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Statistical characterization of the pore space of random systems of hard spheres

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ABSTRACT

An improved statistical characterization of disordered structures such as metallic glasses, random porous media, or granular matter is presented. Suitable structure models follow the idea of dense random packed spheres, where the spheres represent atoms and particles in the case of metallic glasses and porous or granular matter, respectively. The geometry of the empty space between the atoms or particles is described by means of the already otherwise successful concept of so-called contact distributions. Their exact mathematical forms are unknown for hard sphere systems. Knowledge on these is obtained by means of Monte Carlo simulations of the structure models. The numerical results are approximated by simple and general mathematical expressions, with parameters that can be easily determined. These may serve as additional tools for the structural characterization of disordered matter, including systems of partly penetrable spheres.

1. Introduction

The statistical characterization of random many-particle systems and of porous structures is an important problem in the context of the study of non-crystalline microstructures with the aim to understand its relation to macroscopic properties [1]. Though there is considerable progress in experimental techniques and data processing (see, e.g., [2–4]) the experimentally accessible information on the structure of non-crystalline solids is basically limited. The only way out seems to be the combination of measurement, modeling, and statistical analysis of models fitting experimental data.

One example for this method is the reversed Monte Carlo modeling of atomic structure (see, e.g., [5] for the combination of an extended X-ray fine structure spectroscopy (EXAFS) study of amorphous $Ni_{80}P_{20}$ alloys with reversed Monte Carlo). Another important concept for the generation of models of disordered structures is the model of dense random packing of spheres. This model was proposed by Bernal [6] as an approach to the structure of simple liquids. It has been generalized and applied to, e. g., metallic glasses [7–9], porous media [10,11], and granular matter [12]. Early reviews of construction algorithms and applications to amorphous metals and alloys were published by Cargill [13] and Finney [14]. Recent developments will be discussed below.

Once a structure model has been generated then various methods are available for its statistical analysis. An important direction is the study of the geometry of the pore space. For systems of hard spheres, an important approach is the Voronoi–Delaunay method of Medvedev, see Refs. [15,16]. It is directed to the interstitial spaces between the spheres. The present paper, however, considers the fact that the pore space does not consist of isolated pores with a simple geometry. In contrast, often it is infinitely connected, so that it does not make sense to speak about single pores.

In such a situation the so-called contact distributions are useful. They belong to a unified concept of stochastic geometry, see Refs. [10,17]. The linear contact distribution function, $H_l(z)$, describes the linear extent of the pore space and is closely related to the chord length probability density, $p(z)$, and the lineal-path function, $L(z)$, as described in Ref. [1]. The spherical contact distribution $H_s(r)$ characterizes in some way the size of the pores and is closely related to the pore size distribution [18] and the nearest neighbour distribution [1,19], historically also called Hertz distribution [20]. Formulas for the spherical contact distribution function are of great value for deriving formulas for porosity and specific surface for cherry-pit models, see Ref. [21]. (A cherry-pit model is generated starting from a hard sphere structure. The radii of the spheres are enlarged by an arbitrary factor so that the spheres are no longer 'hard' but interpenetrate partially. One obtains a two-phase structure which is called cherry-pit model.)

Fig. 1 illustrates the definition of these distributions. The chord length distribution is measured as follows: A straight line is chosen at random. The intersection of this line with the spheres system divides the line in chords inside the pore space (bold lines in Fig. 1A) and in segments inside the hard phase. The frequency of chords with length z is described by the chord length probability density $p(z)$. The linear

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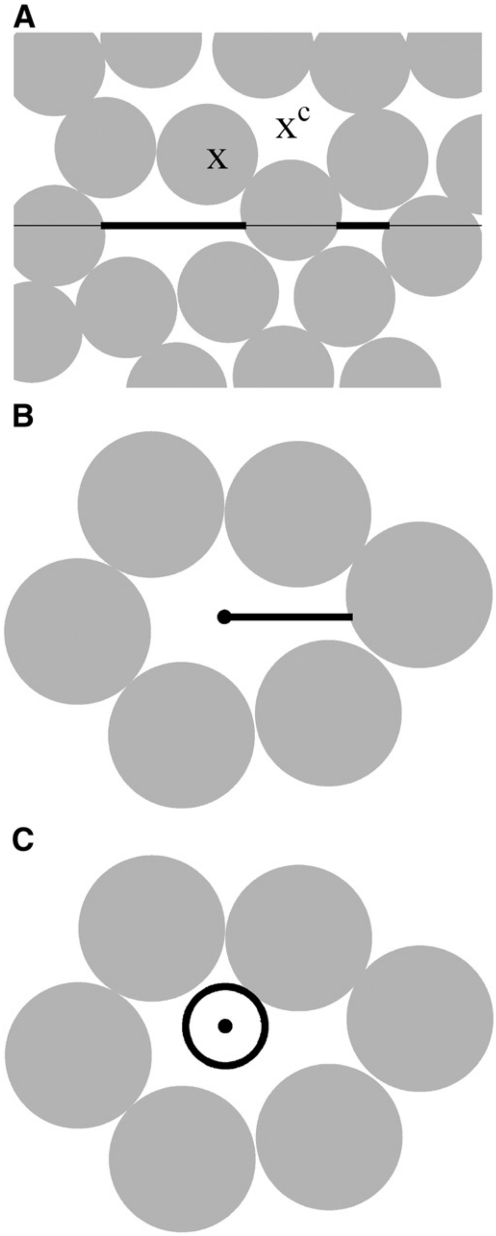

