On the caging number of two- and three-dimensional hard spheres

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Local structural arrest in random packings of colloidal or granular spheres is quantified by a caging number, defined as the average minimum number of randomly placed spheres on a single sphere that immobilize all its translations. We present an analytic solution for the caging number for two-dimensional hard disks immobilized by neighbor disks which are placed at random positions under the constraint of a nonoverlap condition. Immobilization of a disk with radius $r=1$ by arbitrary larger neighbor disks with radius $r \geq 1$ is solved analytically, whereas for contacting neighbors with radius $0<r<1$, the caging number can be evaluated accurately with an approximate excluded volume model that also applies to spheres in higher Euclidean dimension. Comparison of our exact two-dimensional caging number with studies on random disk packing indicates that it relates to the average coordination number of random loose packing, whereas the parking number is more indicative for coordination in random dense packing of disks. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1991852]

I. INTRODUCTION

Contact numbers in sphere packings have in several cases a special physical significance. The *kissing* number represents the maximum number of spheres that can be placed simultaneously on the $d-1$ dimensional surface of a d-dimensional sphere S. For disks in a plane ($d=2$) the kissing number is six and for three-dimensional spheres the number is 12.[1] These maximum contact numbers occur in regular close-packed sphere solids as encountered, for example, in colloidal crystals.[2] The kissing number is a single-valued quantity, in contrast to the distributed contact numbers found by placing spheres on randomly chosen, fixed positions on the surface of S until the probability for finding sufficient parking space vanishes. This distributive contact number, the *parking* number, equals 8.7 for three-dimensional spheres.[3] It is the average outcome of a random parking process with the constraint that spheres are forbidden to overlap. This parking process models irreversible adsorption and has been generalized[3] to the attachment of spheres with arbitrary size on the surface of S. Thus, the kissing number is the absolute maximum contact number achieved for regular close-packed spheres while the parking number is a lower constrained maximum that has more relevance for less dense "amorphous" sphere stackings. To increase the coordination of S above the parking value the disordered neighbors must be rearranged (at least partly) into a more ordered configuration.

One might identify the parking number as the typical number of spheres required to immobilize a sphere in a random packing. However, the parking process is merely a maximization under the constraint of random positioning and nonoverlap which pays no heed to the issue whether or not sphere S is able to translate. Of course, the parked neighbors *do* restrict the mobility of S and, in fact, when the number of contacting neighbors equals the parking number, S will be unable to translate. An important point is that to achieve this arrest, on average much less spheres are required than the parking number. Thus, to describe the local arrest of a single sphere, a *caging* number has been introduced[4–6] defined as the average *minimum* number of randomly placed spheres that blocks all translational degrees of freedom of sphere S. The construction of such geometric cages has been discussed in detail elsewhere (see, for example, the simulations of sphere caging in arbitrary Euclidean dimension in Ref. 5). In essence, a cage is constructed via the parking process referred above, with the additional rule that the process is terminated when S is caged. Consequently, the resulting caging contact numbers fall significantly below the parking and kissing numbers in any Euclidean dimension.[6]

To avoid confusion we note here that caging effects in transport phenomena are time dependent, in contrast to our static definition of caging. In dense colloidal fluids, for example, local structural arrest is described in terms of slowly fluctuating neighbor cages that trap spheres, on approach of a glass transition, over increasing time intervals. In our present analysis a cage is purely geometric, as in a static snapshot of thermal colloids or a packing of macroscopic "granular"

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spheres. This is not to say that the caging number is irrelevant for thermal spheres, because the progressive arrest of spheres near a glass transition is ultimately caused by purely geometrical restrictions.[7] So calculation of caging numbers is useful to better understand or perhaps even quantify coordination numbers in random sphere packings or colloidal sphere glasses, a point to which we return in the Discussion in Sec. VI.

The main challenge in a geometrical caging problem is to account for excluded volume effects, which cause positions of contacts on a sphere to be strongly correlated. For randomly parked, overlapping neighbor spheres, i.e. for a distribution of completely uncorrelated contact points on the surface of sphere S, caging numbers have been calculated analytically for spheres of arbitrary dimension.[5] For nonoverlapping hard spheres, however, caging numbers have only been determined by computer simulation.[5] We report in Sec. III an analytical solution for the caging number of a two-dimensional hard sphere with radius $r=1$ for neighboring spheres with radius $r\geqslant 1$, which is validated by numerical calculations. In Sec. IV, we also investigate the caging number for contacting neighbor spheres with radius $0<r<1$. We compare caging numbers with parking numbers, which exhibits an interesting difference depending on sphere size ratio. In Sec. V, we discuss the caging number for three-dimensional hard spheres. In Sec. II, we first briefly reexamine the caging number for uncorrelated contacts for comparison with the results for correlated contacts in later sections and to provide a more concise derivation than given previously.[5]

II. CAGING BY UNCORRELATED CONTACTS

Let p_n be the probability that n arbitrarily placed contacts cage sphere S. The probability that n contacts do not cage S equals

$$1-p_n=\sum_{k=n+1}^{\infty}P(k), \tag{1}$$

where $P(k)$ is the conditional probability that k contacts cage S, given that $k-1$ contacts still allow sphere S to translate. The caging number is defined as the expectation value,

$$\langle\gamma\rangle=\sum_{k=0}^{\infty}kP(\gamma=k)=\sum_{n=0}^{\infty}\sum_{k=n+1}^{\infty}P(\gamma=k)=\sum_{n=0}^{\infty}1-p_n. \tag{2}$$

The contacts on the surface of S may stem from the touching spheres or any other neighbor shapes such as cylinders or thin rods.[8] If the neighbors are particles that cannot interpenetrate each other, the contacts are correlated. When the neighbors are allowed to overlap without any restriction, the contacts on S are uncorrelated (the neighbors are randomly inserted) and the contact distribution is equivalent to a set of blocking points placed at random, fixed positions on the surface of S.

