e.,

$$\Delta_c(G) = \min(\Delta_0, \Delta_1), \quad (3)$$

where Δ_i is the volume of the fundamental cell of lattice Λ_i ($i = c, 0, 1$); both Λ_0 and Λ_1 have six points on the boundary of G , and $(1, 0) \in \Lambda_0$, $(2^{-1/2p}, 2^{-1/2p}) \in \Lambda_1$ (the lattices are defined uniquely under these conditions). It has been shown that the critical lattice of G gives the densest lattice packing of $\frac{1}{2}G$ [1], which is defined by

$$|x|^{2p} + |y|^{2p} \leq \frac{1}{2^{2p}}. \quad (4)$$

Many works that followed were devoted to this conjecture [15, 16, 17, 18, 19, 20, 21, 22, 23]. In particular, Davis obtained the proper intervals of p , in which one of the families of lattices is the critical lattice [15], i.e., there exists a constant p_0 , with $1.285 < p_0 < 1.29$, such that

$$\Delta_c(G) = \begin{cases} \Delta_1 & 0.5 \leq p \leq 1, p \geq p_0, \\ \Delta_0 & 1 \leq p \leq p_0. \end{cases} \quad (5)$$

Mordell proved the conjecture for $p = 4$ [16]; and Malyshev et al. [23] proved the conjecture for $p \geq 6$ using a parametrization method introduced by Cohn [17]. In addition, Kukharev worked out a method for examination of Minkowski's conjecture for every specific p (except for p near 0.5, 1 and p_0) and checked the conjecture for $p = 0.65, 0.7, 0.75, 0.8, 0.85, 1.1, 1.15, 1.5, 2.0, 2.5$ [21, 22]. Note that the validity of the conjecture for the trivial cases when $p = 0.5$ or ∞ (square) and $p = 1$ (circular disk) are well known.

Recently, Elkies et al. [24] obtained improvements to the Minkowski-Hlawka bound [25] on the maximal lattice-packing density for many centrally symmetric convex bodies by generalizing the method proposed by Rush [26] for convex bodies symmetrical through the

coordinate hyperplanes. In particular, Elkies et al. showed that for very large dimensions ($d \rightarrow \infty$), a small change of p from unity can give an exponential improvement on the lower bound of the maximal lattice-packing density of superballs.

The results in Ref.[24] motivates us to consider whether or not such a dramatic improvement of packing density could actually occur in low dimensions (e.g., $d = 2, 3$). Here we construct the densest known packings of superdisks suggested by MD simulations and show that one can also get a significant increase of the maximal packing density ϕ_{max} of superdisks as p changes from unity, i.e., as one moves off the circular-disk point. For $p \neq 1$, the rotational symmetry of a circular disk is broken (see Fig. 1), which results in a cusp in ϕ_{max} at $p = 1$, i.e., the initial increase of ϕ_{max} is linear in $|p - 1|$. We note that the mechanism of increasing the density of superdisk packings is different from that for random packings of ellipses or random and crystal packings of ellipsoids [12, 27], in which a larger average number of contacts for each particle than that in sphere packings is required. The densest Bravais lattice packing of ellipses (ellipsoids), in which the six (twelve) contacts per particle is maintained, does not give an improvement on the maximal packing density. However, one can take advantage of the four-fold rotational symmetry of superdisks, i.e., arrange them with proper orientations on the sites of certain lattices, to construct packings with a dramatically improved density but with six contacts per particle.

We use a recently developed event-driven molecular dynamics (MD) algorithm to generate dense (ordered and disordered) packings of superdisks [28]. The MD simulation technique generalizes the Lubachevsky-Stillinger (LS) sphere-packing algorithm [29] 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 (unit 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 unit 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 maximum value.