Fig. 1. Measurement of chord length distribution (A), linear contact distribution (B), and spherical contact distribution (C) in the pore space (X^c) outside the solid phase (X, gray). See text for detailed explanation.

contact distribution is determined by generating a random test point in the pore space (small disc in Fig. 1B), drawing a ray from the random point in prescribed direction, and measuring the distance from the test point to the intersection with the nearest sphere surface (bold line in Fig. 1B). The linear contact distribution function, $H_l(z)$, is the distribution function of the random distances determined in this way. The spherical contact distribution, $H_s(z)$, is the distribution function of the distance from a random test point situated in the pore space (small disk in Fig. 1C) to the nearest point of the hard phase. This distance is equal to the radius of the sphere centered at the test point and contacting the hard phase.

In the present paper, the two functions $H_l(r)$ and $H_s(r)$ are investigated for systems of hard spheres. For the case of equilibrium systems, [1] contains formulas which are discussed here, while for packings of hard spheres simulations and a large sample of a real packing of spheres are the basis.

Surprisingly, the contact distributions seem to be for both model types quite similar, while, of course, the topological structure differs greatly: In equilibrium systems the spheres are all isolated, but in packings they have many contacts and usually there are no isolated spheres.

From the practical point of view it is the main progress achieved by the present study that the contact distribution functions can be approximated by simple mathematical expressions. This is expected to be useful for the discussion of physical properties of disordered media in terms of structural characteristics, for example, the distribution of excess free volume in metallic glasses and its impact on mechanical behavior.

2. Explanation of the models and the statistical descriptors

2.1. Hard sphere system models

In the following a porous medium is considered, where X is the hard phase and its complement, X^c, the pore space (see Fig. 1). This X is always a many-particle system built of hard spheres, which is statistically homogeneous or homogeneous ('stationary' in terms of [10]) and isotropic.

This paper considers two types of random systems of hard spheres:

1. Hard sphere systems in equilibrium as in Ref. [1], p. 66. Such a system is determined by the hard sphere potential, and its distribution heavily depends on particle density or porosity. In such a system all spheres are isolated, but the inter-particle distances can be very short. For this model many approximations have been developed by means of methods of statistical physics.
2. Packed hard spheres as discussed in Ref. [1], p.88. For this second structure, there is today no mathematical model. But there are real structures which give an idea of the meaning of such systems and offer the possibility to estimate statistical characteristics [22]. Several simulation algorithms try to generate such systems numerically. An example is the force-biased algorithm (FBA) [23], which goes back to Jodrey and Tory [24].

Basically, FBA is a method where a random initial arrangement of spheres is subjected to repeated compression and rearrangement in order to obtain densely packed systems of hard spheres. During compression, the spheres may interpenetrate. Overlapping spheres are then shifted in such a way that the degree of overlapping is reduced. The shifting distance is calculated by means of a quantity which is similar to a force in classical mechanics. This 'force' can be defined differently. In the present paper, a variant is used which makes the FBA very fast [23]. This variant was tested and compared to results obtained by other simulation techniques. The maximum packing fraction of mixtures of spheres with two different diameters obtained using FBA and by a different method [25] agreed very well in a broad range of size ratio and composition. In recent studies [26,27] the FBA method was successfully compared to the modelling technique proposed by Miracle [28] where the idea of atomic size distribution plots was used to improve the general understanding of amorphous structures.

The volume or covering fraction of X is denoted by ϕ and the specific surface density (mean surface content of X per volume unit) by s. The porosity is then $1-\phi$.

These descriptors can in principle be also defined for more general two-phase structures, not only for such related to spheres, and also many of the following formulas hold true in the general case.

2.2. Linear contact distribution function

The lineal-path function $L(z)$ is the probability that a randomly placed line segment of length z lies completely in the pore space X^c, outside the system X of spheres. The linear contact distribution function $H_l(z)$ is a conditional complement to $L(z)$, it is the probability that the segment is not completely in the pore space under the condition that one of its endpoints is in the pore space. Thus

$$H_l(z) = 1 - \frac{L(z)}{1-\phi}. \tag{1}$$

The function $H_l(z)$ can be interpreted as the distribution function of the distance from an arbitrary test point in X^c to the next point in X in some prescribed direction (see Fig. 1).