The probability that n contacts do not cage a d-dimensional sphere equals the probability that one equator on S can be found such that all n contacts share the same hemisphere of S. For example, a one-dimensional sphere can only translate along a straight line, so there are only two "hemispheres." The probability that all uncorrelated contacts are on one hemisphere is therefore

$$1-p_n=\left(\frac{1}{2}\right)^{n-1}\quad\text{for } n>0 \text{ and } p_0=0, \tag{3}$$

which on substitution in (2) yields for the caging number for uncorrelated contacts on a one-dimensional sphere,

$$\langle\gamma\rangle=1+\sum_{n=1}^{\infty}\left(\frac{1}{2}\right)^{n-1}=3\quad\text{for } d=1. \tag{4}$$

For two-dimensional spheres the caging problem for uncorrelated contacts is more complicated because from an infinite set of possible hemispheres one has to determine whether or not at least one member is common to all n contacts. The general problem for a d-dimensional sphere has been solved by Peters *et al.*[5] Here we present an alternative treatment for $d=2$ employing a formula derived by Wendel[9] for the probability of finding n randomly placed points on the same hemisphere of a d-dimensional sphere (see Appendix A):

$$p_{d,n}=\begin{cases}\left(\frac{1}{2}\right)^{n-1}\sum_{k=0}^{d-1}\binom{n-1}{k} & \text{for } n>d,\\ 1 \quad \text{for } 0\leqslant n\leqslant d.\end{cases} \tag{5}$$

Thus for two-dimensional spheres,

$$p_{2,n}=\begin{cases}1-p_n=n\left(\frac{1}{2}\right)^{n-1} & \text{for } n\geqslant 2,\\ 1 \quad \text{for } n=0,1,\end{cases} \tag{6}$$

which according to (2) yields for the caging number for uncorrelated contacts in two dimensions,

$$\langle\gamma\rangle=1+\sum_{n=1}^{\infty}n\left(\frac{1}{2}\right)^{n-1}=5\quad\text{for } d=2. \tag{7}$$

Equations (4) and (7) are instances of the general result $\langle\gamma\rangle=2d+1$ for uncorrelated contacts, rederived in Appendix B using the Wendel formula (5). The caging number $\langle\gamma\rangle=2d+1$ for d-dimensional spheres is clearly an upper bound because the nonoverlap condition for hard spheres increases the average distance between contacts and, hence, will decrease the number of contacts needed for caging, as demonstrated in the next section for two-dimensional spheres.

III. CAGING BY THREE HARD DISKS

The caging of disk S by nonoverlapping hard spheres of any size has the trivial solution $\gamma=2$ in one dimension. In two dimensions, the caging probability for three disks can be exactly calculated taking into account the nonoverlap condition. For finite-size caging disks, there is a minimum angle given by a triangle of three contacting spheres that is equal to

$$\alpha=2\arcsin[r/(r+1)]. \tag{8}$$

where r is the size ratio of the radii of the caging disks with respect to S (see Figs. 1 and 2). Hence, each contact on the circumference of S excludes an arc with angle α on each side of it for any other contact. S is caged when the largest arc

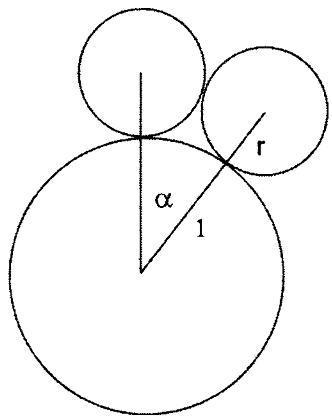

FIG. 1. (a) Hard disks are not allowed to overlap. This leads to an excluded arc on the circumference of the central disk.

between any two adjacent contacts is smaller than π. The caging number as a function of r must satisfy two limiting cases. When r tends to zero, the caging number $\langle\gamma\rangle=5$ for uncorrelated particles should be recovered. On the other hand, for sufficiently large r, a two-dimensional disk S can only accommodate a maximum of three contacting neighbors and since two disks cannot cage S, it follows that the caging number should monotonically decreases from five to three for increasing r. A numerical solution (Fig. 3) indeed confirms this behavior. The caging number diminishes rapidly when the point contacts at $r=0$ start to inflate, to saturate

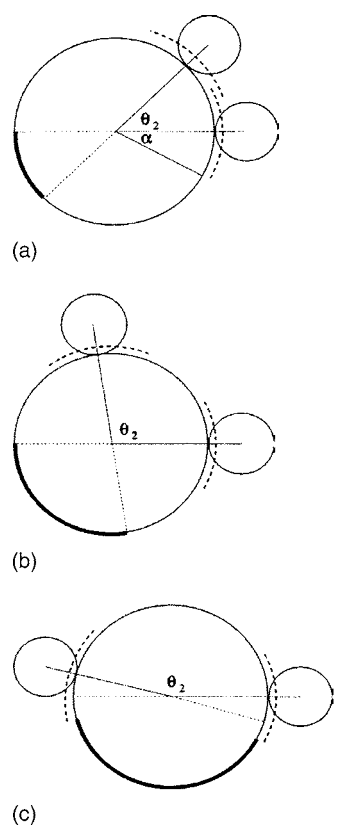

FIG. 2. Illustration of excluded arcs (thick dashed lines), free segment, and caging segment (thick line). The thin dashed lines indicate the "image" points of the contacts with respect to the sphere center. (a) Overlapping excluded arcs; (b) disjoined excluded arcs; (c) image points in excluded volumes.