Our aim is to produce dense packings of superdisks and to identify the densest packing structures if possible. Extensive experience with spheres and circular disks has shown that, for reasonable large packings, sufficiently slowing down the growth of the density, so that the hard-particle system remains close to the equilibrium solid branch of the equation of state,

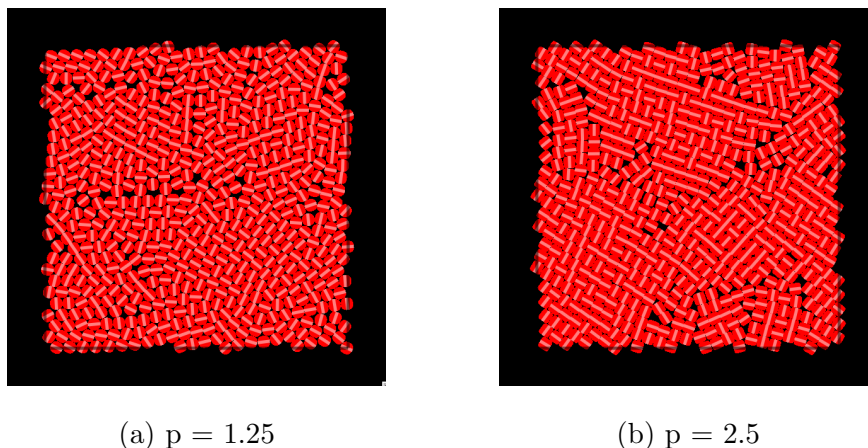


FIG. 2: Large packings of superdisks with different deformation parameters generated by MD simulation. The number of particles in the unit cell is $N = 625$. The white “chord” in each superdisk indicates one of its symmetry axes. The boundaries of the simulation box are shown by dark lines.

leads to packings near the face-centered-cubic lattice and triangular lattice, respectively [30, 31]. However, this requires impractically long simulation times for large superdisk packings. We note that in two dimensions, because the densest local packing of circular disks (a 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 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 (see Fig. 2), which implies the densest equilibrium state (densest packing) of superdisks is consistent with the structure of the densest local clusters that tessellate space. Thus, we should be able to identify the *possible* densest packings of superdisks by running the simulation for unit cells with a small number of particles (e.g., from 4 to 16 particles).

Two types of lattice packings of superdisks, which gives the maximal packing density among all packings generated by simulations for different values of deformation parameter p , are shown in Fig. 3. Note that we do not exclude the possibility of the existence of denser periodic packings with complex basis, although we didn’t find any of these packings by examining the dense grains of large packings of superdisks, which would contain denser clusters if they exist. Given that the superdisks are defined by Eq. (4), it is clear that the

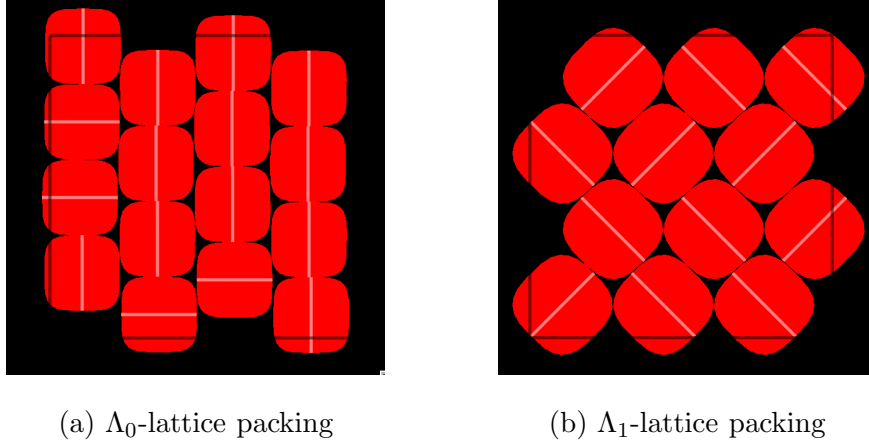


FIG. 3: Two types of lattice packings of superdisks that have the maximal packing density for different deformation parameter p . In the figures (a) and (b), $p = 2.0$ and $p = 1.5$, respectively. In both cases Λ_1 -packing is denser. The white “chord” in each superdisk indicates one of its symmetry axes. The boundaries of the simulation box are shown by dark lines.