The chord length probability density function $p(z)$ is the probability density function of the chord lengths, where "chords" are the line segments outside of X on an infinitely long line (see Fig. 1). It is well known, see Ref. [1], p. 47, that the chord length density function is related to the lineal-path function by

$$p(z) = \frac{\ell_c}{1-\phi}\frac{d^2L(z)}{dz^2}, \tag{2}$$

where ℓ_c is the mean chord length given by

$$\ell_c = \int_0^\infty zp(z)dz. \tag{3}$$

Equivalent to Eq. (2) is the formula

$$H_l(z) = \frac{1}{\ell_c}\int_0^z [1-P(t)]dt \tag{4}$$

with

$$P(t) = \int_0^t p(u)du. \tag{5}$$

For general X (not only such constructed by spheres) the following well-known formula holds:

$$\ell_c = \frac{4(1-\phi)}{s}, \tag{6}$$

see Ref. [10], p. 209. Note that in the case of a many-particle system with mean particle volume $\bar{v}$ and mean surface area $\bar{s}$, it is

$$\phi = \lambda\bar{v}, \tag{7}$$

and

$$s = \lambda\bar{s}, \tag{8}$$

where λ is the mean number of particles per volume unit.

Then

$$\ell_c = \frac{4(1-\lambda\bar{v})}{\lambda\bar{s}}, \tag{9}$$

and in the case of identical spheres with diameter D

$$\ell_c = \frac{2(1-\phi)}{3\phi}D. \tag{10}$$

Eq. (4) yields for the derivative $h_l(z)$ of $H_l(z)$ at $z=0$

$$h_l'(0) = \frac{1}{\ell_c}. \tag{11}$$

This shows that the density function $h_l(z)$ corresponding to $H_l(z)$ satisfies the two relations

$$\int_0^\infty rh_l(r)dr = \ell_c \tag{12}$$

and

$$h_l(0) = \frac{1}{\ell_c}. \tag{13}$$

A well-known probability density function $f(x)$ which satisfies

$$\int_0^\infty xf(x)dx = \ell_c \tag{14}$$

and

$$f(0) = \frac{1}{\ell_c} \tag{15}$$

is the exponential density function

$$f(x) = \mu e^{-\mu x} \tag{16}$$

with $\mu = \frac{1}{\ell_c}$. Note that in the case $h_l(r) = \mu e^{-\mu r}$ one obtains by Eq. (4)

$$p(z) = \mu e^{-\mu z}, \tag{17}$$

i.e. then chord length and linear contact distribution coincide.

2.3. Spherical contact distribution function

The spherical contact distribution $H_s(z)$ is the distribution function of the random distance from a random test point in X^c to the nearest point of X [10], see Fig. 1C. In the notation of Ref. [1], p.48, it is

$$H_s(z) = 1 - F(z). \tag{18}$$

The probability density function related to $H_s(z)$ is here denoted by $h_s(z)$, $h_s(z) = H'_s(z)$; in Ref. [1] it is denoted as $P(\delta)$. It appeared first in Ref. [29] in the context of pore size characterization. A well-known relation states a general relation between $h_s(0)$, ϕ and s:

$$h_l(0) = \frac{s}{1-\phi}, \tag{19}$$

see Ref. [1], formula (2.79) and Ref. [10], formula (6.2.4).

3. The linear contact distribution for hard sphere systems

3.1. Identical spheres

It is surely extremely difficult to obtain the exact form of the lineal statistical measures for both many-particle systems with hard spheres. But approximations are available. For the case of the equilibrium system with identical spheres of diameter D, the paper [30] uses a series expansion to obtain an approximation for $L(z)$ and $p(z)$: the exponential distribution (Eq. 17) with $\mu = 1/\ell_c$ with ℓ_c as given in Eq. (10). The exponential distribution was also empirically observed in Refs. [31–33].

This is a remarkable result: The exponential distribution is the exact form of the linear contact distribution for the case of a completely random distribution of the sphere midpoints and fully penetrable spheres, see Ref. [1]. So it is obvious that the linear contact distribution and all other linear statistical measures are not powerful in model testing. However, it is quite satisfying that the distribution depends only on one parameter: Also the equilibrium model depends only on the single parameter ϕ, if D is given. Thus one can expect no significant differences when physical properties are strongly related to linear statistical measures.

In order to explore the form of the linear contact distribution for random packings of hard spheres, the authors carried out simulations. The following reports the results of these simulations.

Random packings of 10,000 identical hard spheres were generated by means of the force-biased algorithm [23]. Then for 10^6 random test points outside the spheres the lengths of the line segments 'test point → nearest sphere point' in given direction were determined. This yielded samples of lengths corresponding to $H_l(z)$ and $h_l(z)$. By means of a kernel estimator [34] estimates of $h_l(z)$ were obtained.

Fig. 2 shows the function $log(h_l(z))$ for $\phi = 0.65, 0.654, 0.66, 0.67, 0.69, 0.70, 0.71$ as obtained by simulation and the theoretical linear functions $a–bz$ that belong to the exponential distribution with parameters given by $\mu = 1/\ell_c$. Obviously, the exponential distribution is an excellent approximation for the linear contact distribution also for the simulated packings. Only for the larger values of ϕ small deviations appear. The fluctuations of the simulated curves increase with increasing z/D values. Note that the fluctuations are not errors which could be described by error bars but are exact results for the specific model consisting of 10,000 spheres. In other words the fluctuations are due to the finite size of the simulation box. This applies for all figures presenting simulation results as well.