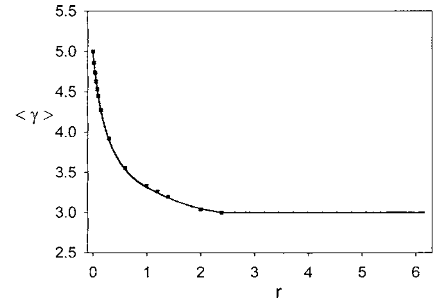

FIG. 3. Plot of two-dimensional caging number $\langle\gamma\rangle$ as a function of the radius of the contacting disks. Triangles represent the approximation with excluded length given by (15) and the computer simulation is shown with circles.

already in the range $r=1-2$. For equal-sized disks, $\alpha=\pi/3$, Bideau *et al.*[10] showed that for a configuration with maximum disorder four disks are an upper limit for the contact number. Four disks do *not* cage S when they touch each other forming a connected row of four, as in a hexagonal unit with two disks missing. In this case the largest arc corresponds exactly to π. Since the probability for this configuration to occur is zero for randomly placed disks, $p_{2,4}=1$. Therefore, for $\alpha>\pi/3$ or equivalently $(r>1)$, the calculation of $p_{2,3}$ is sufficient to obtain the caging number. For the sake of generality, $p_{2,3}$ will be given for arbitrary values of α.

Let us denote the angular coordinates of the three contact points by θ_1, θ_2, and θ_3, where the index indicates the ordering of the successive additions. Since the position of the first contact is arbitrary, we can choose $\theta_1=0$. Since the "upper" and "lower" half circles are as of yet equivalent, we can restrict θ_2 to values $0<\theta_2\leqslant\pi$. Furthermore, because of the excluded volume, θ_2 must satisfy $\theta_2\geqslant\alpha$. To calculate $p_{2,3}$, we need to calculate for each possible choice of θ_2 the probability that the third contact cages the sphere and average this probability over all possible values for θ_2. For a given θ_2, this probability is equal to the lengths of the segments of the circle in which the third contact point cages the sphere, divided by the length of the total available space for the third contact.

For $\alpha<\pi/3$ or equivalently $(r<1)$, three different situations have to be considered as θ_2 increases, see Fig. 2. For $\alpha<\theta_2<2\alpha$, the excluded volumes of the two disks overlap (no third disk can be placed in between), and the total available length for placing the third contact is $2\pi-\theta_2-2\alpha$. In order to cage the sphere, the third contact must be placed such that there is no free arc of length π or more. It can be easily seen from Fig. 2(a) that this happens only in the segment located in between the two "image" points of the two first contacts with respect to the sphere center. Therefore, the length of this segment is just θ_2. For $2\alpha<\theta_2<\pi-\alpha$ [Fig. 2(b)], the excluded volumes are disjoint (now, the third disk can also be placed between the two first), and the total available segment length for the third contact is always equal to $2\pi-4\alpha$, whereas the length of the caging segment is still equal to θ_2. Finally, for $\pi-\alpha<\theta_2<\pi$ [Fig. 2(c)], the image points of the first two contacts fall into the excluded volume. The total available length is still $2\pi-4\alpha$, but the length of the caging segment is reduced to $2\pi-2\alpha-\theta_2$. The expression for $p_{2,3}$ that results from putting the three pieces together is

$$p_{2,3}=\frac{1}{\pi-\alpha}\left(\int_{\alpha}^{2\alpha}\frac{\theta_2}{2\pi-2\alpha-\theta_2}d\theta_2+\int_{2\alpha}^{\pi-\alpha}\frac{\theta_2}{2\pi-4\alpha}d\theta_2+\int_{\pi-\alpha}^{\pi}\frac{2\pi-2\alpha-\theta_2}{2\pi-4\alpha}d\theta_2\right). \quad (9)$$

Similar considerations apply in the case $\alpha>\pi/3$. Only, since now $2\alpha>\pi-\alpha$, the image points enter the excluded volumes before the latter get disjoint. Therefore, the bounds of the individual integrals have to be changed, and the total and caging segment lengths reevaluated for the second integral, which gives

$$p_{2,3}=\frac{1}{\pi-\alpha}\left(\int_{\alpha}^{\pi-\alpha}\frac{\theta_2}{2\pi-2\alpha-\theta_2}d\theta_2+\int_{\pi-\alpha}^{2\alpha}\frac{2\pi-2\alpha-\theta_2}{2\pi-2\alpha-\theta_2}d\theta_2+\int_{2\alpha}^{\pi}\frac{2\pi-2\alpha-\theta_2}{2\pi-4\alpha}d\theta_2\right). \quad (10)$$

The evaluation of these integrals yields, for $\alpha>\pi/3$,

$$p_{2,3}=\frac{1}{\pi-\alpha}\left(\frac{7}{2}\alpha-\frac{5}{4}\pi+(2\pi-2\alpha)\ln\frac{2\pi-3\alpha}{\pi-\alpha}\right). \quad (11)$$

Note that this expression is valid only for $\alpha\leqslant\pi/2$; for $\alpha=\pi/2$, $p_{2,3}=1$, which corresponds to the fact that three disks with $\alpha>\pi/2$ cannot be placed on the same hemicircle, and thus S is always caged.

