Regular Packings on Periodic Lattices

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We investigate the problem of packing identical hard objects on regular lattices in d dimensions. Restricting configuration space to parallel alignment of the objects, we study the densest packing at a given aspect ratio X. For rectangles and ellipses on the square lattice as well as for biaxial ellipsoids on a simple cubic lattice, we calculate the maximum packing fraction $\varphi_d(X)$. It is proved to be continuous with an infinite number of singular points $X_\nu^{\min}$, $X_\nu^{\max}$, $\nu = 0, \pm 1, \pm 2, \ldots$. In two dimensions, all maxima have the same height, whereas there is a unique global maximum for the case of ellipsoids. The form of $\varphi_d(X)$ is discussed in the context of geometrical frustration effects, transitions in the contact numbers, and number-theoretical properties. Implications and generalizations for more general packing problems are outlined.

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The question of how densely objects can fill a volume has attracted both mathematicians and physicists for centuries. One famous problem is that of packing spheres. In 1611, Kepler conjectured that the fcc and hcp lattice configurations of identical spheres yield the highest packing fraction $\varphi_{\max}^{d=3} = \pi/\sqrt{18} \cong 0.7404$. Gauß was able to show in 1831 that these are the optimal periodic packings of spheres, but only very recently it was proved that they are optimal within all possible arrangements [1]. Even for disks in the plane, the corresponding proof of optimality of the hexagonal packing with $\varphi_{\max}^{d=2} = \pi/\sqrt{12} \cong 0.9069$ was only found in 1942 [2]. Apart from its theoretical attraction along with its relation to coding theory [3], packing is a problem of practical relevance. Not only have practitioners long known that a densest packing of oranges or cannon balls can be achieved via hexagonal layering but, more recently, packing problems have received substantial attention in engineering and operations research as problems of optimizing yields in production or minimizing leakage currents in integrated circuits (see, e.g., Ref. [4]).

In physics, periodic packings [3,5,6] are relevant for describing and understanding crystalline materials. In contrast, random close packings (RCPs) [7], i.e., maxima of the packing fraction under some local dynamics starting from loosely packed configurations, have been used to model glasses [8] and granular materials [9]. For spheres in 3D, random close packing leads to a packing fraction $\varphi_{\mathrm{RCP}}^{d=3} \approx 0.64$, significantly below $\varphi_{\max}^{d=3}$. The hard objects considered in such packings need not be spheres, but can be more general convex bodies. Although recently there has been extensive numerical work using techniques from dynamic programming and heuristic optimization, complemented by experiments, for studying periodic packings [10] or random close packing [11] for nonspherical objects, there is a lack of analytical understanding of these problems. For random close packing, it has been observed that the packing fraction increases over $\varphi_{\mathrm{RCP}}^{d=3} \approx 0.64$ as spheres are replaced by ellipsoids, and might even approach $\varphi_{\max}^{d=3} = \pi/\sqrt{18} \cong 0.7404$ in some cases [11]. Concerning periodic packings, an affine transformation maps the fcc or hcp sphere packing to a periodic lattice packing of identically aligned ellipsoids with maximum packing fraction $\varphi_{\max}^{d=3} = \pi/\sqrt{18}$. It has been predicted in Refs. [12,13] that nonparallel arrangement of ellipsoids of revolution may lead to packing fractions exceeding $\pi/\sqrt{18}$. Such superdense packings of ellipsoids were studied recently in more detail [14,15]. Particularly, it has been shown that $\varphi \cong 0.7707$ for all aspect ratios $X \geq \sqrt{3}$ [14].

We make progress in the analytical understanding of the problem of packings of nonspherical bodies by taking a complementary approach. Instead of finding the lattice structure that maximizes the packing fraction for a given type $\mathcal{K}$ of objects, we start out from a fixed Bravais lattice Λ and attach a body $\mathcal{K}$ of the same shape and orientation $\boldsymbol{\omega}$ to each lattice site (at its center of mass, say). We then determine the maximum packing fraction as a function of $\mathcal{K}$, i.e., as a function of the parameters characterizing its shape and orientation. To the best of our knowledge, this problem has not been studied before. Our approach may contribute to describing, for instance, plastic crystals, i.e., lattices with a molecule fixed at each site. In particular, aromatic molecules can be approximately described by hard ellipsoids. Similarly, applications are envisaged in operations research and manufacturing. Finally, insight into the frustration effects generated by the competing length scales of $\mathcal{K}$ and Λ could contribute to the understanding of packings without a predetermined lattice structure.