In order to demonstrate the quality of the approximation also numerically, the slopes b of the linear functions in Fig. 2 are listed in the following table together with the theoretically values of $\mu = \frac{1}{\ell_c}$ with ℓ_c as given by Eq. (10) (Table 1).

It is interesting to consider as reference structures crystalline spheres system with volume fraction $\phi = \pi/\sqrt{18}$, which is the volume fraction of face-centred cubic (fcc) and hexagonal closed packing (hcp) structures. For very high densities ϕ, i.e., for $\phi \to \pi/\sqrt{18}$, it is expected that the simulated sphere packings become nearly crystalline, approximate regular packings, which may then serve as reference systems. The authors' simulations suggest a 'convergence' towards packings with statistical properties similar to those of fcc packings, see also the discussion in Ref. [35]. Packings with local hcp order were not observed in Ref. [35], but will be considered here as well because of their packing fraction of $\phi = \pi/\sqrt{18}$.

Therefore, it is interesting to consider the chord length distributions and linear contact distributions also for regular packings. Fig. 3 shows analogously to Fig. 2 $logh_l(z)$ for fcc and hcp packings. Again these curves can be well approximated by straight lines that belong to exponential distributions with parameter $\mu = 1/\ell_c$ and ℓ_c given by Eq. (10).

Table 1
The slope b of the linear functions approximating $log(h_l(z))$ and the theoretical values of μ.

ϕ	b	μ
0.65	2.84	2.79
0.654	2.94	2.84
0.66	2.93	2.90
0.67	3.02	3.03
0.69	3.19	3.28
0.70	3.46	3.42
0.71	3.64	3.56

By the way, in fcc as well as in hcp packings there can infinite straight cylinders be placed in the pore spaces, as shown in Fig. 4. Therefore, very long chord lengths are indeed possible in these regular packings, which may confirm the use of the exponential distribution as an approximating distribution.

3.2. Random spheres

In the next step also packings of hard spheres of random diameters were investigated. Again the exponential distribution turned out to be an excellent approximation.

Figs. 5 and 6 show the h_l-functions in logarithmic form for some bidisperse packings and packings of spheres with diameters following Gaussian distributions. Also these can be very well approximated by straight lines and the slopes are given by $\mu = 1/\ell_c$ with ℓ_c as in Eq. (6), where mean volume v and mean surface area s are calculated using the diameter distributions.

4. Spherical contact distributions

The spherical contact distribution is probably still a bit more complicated than the linear one. In the literature different approximations are given. One of them is implicitly given in Ref. [18]. That paper contains an approximation for the spherical contact distribution function $H_s^P(z)$ of the point process of sphere centres. (This is the distribution function of the distance from a random test point to the

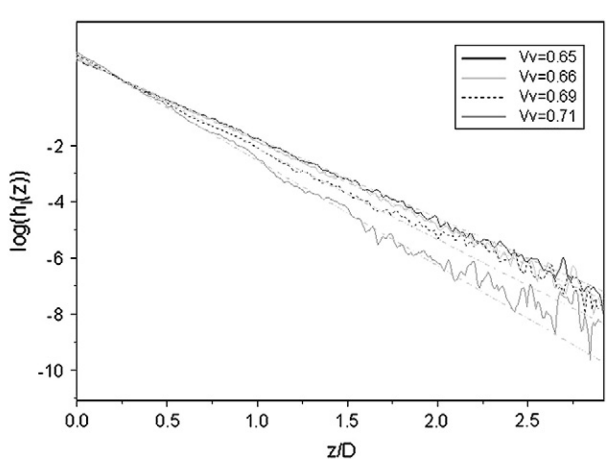

Fig. 2. The functions $log(h_l(z))$ for packings of identical hard spheres with different volume fractions and the approximating linear functions —·—. Variable z is defined in Eq. (1), D is the sphere diameter. The linear form indicates the similarity to exponential distributions.

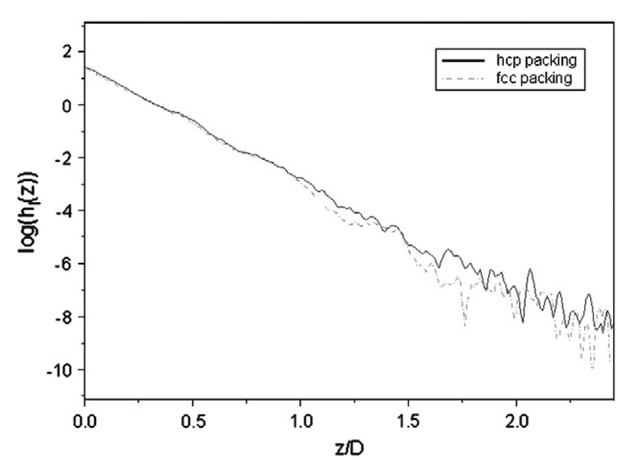

Fig. 3. Functions $log(h_l(z))$ estimated for regular packings of type fcc and hcp. Their nearly linear form indicates some similarity to the exponential distribution.