In particular, for equal-sized disks with $\alpha=\pi/3$, $p_{2,3}=\ln(9/4)-1/8$, which upon substitution in (2) yield the two-dimensional caging number $\langle\gamma\rangle=1+1+1+9/8-\ln(9/4)\cong3.314\,07$. This result equals the value found from simulations in Ref. 5 and those described in the next section. The result for correlated contacts is, as expected, below the caging number for uncorrelated contacts because of excluded volume effects. The caging number is also lower than the parking number for two-dimensional disks, since one can always park four equal-sized disks at random on a central disk. We determined the parking number for two-dimensional disks numerically to be 4.484.

IV. CAGING AND PARKING NUMBERS FOR HARD DISKS OF DIFFERENT SIZE

No analytical solution is yet available for the caging number for $r<1$ ($\alpha<\pi/3$), since there are noncaging configurations with four and more contact points. Therefore, an evaluation of the caging number would require the calculation of $p_{2,n}$ for $n>3$ while taking into account the sequential addition of disks, which is very cumbersome. Fortunately, as a good approximation an exact calculation can be performed for a slightly modified problem. The condition of sequentially adding disks is replaced by positioning n disks simultaneously. The new problem is defined as follows.

Let a central disk of unit radius be surrounded by n disks of radius r. Count all possible configurations for the n surrounding disks and determine the fraction that has all n disks in a hemisphere of the central disk. This can be done in the following way: The space of configurations is defined by the positions of the small disks. All configurations in which all n disks are separated from each other by the same angles are equivalent because one can always transform one configuration into the other by rotating the reference axes. Therefore, only the angle differences between disks are useful variables in two dimensions. Let θ_i again be the angle of the ith contact with respect to an arbitrary reference axis; this time, since all contacts are present from the start, the index can count the contacts counterclockwise. We define the angle differences as $\varphi_i=\theta_{i+1}-\theta_i$ for $i=1$ to $n-1$ and $\varphi_n=\theta_1+2\pi-\alpha_n$ in order to make all $\varphi_i>0$. For n contacts there are n differences. However, they are not all independent since

$$\sum_{i=1}^{n}\varphi_i=2\pi. \quad (12)$$

The total number of configurations is the number of possible ways to choose sets of φ_i satisfying (12). For continuous variables this becomes the volume of phase space spanned by the φ_i. This can be written as, preserving the symmetry between all variables,

$$V=\int d\varphi_1\int d\varphi_2\ldots\int d\varphi_n\,\delta\left(\sum_{i=1}^{n}\varphi_i-2\pi\right), \quad (13)$$

where δ is the Dirac delta function. The integration bounds are determined as follows: For point contacts, there is no other restriction than $0\leqslant\varphi_i\leqslant2\pi$. For finite-size disks, φ_i has to be larger than the angle α. There is also a maximum angle: n disks touching each other occupy $(n-1)\alpha$, so the maximum "gap" is $2\pi-(n-1)\alpha$. Including the theta functions conveniently incorporates these restrictions on the phase-space volume,

$$V=\int d\varphi_1\int d\varphi_2\ldots\int d\varphi_n\,\delta\left(\sum_{i=1}^{n}\varphi_i-2\pi\right)\times\theta(\varphi_1-\alpha)\theta(\varphi_2-\alpha)\ldots\theta(\varphi_n-\alpha). \quad (14)$$

This way the integration bounds can stay open ($-\infty$ to $+\infty$) and adding the theta function is equal to starting at angle α. This is also a convenient way to take into account the upper boundary without breaking the symmetry between the variables. One can see that the value of the entire integral is independent of the ordering of the integration variables.

The fraction of noncaging configurations is given by the configurations where at least one $\varphi_i>\pi$. There can be only one such φ_i because of the constraint (12). The volume of phase space filled by such configurations can therefore be calculated as

$$V=\sum_{l}\int d\varphi_1\int d\varphi_2\ldots\int d\varphi_n\,\delta\left(\sum_{i=1}^{n}\varphi_i-2\pi\right)\times\theta(\varphi_1-\alpha)\theta(\varphi_2-\alpha)\ldots\theta(\varphi_n-\alpha)\theta(\varphi_l-\pi), \quad (15)$$

where the new element is the last theta function which counts only the configurations with $\theta_l>\pi$. The outer sum is necessary because any of the φ_i can become greater than π. Since all variables are symmetric, this can immediately be simplified, giving for the total probability of finding all disks on the same hemisphere,

$$p_{2,n} = \frac{n \int d\varphi_1 \int d\varphi_2 \ldots \int d\varphi_n \delta\left(\sum_{i=1}^{n} \varphi_i - 2\pi\right) \theta(\varphi_1 - \alpha) \ldots \theta(\varphi_{n-1} - \alpha) \theta(\varphi_n - \pi)}{\int d\varphi_1 \int d\varphi_2 \ldots \int d\varphi_n \delta\left(\sum_{i=1}^{n} \varphi_i - 2\pi\right) \theta(\varphi_1 - \alpha) \ldots \theta(\varphi_n - \alpha)}. \quad (16)$$

Note that this is an exact formula valid for any α (and thus r) and n. Rather than evaluating the integrals explicitly, we will use a graphical method that immediately gives the result for the $p_{2,n}$.

First the probability for the three disks will be discussed and then it will be extended to n disks. The total phase space is spanned by $\{\varphi_1, \varphi_2, \varphi_3\}$. The Dirac δ function restricts the phase space to a plane that can be defined by the points $(2\pi, 0, 0)$, $(0, 2\pi, 0)$, and $(0, 0, 2\pi)$. For point contacts the theta functions exclude all $\varphi_i < 0$ and $\varphi_i > 2\pi$. The resulting domain of phase space is an equilateral triangle. This is known (up to a rescaling) as the Gibbs simplex, used abundantly in ternary alloy phase diagrams.