Consider a class of identical d-dimensional convex bodies $\mathcal{K}$ whose shape depends merely on their "length" l and "width" w, and consequently are characterized by a single parameter $X = l/w$, the aspect ratio. As a general example one might think of a d-dimensional ellipsoid of revolution. Fixing the aspect ratio X and orientation $\boldsymbol{\omega}$, proportional rescaling of the bodies allows one to reach the maximum packing fraction without overlaps, $\varphi_d(X, \boldsymbol{\omega})$. This fraction varies with $\boldsymbol{\omega}$, and we are interested in the maximum packing fraction irrespective of orientation, $\varphi_d(X) = \max_{\boldsymbol{\omega}} \varphi_d(X, \boldsymbol{\omega})$. The maximum $\varphi_d(X)$ is continuous as a function of X. Here, we only outline the idea of the rigorous proof [16]. Let us assume that $\varphi_d(X)$ is discontinuous at some $X_0 = l_0/w_0$, where, e.g., it jumps from φ_- to $\varphi_+ > \varphi_-$, with $\varphi_\pm = \lim_{\varepsilon\to 0}\varphi_d(X_0 \pm \epsilon)$. The convex bodies at φ_- and φ_+ are characterized by (l_-, w_-) and (l_+, w_+), respectively. Both pairs differ from each other, as $\varphi_- \neq \varphi_+$. Of course, it is $l_+/w_+ = l_-/w_- = X_0$. Now, starting from the configuration at φ_+, we continuously decrease the length of the hard objects. Consequently, without change of orientation, both the aspect ratio X and the corresponding packing fraction $\tilde{\varphi}_d(X)$ decrease continuously from X_0 and $\varphi_+ = \tilde{\varphi}_d(X_0)$, respectively. Below but arbitrarily close to X_0, $\tilde{\varphi}_d(X)$ must be arbitrarily close to φ_+, due to its continuity. On the other hand, it is $\varphi_d(X) \geq \tilde{\varphi}_d(X)$ for all $X \leq X_0$, since $\varphi_d(X)$ is the maximum packing fraction by definition. Therefore, even if $\varphi_d(X) = \tilde{\varphi}_d(X)$ holds (instead of $\geq$) for all $X \leq X_0$, we get $\varphi_- = \lim_{\varepsilon\to 0}\varphi_d(X_0 - \epsilon) = \varphi_+$. This contradicts the original assumption $\varphi_+ > \varphi_-$. Consequently, φ_d must be continuous.

We now turn to the calculation of $\varphi_d(X)$ for specific hard objects. As an example in two dimensions (2D), we study a square lattice with lattice constant $a = 1$. Consider first the case of rectangles of length l and width w. Imagine two identical rectangles with common direction $\mathbf{e} = (\cos\omega, \sin\omega)$, of their long side, attached with their centers to lattice sites $(0, 0)$ and $\mathbf{R}_{jk} = (j, k)$, respectively. In the following, we assume that $j \geq 0$ and $k \geq 0$ are coprime integers; i.e., they do not have a common divisor other than 1. For fixed aspect ratio X, it is obvious that the rectangles will attain maximum volume $v_2(l, w)$ if they touch each other and line up precisely along their short or long sides, cf. Fig. 1. Combining this and the periodicity of the packing, it is straightforward to prove that $\mathbf{e}$ must be parallel to $\mathbf{R}_{jk}$ [16]. In other words, for given X maximum packing fractions will always occur for "rational" orientations $\omega = \arctan(k/j)$ of the rectangles. Maximal packings for specific X can be constructed using the concept of lattice lines. The line $L_{jk}^{(0)}$ through the origin is defined by the lattice vector $\mathbf{R}_{jk} = (j, k)$. The distance of adjacent lattice sites on $L_{jk}^{(0)}$ equals $l_{jk} = \sqrt{j^2 + k^2}$. The square lattice can be decomposed into a set of parallel lattice lines $L_{jk}^{(\sigma)}$, $\sigma = 0, \pm 1, \ldots,$ of distance w_{jk}, where $w_{jk} l_{jk} = v_0 = 1$ (cf. the dashed lines in Fig. 1). Choosing $l = l_{jk}$ and $w = w_{jk}$, i.e., $X = X_{jk}^{\max} = l_{jk}/w_{jk} = j^2 + k^2$, leads to a perfect tiling with $\varphi_{\max} = \varphi_2(X_{jk}^{\max}) = l_{jk} w_{jk} = 1$, for all coprime