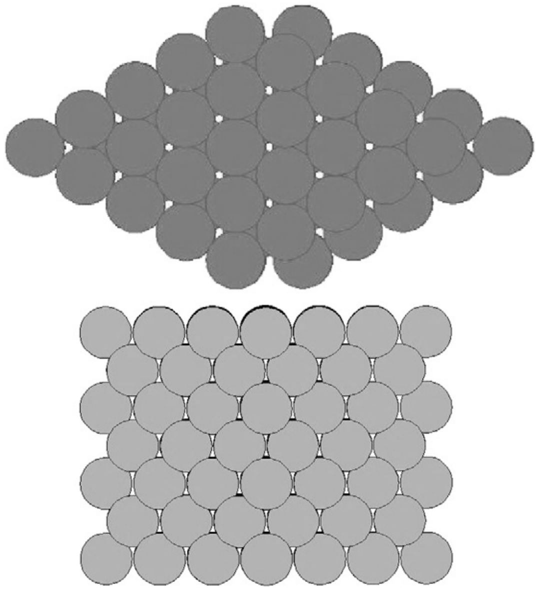

Fig. 4. Cross-sections through regular sphere packings. The small white objects are cross-sections of infinite (non-circular) cylinders outside the spheres. hcp (top) and fcc (bottom) with [001] and [110] direction perpendicular to the image plane for hcp and fcc, respectively.

nearest sphere centre.) The $P_0(R)$ in Ref. [18] is the same as $1-H_s^P(R)$ and can be used to obtain the following formula for $h_s(z)$:

$$h_s(z) = \frac{\phi}{(1-\phi)^2}\left\{24(1+2\phi)\zeta^2-36\phi\zeta\right\} \times \\ \times\, exp\left[\frac{\phi}{(1-\phi)^2}\left\{-8(1+2\phi)\zeta^3+18\phi\zeta^2+1-\frac{5}{2}\phi\right\}\right], \quad (20)$$

$$\zeta = z+\frac{1}{2}$$

In this formula the sphere diameter is assumed to be 1.

The authors of Ref. [18] did not clearly write to which model this formula belongs. The derivation is based on the Percus–Yevick approximation, a method that is designed for equilibrium systems. However, in the discussion of the paper it is then used also for packings, simulated ones by Tory and Finney. (Perhaps Gotoh et al. did believe that their formula is applicable for both hard sphere models.)

For the case of the equilibrium model, Ref. [1], p. 143, contains formulas which can be used to obtain the following approximative formula for $h_s(z)$, again for diameter 1:

$$h_s(z) = 24\phi\left(a_0\zeta^2+a_1\zeta+a_2\right)\times \\ \times\, exp\left[-\phi\left(8a_0\zeta^3+12a_1\zeta^2+24a_2\zeta+a_3\right)\right], \quad (21)$$