The noncaging part of the phase space is given by the volume where one $\varphi_i > \pi$. This gives three equilateral triangles with side π (Fig. 4). The stripes are cut off from the phase-space triangle to take into account the excluded volume thetas, i.e., the nonoverlap condition for hard disks. The stripes are cut from the outer rim of the triangle. The remaining inner triangle is the total volume of phase space. Since all subvolumes are equilateral triangles, the ratios of their surfaces are the ratios of the side lengths squared. The side length of the total volume is $2\pi - 3\alpha$ and the side length of one of the three noncaging volumes is $\pi - 2\alpha$. From this the noncaging probability follows:

$$p_{2,3} = \begin{cases} 3(\pi - 2\alpha)^2/(2\pi - 3\alpha)^2 & \text{for } \alpha < \pi/2, \\ 0 & \text{for } \alpha > \pi/2. \end{cases} \quad (17)$$

The argument with the Gibbs simplex is general and can be applied to any n. For example, for $n=4$, the Gibbs simplex is a tetrahedron, and the noncaging volumes are four small tetrahedra located in the corners of the large one. Therefore the immediate generalization,

$$p_{2,n} = \begin{cases} n\left(\dfrac{\pi - (n-1)\alpha}{2\pi - n\alpha}\right)^{n-1} & \text{for } \alpha < \pi/(n-1), \\ 0 & \text{for } \alpha > \pi/(n-1). \end{cases} \quad (18)$$

Note that in the limit $\alpha \to 0$ the probability for point contacts is obtained. Substitution of (18) in (2) gives the approximated caging number as a function of contacting disk radius, as plotted in Fig. 3. The upper boundary of the summation in (2) was adjusted to π/α because only a finite number of disks can be placed on the same hemicircle.

The accuracy of Eq. (18) was verified with a computer simulation of the sequential addition of disks using a method similar to Ref. 5 for equal-sized spheres. The difference between simultaneously positioning n disks and the numerical solution of sequentially adding disks is surprisingly small over the whole range, as shown in Fig. 3. In the numerical simulation, the probability for a given configuration depends on the order in which the disks were placed and is thus nonuniform, whereas for adding n disks simultaneously on the central disk the probability for a given configuration is uniform.

To compare the caging number with the parking number a computer simulation was performed to determine the parking number as a function of contacting disk radius (see Fig. 5). For uncorrelated point contacts the parking number goes to infinity, while for large radii the parking number reaches its minimum value of 2.

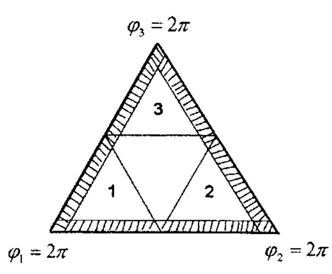

FIG. 4. The phase space spanned by $\{\varphi_1, \varphi_2, \varphi_3\}$ is an equilateral triangle with length 2π. The nonoverlap condition for disks is taken into account by requiring that the minimum of each φ_i is α. Therefore the outer rims of the triangle are stripped off. A disk is noncaged if any of the φ_i is larger than π. This is the case for the three small equilateral triangles.

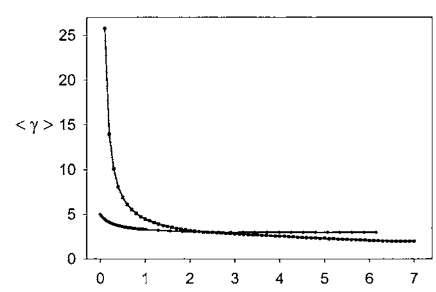

FIG. 5. Caging and parking numbers plotted as functions of contacting disk radius. Parking number (squares) and caging number (circles). Two radii can be identified, $r_{\min}$ and $r_{\max}$. $r_{\min}$ is the intersection point of the caging and parking numbers. $r_{\max}$ is the maximum radius for which a unit sphere can have three contacts. Note the difference in parking and caging number for $r \to 0$ and $r \to r_{\max}$.

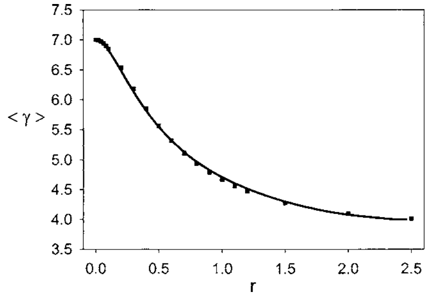

FIG. 6. Plot of three-dimensional caging number $\langle\gamma\rangle$ as a function of the radius of the contacting spheres. The approximation method extended to three-dimensional (triangles). Determination with computer simulation (circles). The flattening of the caging number as $r\rightarrow 0$ is caused by the cosine term in the excluded area in Eq. (19).

V. CAGING NUMBERS FOR THREE-DIMENSIONAL SPHERES

The approach previously discussed can be extended to three-dimensional spheres caged by hard spheres of arbitrary size. A hard-sphere contact excludes an area (a spherical cap) on a unit sphere surface where no other spheres can be placed,

$$A_{\text{excl}} = 2\pi(1-\cos[2\arcsin(r/(r+1))]). \quad (19)$$

The n contacts divide the surface of the three-dimensional sphere into $\left(\frac{1}{2}n^2-\frac{1}{2}n+1\right)$ sectors. Calculation of the total phase space involves double integrals over the area sectors on the sphere, taking into account the nonoverlap condition, which is very hard to do. Instead, we approximate the fraction of noncaging configurations in the same way as for the two-dimensional case. Rewriting the probability for finding n points on a three-dimensional hemisphere yields