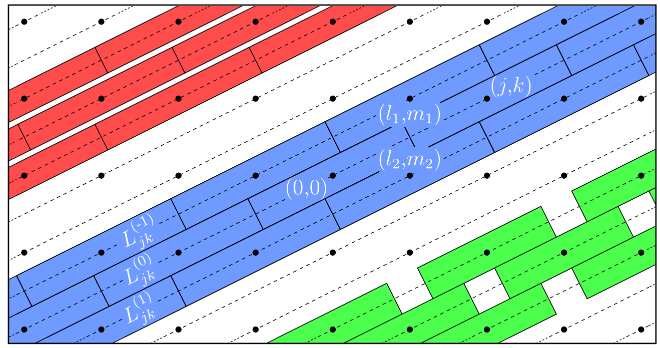

FIG. 1 (color online). Maximum packing configurations of rectangles with aspect ratios $X = 4$ (green, bottom), $X = X_{21}^{\max} = 5$ (blue, middle), and $X = 7$ (red, top), respectively. Lattice lines $L_{jk}^{(\sigma)}$, $\sigma = 0, \pm 1, \ldots,$ for $(j, k) = (2, 1)$ are indicated with dashed lines.

pairs (j, k), cf. the maxima at $\varphi_2 = 1$ in the lower part of the main panel of Fig. 2. The pairs (j, k) can be ordered such that $X_{\nu-1}^{\max} < X_\nu^{\max}$, where $X_\nu^{\max} = X_{j_\nu k_\nu}^{\max}$, $\nu = 0, 1, 2, \ldots$. Since $\mathbf{e}$ must be parallel to $\mathbf{R}_{jk}$, the maximum packing for $X < X_{jk}^{\max}$ and $X > X_{jk}^{\max}$ is obtained by decreasing l below l_{jk} keeping $w = w_{jk}$ and decreasing w below w_{jk} keeping $l = l_{jk}$, respectively (see Fig. 1). Consequently,

$$\varphi_2(X) = \begin{cases} w_{j_\nu k_\nu}^2 X & X_{\nu-1}^{\min} \leq X \leq X_\nu^{\max} \\ l_{j_\nu k_\nu}^2 / X & X_\nu^{\max} \leq X \leq X_\nu^{\min}. \end{cases} \quad (1)$$

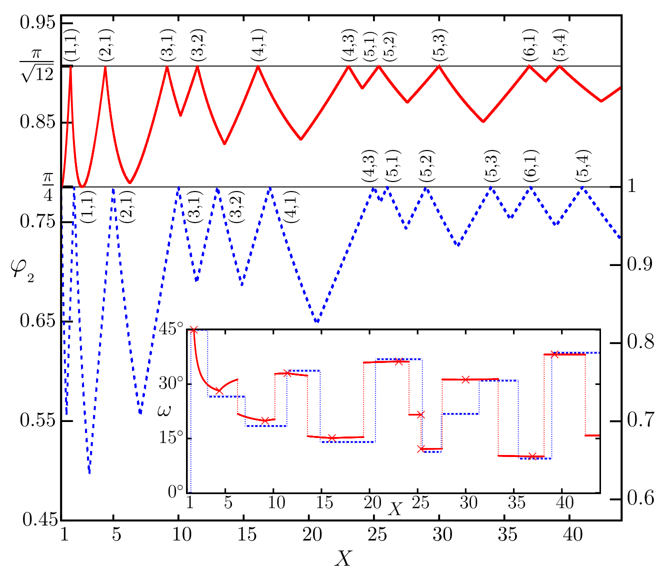

FIG. 2 (color online). Maximum packing fraction $\varphi_2(X)$ for rectangles (dashed line, right scale) and for ellipses (solid line, left scale). Inset: Orientation angle ω as a function of X for rectangles (dashed line) and ellipses (solid line). The crosses correspond to the positions of the maxima of $\varphi_2(X)$ for ellipses.