$$\zeta = z+\frac{1}{2}$$

with

$$a_0 = \frac{1+\phi+\phi^2-\phi^3}{(1-\phi)^3}$$

$$a_1 = \frac{\phi\left(3\phi^2-4\phi-3\right)}{2(1-\phi)^3}$$

$$a_2 = \frac{\phi^2(2-\phi)}{2(1-\phi)^3}$$

$$a_3 = -(a_0+3a_1+12a_2)$$

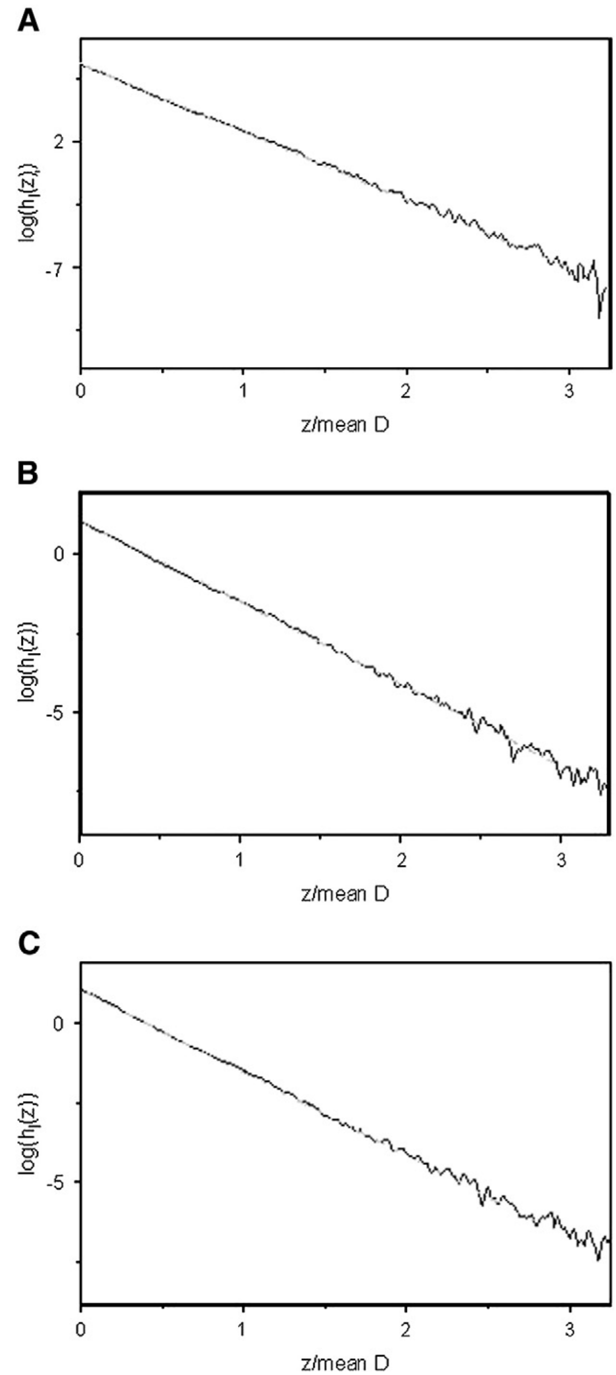

Fig. 5. The functions $log(h_l(z))$ for bidisperse sphere packings with $R_2/R_1=2$ and different relative volumes v_r of the small spheres (v_r gives the fraction of the volume of the packing which is captured by the small spheres): A) $v_r=0.5$ B) $v_r=0.7$ and C) $v_r=0.9$.

Fig. 7 shows the curves for $h_s(z)$ using the formulas from Eqs. (20) and (21) for diameter 1 and $\phi=0.64$.

For comparison three further curves are shown: $h_s(z)$ for

a) a packing simulated with the force-biased algorithm,
b) the natural packing of hard acrylic beads described in Ref. [22] and statistically analyzed as in Ref. [21] and
c) the probability density function of the half normal distribution as discussed below.

This figure encourages to believe that the force-biased algorithm produces hard sphere systems which behave statistically similar as real packings of hard spheres, what was also demonstrated in Ref.

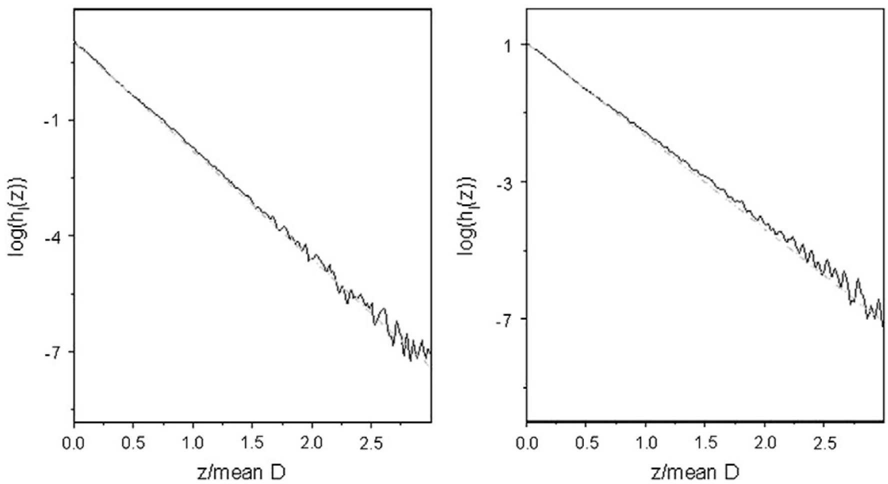

Fig. 6. The function $log(h_l(z))$ for packings with Gaussian diameter distribution with coefficient of variation $\eta = 0.1$ (left) and $\eta = 0.28$ (right).

[21]. Therefore, now results are presented which were obtained by means of the force-biased algorithm for the probability density functions $h_s(z)$ of the spherical contact distribution. The statistical method is analogous to that applied to explore $h_l(z)$. For 10^6 random test points outside the spheres in the simulated packings the lengths of the line segments test point → nearest sphere point in arbitrary direction were determined.

Note that the curves calculated from the formulas proposed in Refs. [1,18] are not monotonous but show a maximum at small z/D. In contrast, in all of our simulations, for identical and random spheres, and for the natural packing, we always observed decreasing $h_s(z)$; also the density function of the half normal distribution is monotonically decreasing. Therefore, at least for random hard sphere packings, the half normal distribution gives a better approximation to $h_s(z)$ than the formulas proposed in Refs. [1,18].