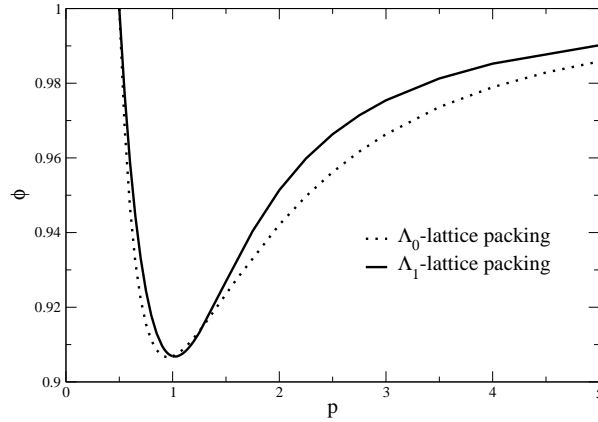


FIG. 4: Densities of Λ_0 -lattice and Λ_1 -lattice packings of superdisks as a function of deformation parameter p .

two types of lattices we found are G -admissible lattices Λ_0 and Λ_1 , respectively. Subsequent analytical calculations suggested by the simulation results gives us the packing densities as a function of p (see Fig. 4) as well as the value of p_0 , i.e., $p_0 \approx 1.2863$. As can be seen from Fig. 4, the packing density increases dramatically as p moves away from the circular-disk point ($p = 1$). It is worth noting that our MD algorithm can be employed to verify Minkowski’s conjecture for all values of $p \geq 1$ to a very high numerical accuracy in principle.

As the deformation parameter p changes from unity, the rotational symmetry of circular disks is broken, i.e., superdisks only possess four-fold rotational symmetry. Donev et al. studied the effects of broken symmetry introduced by stretching circular disks (spheres) into ellipses (ellipsoids) on the random packings of these particles [27, 32], e.g., how the average contact number and packing density change as a function of the maximum aspect ratio of the ellipses and ellipsoids. Donev et al. also constructed a family of unusually dense crystal packings of ellipsoids, by taking advantage of the broken symmetry via the new rotational degrees of freedom that result for nonspherical particles [12]. Densest packing of ellipses can be trivially obtained by an affine transformation of triangular-lattice packing of circular disks, which produces a lattice packing of ellipses with the packing density unchanged (i.e., $\phi_{max} \approx 0.91$). As stated earlier, this can be shown by enclosing each ellipses with a hexagon with the smallest area which tessellates the space [11].

The broken symmetry of superdisks, introduced by deforming the circular disks, affects the packing density in a non-trivial way. In particular, we focus on the maximal packing density ϕ_{max} , which is a property of equilibrium superdisk system in solid state, as a function of p . There are two discontinuities of the derivative $\phi'_{max}(p)$ at $p = 1$ and $p = p_0$, respectively (see Fig. 4). Thus, as p changes from 1, ϕ_{max} will increase in a cusp-like manner. By expanding $\phi_{max}(p)$ around $p = 1$, we get

$$\phi_{max} = \phi_0[1 - 0.009(p - 1) + O((p - 1)^2)] \quad (6)$$

for $0.5 \leq p \leq 1$ and

$$\phi_{max} = \phi_0[1 + 0.01(p - 1) + O((p - 1)^2)] \quad (7)$$

for $p \geq 1$, where $\phi_0 = 0.906\dots$ is the density of triangular-lattice packing of circular disks. In other words, the initial increase in the density is linear in $|p - 1|$, which is analogous to the effects of asphericity of ellipses (ellipsoids) on the density of random packings of these particles [32]. The increase of the density of packings of ellipses (ellipsoids) is related to the increase of the average number of contacts per particle. The Bravais lattice packing of ellipses, which can be obtained by an affine transformation of the triangular-lattice packing of circular disks, does not have an improvement on the maximal packing density since the six contacts per particle is maintained. Here the increase of the maximal packing density

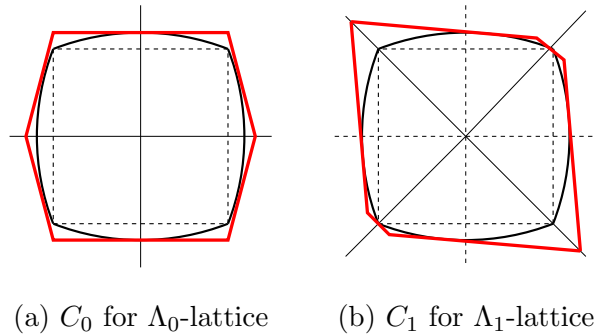


FIG. 5: The enclosing cells C_0 and C_1 of superdisk with $p = 2.0$ for Λ_0 -lattice and Λ_1 -lattice, respectively.

of superdisks with certain $p \neq 1$ is due to the fact that the four-fold rotationally symmetric shape of superdisk is more efficient for filling space, which we will discuss in detail in the following.