The positions $X_\nu^{\min} = l_{j_\nu k_\nu} l_{j_{\nu+1} k_{\nu+1}}$ follow from the matching condition $(l_{j_\nu k_\nu})^2 / X_\nu^{\min} = (w_{j_{\nu+1} k_{\nu+1}})^2 X_\nu^{\min}$ and $l_{j_{\nu+1} k_{\nu+1}} w_{j_{\nu+1} k_{\nu+1}} = 1$. $\varphi_2(X)$ is shown in Fig. 2, together with the optimal orientation $\omega(X)$ in the inset.

We now turn to the case of packing ellipses on the square lattice. A naive approach would be to inscribe them into the rectangles considered above. The resulting packing fraction of ellipses is then just $\pi/4$ that of the rectangles. In reality, however, maximally packed ellipses do not, in general, touch each other "head" to "tail," nor are they oriented parallel to the lattice lines, cf. Fig. 3. In contrast to the highly degenerate case of packing rectangles which touch along whole line segments, packings of general, smooth convex bodies are characterized by K contact points per body of which, due to inversion symmetry, only $K/2$ are independent. The three parameters describing an ellipse (two half axes and the orientation angle) are underdetermined in the generic case of $K = 4$ contact points (resulting in $K/2 = 2$ equations), yielding a continuum of solutions as a function of X. The case of $K = 6$ contacts is nongeneric, leading to a discrete set of maxima in $\varphi_2(X)$. For this situation, put one ellipse at the origin, such that the sites of the other ellipses are at $\pm(l_i, m_i)$, $i = 1, 2$, and $\pm(j, k) = \pm(l_1 + l_2, m_1 + m_2)$, cf. Fig. 3. Note that $0 \le l_i \le j$, $0 \le m_i \le k$. Then, the three corresponding contact vectors $\mathbf{c}_i = \frac{1}{2}(l_i, m_i)$, $i = 1, 2$, and $\mathbf{c}_3 = \frac{1}{2} \times (j, k) = \mathbf{c}_1 + \mathbf{c}_2$ uniquely determine the three coefficients a, b, and c in the ellipse equation $ax^2 + 2bxy + cy^2 = 1$. This allows us to determine the lengths of the half axes and thus the aspect ratio to be

$$X_{jk}^{\max} = (\alpha_+ + \sqrt{\alpha_-^2 + \alpha_0^2})/\sqrt{3},$$
$$\alpha_i = \mathbf{c}_1 \cdot \boldsymbol{\varepsilon}_i \mathbf{c}_1 + \mathbf{c}_2 \cdot \boldsymbol{\varepsilon}_i \mathbf{c}_2 + \mathbf{c}_1 \cdot \boldsymbol{\varepsilon}_i \mathbf{c}_2, \qquad (2)$$

where

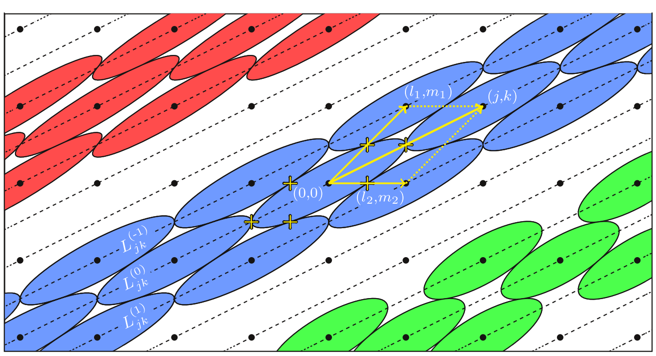

FIG. 3 (color online). Maximum packing configurations of ellipses with aspect ratios $X = 3$ (green, bottom), $X_{21}^{\max} = \sqrt{29 + 8\sqrt{13}}/\sqrt{3} \cong 4.4$ (blue, middle), and $X = 6$ (red, top). Lattice lines for $(j, k) = (2, 1)$ (dashed lines) and contact points (crosses).

$$\boldsymbol{\varepsilon}_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and

$$\boldsymbol{\varepsilon}_\pm = \begin{pmatrix} 1 & 0 \\ 0 & \pm 1 \end{pmatrix}.$$

The corresponding packing fraction is $\varphi_{\max} = \varphi_2(X_{jk}^{\max}) = \pi/\sqrt{12}$ for all (j, k), identical to the packing fraction of hcp disks. In fact, each such maximal ellipse packing can be continuously deformed via an affine transformation into a packing of disks. On increasing (decreasing) X from $X_{jk}^{\max}$, the shortest (longest) contact vector disappears, and the remaining four contacts allow us to determine the coefficients a, b, and c, and therefore $\varphi_2(X)$ and $\omega(X)$ in between the maxima $X_{jk}^{\max}$ as a function of X in a closed-form expression.