Fig. 8 shows the results for packings of identical spheres with volume fractions $\phi = 0.65, 0.654, 0.66, 0.67, 0.69, 0.70$ and 0.71. The functions $log(h_s(z))$ are nearly linear in dependence on z^2/D^2. More precisely, the functions $h_s(z)$ can be well approximated by the doubled positive part of the density function of a normal distribution with mean value zero, i.e.

$$h_s(z) = \frac{2}{\sqrt{2\pi}\sigma} exp\left(-\frac{z^2}{2\sigma^2}\right), \text{ for } z \geq 0, \tag{22}$$

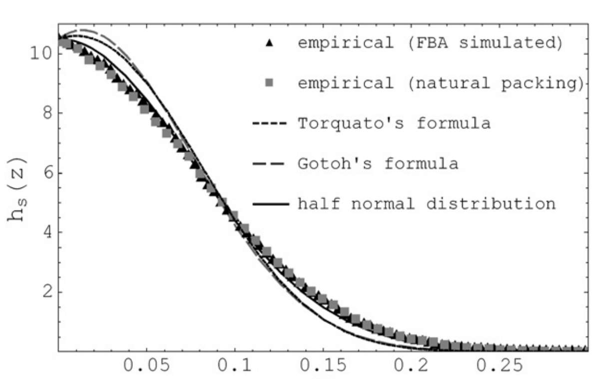

Fig. 7. The functions $h_s(z)$ for hard sphere systems with $D = 1$ and $\phi = 0.64$ as given by the approximations of Gotoh et al. and Torquato, for a real packing of acrylic beads and for a packing simulated with the force-biased algorithm. These four curves are compared with the half normal density function with adapted parameter σ.

The corresponding mean is

$$m_s = \sqrt{\frac{2}{\pi}}\sigma. \tag{23}$$

In the statistical literature this distribution is called 'half normal distribution', see Ref. [36].

Eqs. (19) and (20) yield the following relation for the parameter σ of the half normal distribution:

$$\sigma = \frac{2(1-\phi)}{\sqrt{2\pi}s} \tag{24}$$

or, in terms of ϕ and D,

$$\sigma = \frac{(1-\phi)D}{3\sqrt{2\pi}\phi}. \tag{25}$$

Fig. 9 shows the values of σ in Eq. (22) in comparison with statistically estimated values $\hat{\sigma}$ from the 10^6-samples, assuming half normal distribution. The estimator is

$$\hat{\sigma} = \sqrt{\frac{\pi}{2}}\bar{x}, \tag{26}$$

where $\bar{x}$ is the mean of the 10^6 lengths. Here the formula for the mean of the half normal distribution is used.

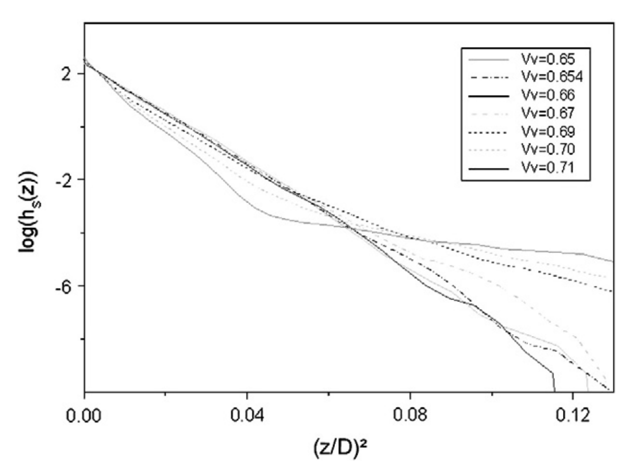

Fig. 8. The functions $log(h_s(z))$ for packings of identical spheres with volume fractions from $\phi = 0.65$ to $\phi = 0.71$. The abscissa is scaled as $(z/D)^2$.

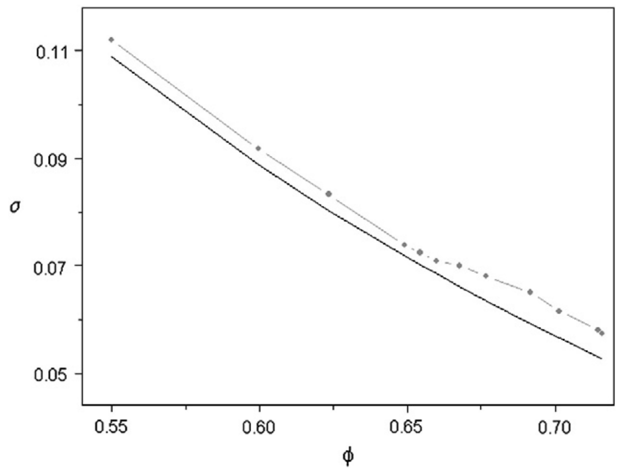

Fig. 9. The relationship between ϕ and σ as obtained statistically (data points) and according to formula (22) (solid line), here $D=2$.

The authors do not have a mathematical explanation for the occurrence of the half normal distribution; it has nothing to do with the central limit theorem. It is clear that the approximation cannot be true for very large values of z: While the half normal distribution has an infinite tail, the tail of $h_s(z)$ must be finite, since it is impossible to place arbitrarily large spheres in the pore space of dense systems of spheres, while, as Fig. 3 shows, very long line segments can be placed). The spherical contact distribution of a Boolean model differs from the form given by the half normal distribution; it has an infinite tail.