$$p_{3,n} = \left(\frac{1}{2}n^2-\frac{1}{2}n+1\right)\left(\frac{2\pi-(n-1)A_{\text{excl}}}{4\pi-nA_{\text{excl}}}\right)^{n-1}, \quad (20)$$

where now areas are used instead of angles with respect to (18). However, $A_{\text{excl}}=\pi$ for $r=1$. This means that according to (20) the probability of finding three spheres on a hemisphere is zero. This is clearly invalid. The area in (19) is the area excluded for other sphere centers. These other sphere centers exclude the area themselves and thus the part of the excluded area is shared and double counted in (20). To get a more meaningful result, the excluded area in (20) is taken to be the area that belongs exclusively to a single sphere contact, namely,

$$A_{\text{excl}} = 2\pi(1-\cos[\arcsin(r/(r+1))]). \quad (21)$$

Using (20) and (21) to calculate (2) with upper boundary $2\pi/A_{\text{excl}}$ gives the caging number as a function of contacting sphere radius, as shown in Fig. 6. Again the approximation agrees well with the simulation over the whole range. The caging number found numerically is 4.71 for equal-sized spheres, in agreement with the numerical value 4.79±0.02 found in Ref. 5.

VI. DISCUSSION

We have rederived the general caging number for spheres of Euclidean dimension d using the Wendel formula (5). The minimum number of contacts required to cage a sphere is $d+1$, but on average an additional number of d spheres is needed in view of the caging number $\langle\gamma\rangle=2d+1$. This result for uncorrelated contacts is clearly an upper limit for the caging number for correlated sphere contacts. Our analytical result for equal-sized disks $\langle\gamma\rangle=3.314$, which agrees precisely with simulation results, illustrates that excluded volume effects indeed reduce the caging number substantially. The physical significance of this two-dimensional caging number becomes clear in comparison with other studies on hard disks.

Williams[11] attempted, using a local arrest criterion, to calculate the average contact number that stabilizes a two-dimensional random packing and found an average contact number of 3.2. Uhler and Schilling[12] showed that the contact number found by Williams is not correct because not all configurations had been taken into account. They estimated the coordination number for a loose-packed configuration by calculating the probability of a disk having n neighbors in a stable configuration. The central disk is stable if it cannot move without moving any of its neighbors. The value obtained for the average n is in the range of 3.33–3.42. We present here an analytical solution for the problem posed by Williams and extended the problem to disks with size ratio larger than 1. Furthermore, we extended the approach from Uhler and Schilling to disks and spheres of arbitrary size. Computer simulation of disk packing was performed by Hinrichsen *et al.* who found a coordination number around 3 (Ref. 13) and implied that the generated disk packing was very close to a random loose packing configuration. The interesting finding is that at least for two-dimensional spheres the caging number seems to be related to random loose packing. This raises the question whether it is also possible to identify a contact number relevant for random *close* packing.

Uhler and Schilling attempted a local description for random dense packing but could not find a satisfying analytical approach. Experiments performed by Quickenden and Tan on random dense disk packings[14] yielded a coordination number of 4. The parking number for equal-sized disks is 4.484, which is indeed closer to the experimental value from Ref. 14 than the caging number. A random close packing is a *maximum* in volume fraction, while the parking number is the average maximum number of disks that can be parked on a central disk. The difference between the parking number and the coordination number in a packing is probably due to global correlations between disks, so the parking number seems to be merely an indication for the average coordination number in a random dense packing.

It can hardly be a coincidence that the caging number is close to contact numbers found in random loose packings. In random loose packing there is no long-range ordering and the packing should be static. From the static condition it follows that the net sum of forces on a particle is zero. The "loose" in random loose packing signifies the lowest reachable volume fraction that satisfies the two mentioned conditions. The caging of spheres described in this work yields a local description of random configurations of spheres. Each of these configurations satisfies the condition that a combination of forces can be chosen which makes the net sum of forces on the central sphere zero. The generation of a single configuration is stopped as soon as the central sphere is caged. Thus a minimum number of spheres is added and thus the local volume fraction is also a minimum or at least close to it. A random loose packing could therefore be modeled as a distribution of these cages since each cage satisfies the requirements for random loose packing. The distribution of cages needs to be such that no long-range order is introduced.

The parking and caging numbers, it should be noted, constitute a local description of coordination numbers in random packings. Global correlations in a packing due to collective effects of particles are not taken into account. For random loose packing the collective effects, as mentioned earlier, seem small enough to allow a purely local description via the caging number. However, for random close packing more global correlations, as manifested, for example, by the full pair-distribution function, cannot be ignored. In the field of dynamical arrest lattice models have been developed to incorporate collectivity.[15,16] It is interesting to see in future work, whether the concepts of these lattice models can be used to incorporate global effects in our continuum model.

In lack of an analytical solution for caging by disks with a size ratio $r<1$ we have used an approximation to account for excluded volume effects that reproduces the numerical results quite well. The difference in value between the approximation and computer simulation of the caging number are due to rewriting the problem from sequentially placing n disks to stating that there are already n disks present, which modifies the probability distribution.