The result for $\varphi_2(X)$ and $\omega(X)$ is displayed in Fig. 2. Since $\varphi_2(1/X) = \varphi_2(X)$, only the regime $X \ge 1$ is shown. The maximum packing fraction is singular at $X_\nu^{\max}$ for all ν. The orientation $\omega(X)$ is discontinuous at those $X_\nu^{\min}$ at which $\varphi_2'(X)$ is discontinuous and at those $X_{jk}^{\max}$ which are degenerate, such as $X_{51}^{\max} = X_{52}^{\max}$ (cf. Fig. 2). At these points there are two degenerate maximal packings with the same packing fraction and aspect ratio but different orientations. The global maximum value of $\varphi_{\max} = 1$ and $\varphi_{\max} = \pi/\sqrt{12}$ for rectangles and ellipses, respectively, is attained for an infinite number of packings, uniquely labeled by (j, k). From Fig. 2 it appears plausible that $\lim_{X\to\infty} \varphi_2(X) = \varphi_{\max}$, which indeed can be proved [16].

The relation of the contact points can be understood from a number-theoretical point of view. Note that the centers (l_i, m_i), $i = 1, 2$, of two ellipses touching the central one at (0, 0) also define lattice lines $L_{l_i m_i}^{(0)}$ with direction (l_i, m_i). These are the directions closest to that of $L_{jk}^{(0)}$ provided that l_i and m_i are coprime and $0 \le l_i \le j$, $0 \le m_i \le k$. In mathematical terms, this means that m_i/l_i, $i = 1, 2$, are given by the best principal and best intermediate rational approximant [17] of k/j. They follow from the finite continued fraction expansion of k/j,

$$k/j = a_0 + 1/[a_1 + 1/[a_2 + \cdots + 1/[a_{n-1} + 1/a_n]\cdots]], \qquad (3)$$

where a_i, $i = 1, \ldots, n$ ($a_n \ge 2$) are positive integers that are uniquely determined by k/j. Then, it is $l_1 = s_{n-1}$, $m_1 = r_{n-1}$, where the best principal approximant r_{n-1}/s_{n-1} follows from Eq. (3) for $a_n = \infty$, and $l_2 = s_{n,a_n-1}$, $m_2 = r_{n,a_n-1}$ follows analogously from the best intermediate approximant $r_{n,a_n-1}/s_{n,a_n-1}$ obtained from Eq. (3) replacing a_n by $a_n - 1$. Since coding problems are strongly linked to number theory [3], these results also promise insight into the connection between packing and coding problems.

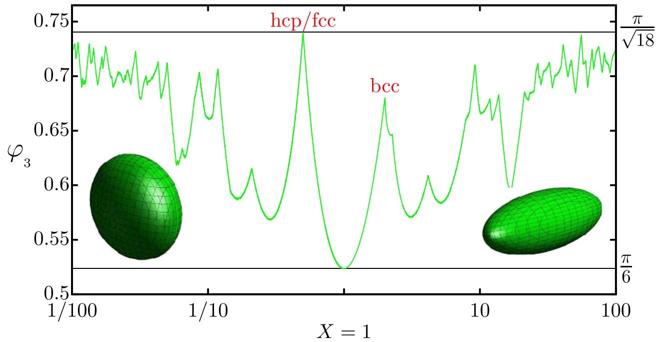

FIG. 4 (color online). Maximum packing fraction for biaxial ellipsoids on an sc lattice on a logarithmic X scale.