In some approximation the finding for identical spheres remains true for the case of random hard spheres. This is shown again for the packings of random spheres considered for the case of linear contact distribution, see Fig. 10. The parameter σ is now determined by Eq. (25), with s calculated by means of Eq. (8) using the second moment of sphere diameters. The curves show also clearly the deviation from the half normal distribution for large z.

5. Discussion

This paper suggests that for both random hard sphere models (with identical or random diameters) the linear contact distribution function is in excellent approximation an exponential function. The parameter of the exponential distribution is given by a simple formula, which appears already in Ref. [30]. The authors observed similar results also for the so-called cherry-pit model [1], but there the parameter formula is more complex. And, as already mentioned, the exponential distribution is the exact distribution in the case of the so-called Boolean model for fully interpenetrating particles and completely random centres. By the way, the exponential form of $h_l(z)$ holds not only for spheres, but also for arbitrary convex particles, see Refs. [1,10].

Since the formulas (6) and (11), which are the heuristic basis of the exponential approximation, are true for general convex particles, one may conjecture that approximative exponential functions will appear also for packings of hard non-spherical convex particles, as long as the packings are isotropic.

Summarizing one may say that exponential lineal-path functions can be assumed for many random structures consisting of hard particles. The fact that a statistically obtained $L(z)$ is an exponential function says therefore only little on the corresponding geometrical microstructure. For small samples, statistical methods are hardly able to detect deviations from exponentiality. This means also that different classes of real structures like simple liquids [6], metallic glasses [7], or granular matter [12] can be characterized by the same type of exponential lineal-path functions regarding their pore structure.

On the other hand, there are of course many models with non-exponential $L(z)$, for example structures complementary to those considered in this paper, when changing the roles of X and X^c. Structures with non-overlapping spherical pores do have quite different linear contact distributions.

The present results show that the exponential form for the linear contact distribution and the half normal distribution form for the spherical contact distribution describe statistical features of a broad class of random hard sphere-based models for non-crystalline and porous solids. The half normal approximation for the spherical contact distribution is shown to be significantly better than the previous approaches in Refs. [1,18].

The authors believe that the knowledge of good approximations for the linear path functions will be useful for studies related to phenomena like diffusion and percolation while the spherical contact distribution seems to be of interest for processes requiring some free volume such as rearrangement or particles in granular matter or

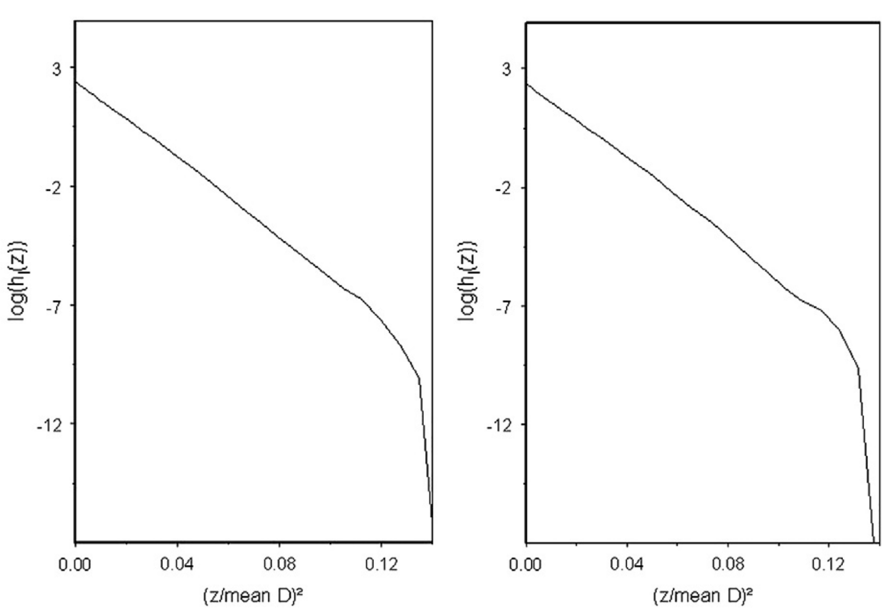

Fig. 10. The function $log(h_s(z))$ for a packing with bidisperse diameters with diameter ratio 2, volume fraction 0.68 and relative volume fraction $v_r=0.5$ of small spheres (left) and with Gaussian distributed diameters with volume fraction 0.65 and coefficient of variation of 0.28 (right).

viscosity and plastic deformation in liquids and amorphous metals, respectively.

6. Conclusions

Contact distributions are shown to enrich the arsenal of tools for the characterization of the class of disordered systems which can be modeled by dense packings of hard spheres. Both the linear and the spherical contact distribution are quantitative measures for the geometrical properties of the pore space of the systems. The linear contact distribution is in good approximation the exponential distribution, while the spherical contact distribution can be well approximated by the so-called half normal distribution. The authors are sure that these conclusions will be valuable for the discussion of physical properties of related materials that depend on quantities like free path length or excess free volume.

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