From Fig. 3 two radii can be identified in the curve for the caging number. The minimum radius at which the caging number is always three and the maximum radius where the central disk just fits in the pore created by three large spheres. These radii are given by

$$r_{\min} = \frac{1}{\sqrt{2}-1} \approx 2.41 \text{ and } r_{\max} = \frac{1}{(2/\sqrt{3})-1} \approx 6.46. \quad (22)$$

Comparing the caging number and the parking number we see that for $r \leq r_{\min}$, the parking number is larger than the caging number as expected. However, for $r > r_{\min}$ the parking number is below the caging number, because in the calculation of the caging number, noncaging configurations are not taken into account. These noncaging configurations are counted in the calculation of the parking number because it is possible to generate configurations with only two disks. For large r the parking number is thus between two and three. This excluded volume effect also occurs in random bidisperse packings where a small disk can get stuck between two large disks while not being caged according to our definition. For small r the parking number is much larger than the caging number. In bidisperse packings, where the number of small particles is much larger than the number of large particles, the number of contacts on large particles clearly exceeds the coordination number in a packing of equal-sized disks. This could be seen as a parking process of small disks on a large disk. It is interesting to study this effect in bidisperse packings in more detail.[17] Sitharam and Shimizu found a coordination number around 3.3 for loose packings and a coordination number around 4.1 for dense packings[18] of a log-normal distribution of disk sizes. Sinelnikov *et al.* found a contact number for a bidisperse disk system on a plane[19] that did not exceed three for a loose packing from the standpoint of mechanical stability. After compression to the center the average contact number was 4. From the caging numbers in Sec. IV for disk contacts of arbitrary size, it is clear that the number of contacts should indeed be in the range from 3.0 to around 4.0 (see Fig. 3).

The approximation in three dimensions shows the same trend as the two-dimensional case. The minimum radius at which the sphere is always caged with four contacts appears to be 2.41, which is the same as in two dimensions. Three disks with this radius always cage a central disk. Now extend the disks to three-dimensional spheres. The central sphere is caged in the plane. Adding a fourth sphere blocks one translation perpendicular to the plane and leaves one free. The probability to have three spheres in one plane that contains the central sphere is infinitesimally small and thus the four spheres will always cage the central sphere. The maximum radius in which the central sphere can fit in the pores of the four larger spheres is given by

$$r_{\max} = \left(\frac{1}{2}\sqrt{6}-1\right)^{-1} \approx 4.45. \quad (23)$$

For equal-sized three-dimensional spheres the caging number $\langle\gamma\rangle=4.71$ is again much smaller than the parking number $\langle z\rangle=8.7$ and smaller than the caging number for point contacts $\langle\gamma\rangle=7$. An analytical expression for the caging of spheres in three dimensions as was found for the two-dimensional case is a very difficult task because not only p_3 has to be calculated but also p_4 until p_8. To find these probabilities one needs to integrate over the surface of a sphere, which is much more complex than the line integrals needed for two-dimensional disks.

VII. CONCLUSIONS

We report an analytical solution for the caging of a two-dimensional sphere by sequentially placed, contacting neighbor disks with a size ratio equal to or greater than unity. The analytical caging number, which fully incorporates excluded volume effects, agrees well with a numerical simulation of the two-dimensional caging problem.

The caging problem for contacting disks smaller than the central disk can be slightly modified to the calculation of the caging probability for n disks placed simultaneously on the central disk. This modified problem can be solved exactly and the outcome approximates the numerical result for caging by sequential addition of neighbor disks quite well. In a similar approximate manner we calculate fairly accurate caging numbers for three-dimensional spheres. Extension to d dimensions is possible provided the $(d-1)$-dimensional excluded volume is known.

Our results for nonoverlapping hard spheres show that excluded volume effects substantially reduce the caging number in comparison with caging by uncorrelated contacts. The latter forms an upper bound for the caging number which we rederive using Wendel's formula for the probability for n randomly placed points to share one hemisphere on a d-dimensional sphere.

We have also numerically evaluated the parking number for non-equal-sized disks. A comparison with caging numbers shows that the latter are indicative for the average contact number in random loose packings of monodisperse spheres, whereas parking numbers seem to approach the average coordination number in random close packing. The physical significance of caging and parking numbers is also apparent in random bidisperse packings where, in addition to caging effects for equal-sized particles, one observes the parking number for many small disks simultaneously contacting a large one.

Our calculations relate to a *local* description of coordination in granular matter or colloidal sphere packings. A next step is to model more global correlations, for example, by including additional shells of neighbors in the caging or parking model for random sphere packing to include collective effects.

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APPENDIX A: THE WENDEL FORMULA

Wendel's useful formula (5) appears to be unknown in the context of sphere arrest. For later reference we briefly rederive it. A contact x_i on a d-dimensional sphere is a d-dimensional vector. A vector y is perpendicular to none of the x_i. (y,x_i) represents a dot product. Then the sequence $s_y=\{\text{sign}(y,x_i)\}$ is a random point in the set $S=\{s\}$ of all ordered N tuples consisting of plus and minus signs. A specified s is said to occur if there is a y such that $s_y=s$.

A d-dimensional sphere is a noncaged sphere if all n points lie on one single hemisphere. If all n points are on the same hemisphere then there exists a vector y for which the sequence $s_+=\{+,+,\ldots,+\}$. By definition the probability that a d-dimensional sphere is not caged, $p_{d,n}$ is the probability that s_+ occurs. Since any s can be changed into any other by reflecting appropriate x_i through the origin it follows that all s are equally likely to happen. Hence

$$2^n p_{d,n} = Q_{d,n}, \tag{A1}$$

where n is the number of contacts, and $Q_{d,n}$ is the number of different s that occur. To calculate $p_{d,n}$ it suffices to know $Q_{d,n}$. A contact point x_i is the normal for a hyperplane X_i that cuts a d-dimensional sphere in two. Then Q is the number of sectors formed by hyperplanes X_i because each sector consists of all vectors y for which s_y has a fixed value.