Finally, we have investigated ellipsoids of revolution on a simple cubic lattice. Analytically, it is possible to proceed in a similar fashion as for the ellipses. The resulting eighth-order polynomial in w^2 can only be solved numerically, however, and the intermediate expressions are rather unwieldy. Therefore, we instead determined $\varphi_3(X)$ numerically by a downhill-simplex minimization algorithm, the result of which is shown in Fig. 4; it agrees with that determined earlier in Ref. [18] and, as expected, shows continuity, too. Similar to the results in 2D, the derivative $\varphi_3'(X)$ seems to be discontinuous at a series of maxima at $X_\nu^{\max}$. It appears to be discontinuous at some, but not all, minima $X_\nu^{\min}$. The symmetry between $1/X$ and X valid in 2D, however, is lost. Most strikingly, the global maximum $\varphi_{\max} = \pi/\sqrt{18}$ for ellipsoids appears to be attained only for the single packing fraction $X_{-1}^{\max} = 1/2$, whereas in 2D there was a countable infinity of degenerate maxima. This maximum corresponds to the highly nongeneric case of each ellipsoid touching 12 neighbors. Consequently, an affine transformation can be applied to map this pattern to closest packing of hard spheres resulting in a fcc or hcp lattice. A second prominent maximum occurs at $X_1^{\max} = 2$ with 8 contact points per ellipse. The corresponding transformed hard sphere packing yields a bcc lattice. It can be shown that $\varphi_3(X) \geq \varphi_{\min} = \pi/6 = \varphi_3(X = 1)$; i.e., the packing fraction of hard spheres on a simple cubic (sc) lattice is a lower bound for $\varphi_3(X)$ [16]. From the numerical results in Fig. 4 we conjecture that, analogous to the 2D case, $\varphi_3(X) \to \varphi_{\max} = \pi/\sqrt{18}$ for $X \to \infty$ and $X \to 0$, respectively.

To conclude, the maximum packing fraction $\varphi_d(X)$ of parallel-aligned convex objects $\mathcal{K}$ characterized by a single aspect ratio exhibits universal features that appear to be independent of $\mathcal{K}$, the underlying Bravais lattice Λ, and even its dimension d. In particular, $\varphi_d(X)$ has been very generally proved to be continuous. In fact, this proof can even be extended to the case of convex bodies characterized by an arbitrary number of aspect ratios. Furthermore, as shown for the case of rectangles and ellipses on the square lattice as well as for biaxial ellipsoids on the sc lattice, there is an infinite number of local maxima and minima at which $\varphi_d(X)$ is singular. The singularities at the minima and at certain, degenerate maxima (see Fig. 2 for the case of ellipses) are correlated to the discontinuities in the orientation of $\mathcal{K}$. For the studied cases, we find that $\varphi_d(X)$ converges to its global maximum for $X \to \infty$ as well as for $X \to 0$. While we were only able to prove this rigorously for the case of rectangles and ellipses, we believe that this property holds far more generally, implying that convex hard objects, on average, pack much better if they become more oblate or prolate.

On the other hand, there are also significant differences between the systems studied in two and three dimensions. For rectangles and ellipses, the global maximum packing fraction $\varphi_{\max} = 1$ (rectangles) and $\varphi_{\max} = \pi/\sqrt{12}$ (ellipses) is attained for an infinite number of discrete aspect ratios $X_{jk}^{\max}$, uniquely labeled by pairs (j, k) of coprime integers. On the contrary, for symmetric ellipsoids with $1/100 \leq X \leq 100$, $\varphi_3(X)$ takes its maximal height $\varphi_{\max} = \pi/\sqrt{18}$ at the single value $X_{-1}^{\max} = 1/2$ only. This qualitative difference can be understood as follows. Consider, for instance, a d-dimensional symmetric ellipsoid which depends on $d + 1$ parameters. In a packing, K contacts lead to $K/2$ equations. In the generic case of $K/2 = d$, the system is underdetermined and φ_d can be found as a function of the aspect ratio X. For the nongeneric case $K/2 = d + 1$, there is always a solution corresponding to the local maxima of $\varphi_d(X)$ at $X_\nu^{\max}$. It appears likely that the competing point symmetries of $\mathcal{K}$ and Λ are responsible for the nonequal heights of these maxima for $d = 3$ and $K = 8$. It is conceivable that this extra frustration might be relieved by considering convex hard objects characterized by three length scales, possibly leading again to an infinity of equal-height maxima. The even more nongeneric situation $K/2 > d + 1$ as realized, e.g., in the global maximum $\varphi_{\max} = \pi/\sqrt{18}$ for our 3D ellipsoids with $K = 12$, corresponds to an overdetermined set of equations such that, at most, only very few solutions can be expected. It is worthwhile to point out that our results for packing on fixed lattices should be closely related to continuum packing with a fixed number of contacts since the latter involves geometric frustration as well.

Of course, it might be a challenge to study packings of the considered type on different lattices. Even richer behavior is expected on weakening the condition of parallel alignment, paving the way for the occurrence of superdense packings in analogy to those recently found for ellipsoids in the 3D continuum [14,15].

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