The other discontinuity at $p = p_0$ corresponds to a jump-like change of the packing structure that evolves as p varies. In particular, as p increases from 1 (Λ_0 -lattice and Λ_1 -lattice coincide at $p = 1$), the packing lattice continuously deforms from triangular-lattice to Λ_0 -lattice till $p = p_0$, where the packing lattice “jumps” from Λ_0 -lattice to Λ_1 -lattice and then proceeds to deform continuously. This is because the superdisk fits the enclosing cell (defined in the following) of Λ_1 -lattice better when p exceeds p_0 .

Analysis of the packing structure is necessary for understanding 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 contact neighbors (see Fig. 5). For a particular lattice packing, the enclosing cells for all superdisks are the same; this enclosing cell must be able to tessellate space. As p varies, the enclosing cell for a particular lattice also deforms continuously, e.g., from hexagon to square as p increases from 1 to ∞ .

For a fixed value of p , the denser lattice packing is the one with the smaller enclosing cell (i.e., the enclosing cell that fits the superdisk better). As can be seen in Fig. 5, the two types of enclosing cells C_0 and C_1 (associated with Λ_0 -lattice and Λ_1 -lattice, respectively) accommodate the curvature around the boundary point $(2^{-1/2p}, 2^{-1/2p})$ and its images, and $(1, 0)$ and its images better, respectively, 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

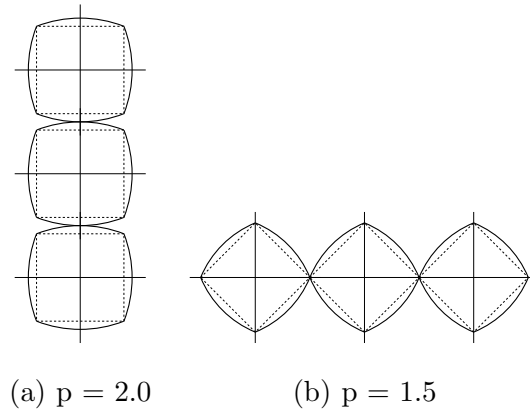


FIG. 6: Two types of superdisk chains, as the building block for lattice packings of superdisks shown in Fig. 3.

denser packing is given by Λ_0 -lattice. As p increases, the curvature around point $(1, 0)$ and its images becomes dominant, thus, the packing jumps to Λ_1 -lattice. For $0.5 \leq p \leq 1$, the curvature around point $(1, 0)$ is always dominant, so the Λ_1 -lattice gives the denser packing for all p in that interval.

It is also of interest to consider the packings as stacks of superdisk chains, as shown in Fig. 6. For example, the lattice packings in Fig. 3(a) and (b) can be constructed by stacking the superdisk chains shown in Fig. 6(a) and (b) horizontally and vertically, respectively. This may seem to be trivial for superdisks, however this view of packing structure enables us to construct dense packings of concave particles and to better understand packings of superballs in higher dimensions.

It is interesting to generalize the above discussion to the case of concave superdisks ($0 < p < 0.5$), as shown in Fig. 7. To construct dense packings of these particles, one needs to take advantage of the concave shape to reduce exclusion-volume effects. (The exclusion volume of a particle is the region around its center in which no other particle centers can be found due to the impenetrability constraint.)

For each concave superdisk, we can define a convex enclosing box as the one has the smallest area among all convex boxes that contain the particle, which is a square in this case [see Fig. 7(a)]. First, we construct 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 impenetrability constraints imposed by the hard particles. This also

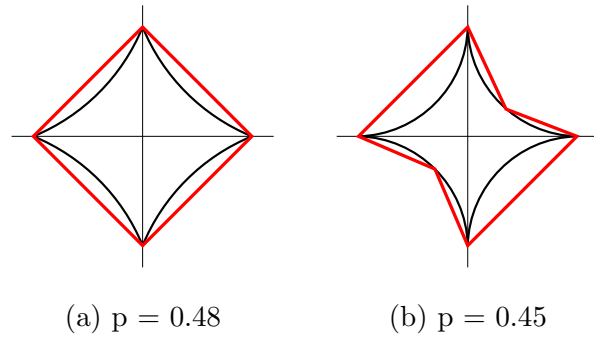


FIG. 7: (a) A concave superdisk with convex enclosing box (a square). (b) A concave superdisk with concave enclosing box (an hour-glass).