Adding a hyperplane X_n cuts a number of sectors Q^1 in two and leaves a number Q^2 intact. Thus $Q_{d,n-1}=Q^1+Q^2$ and $Q_{d,n}=2Q^1+Q^2$. It follows that

$$Q_{d,n} = Q_{d,n-1} + Q^1. \tag{A2}$$

The intersection of the hyperplane X_n and the d-dimensional sphere is a $(d-1)$-dimensional sphere. The sets of intersections $X_i \cup X_n$ are hyperplanes in $(d-1)$-dimensional space. The union of intersections $\cup_{i=1}^{n-1} X_i \cap X_n$ cut the $(d-1)$-dimensional sphere in $Q_{d-1,n-1}$ sectors. Thus there are $Q_{d-1,n-1}$ intersections upon adding X_n. So

$$Q_{d,n} = Q_{d,n-1} + Q_{d-1,n-1}. \tag{A3}$$

This recurrence relation (A3) was also derived by Peters *et al.*[5] and then used to calculate the caging number directly. Here the probability of finding n points on the same hemisphere will be calculated from the same recurrence relation. From (A1) and (A3) it follows

$$p_{d,n} = \tfrac{1}{2}(p_{d,n-1} + p_{d-1,n-1}) \tag{A4}$$

solving this recurrence relation together with the boundary conditions[20]

$$p_{1,n} = \left(\frac{1}{2}\right)^{n-1} \text{ and } p_{d,n} = 1 \quad \text{if } 0 \leq n \leq d$$

gives

$$p_{d,n} = \left(\frac{1}{2}\right)^{n-1} \sum_{k=0}^{d-1} \binom{n-1}{k}. \tag{A5}$$

For example, in two dimensions $(d=2)$ each contact creates two new sectors. Therefore the number of sectors for the rth contact is $2n$. Substitution in (A1) yields then $p_{2,n} = n(1/2)^{n-1}$ as is also found by directly substituting $d=2$ in (A5).

APPENDIX B: DERIVATION OF THE CAGING NUMBER IN *d* DIMENSIONS

Here we derive the caging number for uncorrelated contacts in d dimensions, making use of Wendel's result for the probability of finding n contacts on a d-dimensional sphere. Substitution of Eq. (5) in Eq. (2) produces

$$\begin{aligned}\langle \gamma \rangle_d &= 1 + d + \sum_{n=d+1}^{\infty} \left(\frac{1}{2}\right)^{n-1} \sum_{k=0}^{d-1} \binom{n-1}{k} \\ &= 1 + d + \sum_{n=d}^{\infty} \sum_{k=0}^{d-1} \left(\frac{1}{2}\right)^{n} \binom{n}{k}.\end{aligned} \tag{B1}$$

The first term in the summation of (B1) is the power series

$$\sum_{n=d+1}^{\infty} x^{n-1} = -\frac{x^d}{x-1}. \tag{B2}$$

The other terms in (B1) can be calculated using (B2)

$$\sum_{n=d+1}^{\infty} x^{n-1}\binom{n-1}{k} = \frac{x^k}{k!}\frac{\partial}{\partial x^k}\sum_{n=d+1}^{\infty} x^{n-1} = \frac{x^k}{k!}\frac{\partial}{\partial x^k}\left(\frac{-x^d}{x-1}\right). \tag{B3}$$

The kth derivative of (B2) is

$$\frac{\partial}{\partial x^k}\left(\frac{-x^d}{x-1}\right) = \sum_{i=0}^{k} \frac{(-1)^{k+1-i}\binom{d}{i}k!x^{d-i}}{(x-1)^{k+1-i}}. \tag{B4}$$

Combining pairs of two terms of the summation in (B1), such as $k=0$ and $k=d-1$, $k=1$ and $k=d-2$, gives for the kth pair,

$$\sum_{n=d+1}^{\infty} x^{n-1}\left[\binom{n-1}{k} + \binom{n-1}{d-1-k}\right] = x^k\sum_{i=0}^{k}\frac{(-1)^{k+1-i}\binom{d}{i}x^{d-i}}{(x-1)^{k+1-i}} + x^{d-1-k}\sum_{i=0}^{d-1-k}\frac{(-1)^{d-k-i}\binom{d}{i}x^{d-i}}{(x-1)^{d-k-i}}. \tag{B5}$$

Setting x to $\frac{1}{2}$

$$\left(\frac{1}{2}\right)^{d-1}\left[\sum_{i=0}^{k}\binom{d}{i} + \sum_{i=0}^{d-1-k}\binom{d}{i}\right] = \left(\frac{1}{2}\right)^{d-1}\left[\sum_{i=0}^{d}\binom{d}{i} - \sum_{i=d-k}^{d}\binom{d}{i} + \sum_{i=0}^{k}\binom{d}{i}\right]. \tag{B6}$$

Using

$$\sum_{i=0}^{d}\binom{d}{i} = 2^d \tag{B7}$$

and realizing that the last two terms in (B6) cancel yields

$$\left(\frac{1}{2}\right)^{d-1}\left[\sum_{i=0}^{d}\binom{d}{i}\right] = 2 \tag{B8}$$

In the summation in Eq. (B1) there are $\frac{1}{2}d$ pairs that all contribute two to the summation, if d is even, and $(d-1)/2$ pairs if d is uneven. Inserting (B8) in to the summation in Eq. (B1) leads to

$$\sum_{n=d}^{\infty}\sum_{k=0}^{d-1}\left(\frac{1}{2}\right)^n\binom{n}{k} = \frac{d}{2} * 2 = d. \tag{B9}$$

For uneven d, the single term for $k=(d-1)/2$ needs to be evaluated, this term contributes one, so the sum in (B1) is also equal to d for uneven d. Substitution of (B9) in (B1) yields finally

$$\langle\gamma\rangle_d = 2d + 1. \tag{B10}$$

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