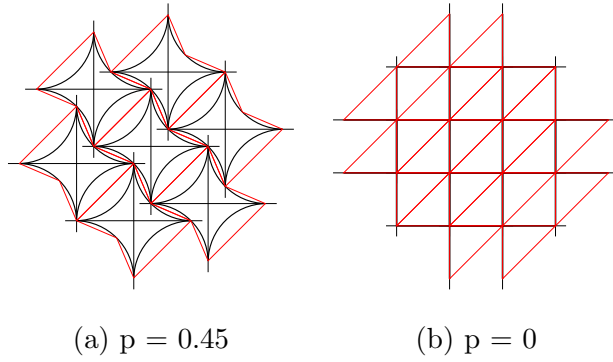


FIG. 8: Examples of dense packings of concave superdisks constructed by using the method described in the text.

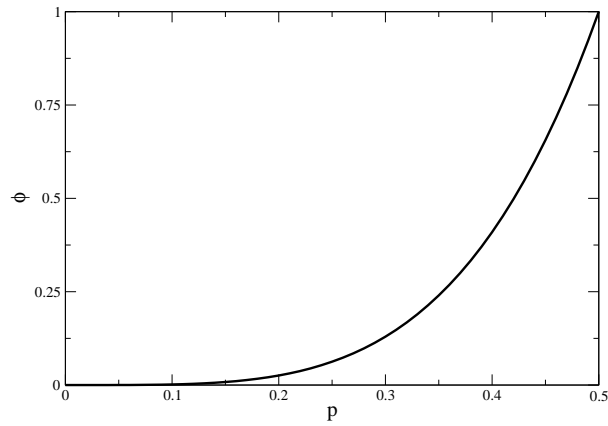


FIG. 9: Densities of the constructed lattice packings of concave superdisks as a function of deformation parameter p .

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 Fig. 7(b)] and 6 contact neighbors. Note that the constructed lattice packings of concave superdisks resemble Λ_0 -lattice packings of superdisks.

Two examples of the dense lattice packings of concave superdisks constructed by using the aforementioned method are shown in Fig. 8. As p decreases from 0.5, the particle shrinks; at the limit $p \rightarrow 0$, the superdisks become “crosses” [see Fig. 8(b)]. Note that at the limiting case of “crosses”, the area of the particle is 0, so is the packing density defined as the area fraction of the space covered by the particles. However, the *number density* of the lattice packing we constructed is *twice* of that for square-lattice packing of crosses, whose enclosing box is a square. The density of the constructed lattice packings of concave superdisks as a function of p is shown in Fig. 9. We emphasize that the existence of denser periodic packings or other lattice packings of these concave particles is also possible.

In summary, we have constructed the densest known packings of superdisks suggested by MD simulations. In particular, we found that the maximal packing densities of superdisks for certain $p \neq 1$ are achieved by one of the two families of lattice-packings, i.e., Λ_0 -lattice and Λ_1 -lattice packings, which provides additional numerical evidence for Minkowski’s conjecture concerning the critical determinant of the region occupied by a superdisk. 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 $p = p_0$, which are effects of the broken symmetry of superdisks. The result that ϕ_{max} increases as p varies from 1 is also consistent with the improvement on the lower bound on the packing density of superballs in arbitrarily high dimensions found by Elkies et al. Based on our observations of the structural properties of lattice packings of superdisks, we also proposed an analytical method to construct dense packings of concave superdisks. We emphasize that a good understanding of packings of superdisks provides the basis for the study of packings of superballs and superellipsoids in higher dimensions.

In future work, we will generate and study both ordered and disordered packings of superballs and superellipsoids in three dimensions, focusing on the role of broken symmetry in influencing the properties of such packings. It is important to adapt the methodology described in Ref. [32] to test the jamming categories [33] of disordered packings of superballs

and superellipsoids in order to study of the maximally random jammed (MRJ) states of packings with such nonspherical particle shapes.

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