Theory of random packings

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Abstract. We review a recently proposed theory of random packings. We describe the volume fluctuations in jammed matter through a volume function, amenable to analytical and numerical calculations. We combine an extended statistical mechanics approach ‘a la Edwards’ (where the role traditionally played by the energy and temperature in thermal systems is substituted by the volume and compactivity) with a constraint on mechanical stability imposed by the isostatic condition. We show how such approaches can bring results that can be compared to experiments and allow for an exploitation of the statistical mechanics framework. The key result is the use of a relation between the local Voronoi volume of the constituent grains and the number of neighbors in contact that permits a simple combination of the two approaches to develop a theory of random packings. We predict the density of random loose packing (RLP) and random close packing (RCP) in close agreement with experiments. Theoretical results are well reproduced by numerical simulations that confirm the essential role played by friction in determining both the RLP and RCP limits. Finally we present an extended discussion on the existence of geometrical and mechanical coordination numbers and how to measure both quantities in experiments and computer simulations.

Keywords: granular matter, random close packing, statistical mechanics

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I. STATISTICAL MECHANICS OF JAMMED MATTER

Conventional Statistical Mechanics uses the ergodic hypothesis to derive the microcanonical and canonical ensembles, based on the quantities conserved, typically the energy $E$ [1]. Thus the entropy in the microcanonical ensemble is $S(E) = k_B \log \{\delta(E - \mathcal{H}(p, q))\}dpdq$, where $\mathcal{H}(p, q)$ is the Hamiltonian. This becomes the canonical ensemble with $\exp[-\mathcal{H}/(\partial S/\partial E)]$. Experiments [2, 3, 4, 5] indicate that systematically shaken granular materials show reversible behavior, and the analogue of the conserved quantity is the volume $V$, thus the micro-canonical ensemble or $V$-ensemble is [6, 7, 8, 9, 10, 11, 12]:

$$\Omega(V) = \exp[S(V)/\lambda] = \int \delta(V - \mathcal{W}(\vec{r}_i)) \Theta_{\text{jam}}(\vec{r}_i) d\vec{r}_i,$$

(1)

where $\Theta_{\text{jam}}(\vec{r}_i)$ is a function that defines the jammed configuration. As a minimum requirement the jamming function $\Theta_{\text{jam}}(\vec{r}_i)$ should ensure touching grains, and obedience to Newton’s force laws. $\vec{r}_i$ denotes the particle positions in the system and $\mathcal{W}(\vec{r}_i)$ is the volume function defining the volume associated with each grain (see below). This gives a canonical ensemble of $\exp[-\mathcal{W}(\partial S/\partial V)]$. Just as $\partial E/\partial S = T$ is the temperature in equilibrium system, the temperature-like variable in granular systems is the compactivity $X = \partial V/\partial S$. In Eq. (1), $\lambda$ is the analogue of the Boltzmann constant.

Thermodynamic analogies may illuminate methods for attempting to solve certain problems, but inevitably fail at some point in their application. The mode of this failure is an interesting phenomenon, illustrated by the compaction experiments of the groups of Chicago, Texas, Paris and Schlumberger [2, 3, 4, 5]. They have shown that reversible states exist along a branch of compaction curve where statistical mechanics is more likely to work. Conversely, experiments also showed a branch of irreversibility where the statistical framework is not expected to work. Poorly consolidated formations, such as a sandpile, are irreversible and a new “out-of-equilibrium” theory is required to describe them. Below we focus on a theoretical description of the reversible branch of the compaction curve focusing on a theory of the random close packed state.

The canonical partition function in the $V$-ensemble is the starting point of the statistical analysis of jamming:

$$Z(X) = \int g(\mathcal{W}) e^{-\mathcal{W}/X} \Theta_{\text{jam}} d\mathcal{W},$$

(2)

where $g(\mathcal{W})$ is the density of states for a given volume $\mathcal{W}$. 

From Eq. (2) we identify three minimal steps in developing analytical solutions which are discussed in the next sections. Section II discusses the need for a volume function in terms of the contact network. Section III discusses the need for a proper definition of jammed state that allows one to define \( \Theta_{\text{jam}} \). Section IV discusses the density of states. Finally in Section V we explain the geometrical and mechanical coordination numbers and how to measure them in Section V.A, and we conclude in Section VI.

II. VOLUME FUNCTION

While it is always possible to quantify the total volume of the system, it is unclear how to treat the volume fluctuations at the grain level. The first step to study the V-ensemble is to find the volume \( W(\vec{r}_i) \) associated to each particle \( \vec{r}_i \) that successfully tiles the system. This is analogous to the additive property of energy in equilibrium statistical mechanics.

Initial attempts included a model volume function under mean-field approximation [6], the work of Ball and Blumenfeld [13] and simpler versions in terms of the first coordination shell [14]. These definitions are problematic since some are not additive, others present problems in polydisperse systems or are proportional to coordination contrary to expectation. In Ref. [15, 16] we have found an analytical form of the volume function in three-dimensions and demonstrated that it is the Voronoi volume of a particle \( i \):

\[
W_{i}^{\text{vor}} = \frac{1}{3} \int \left( \min_{\hat{s}: \hat{s} \cdot \vec{r}_{ij} > 0} \left( \frac{R_{ij}}{2\hat{s} \cdot \vec{r}_{ij}} \right) \right)^3 \, ds,
\]

where \( \vec{r}_{ij} \) is the vector from the position of particle \( i \) to that of particle \( j \), the integration is done over all the directions \( \hat{s} \) forming an angle \( \theta_{ij} \) with \( \vec{r}_{ij} \) as in Fig. 1a, and \( R \) is the radius of the grain. \( R \) will be set to unity for simplicity. While this formula may seem complicated, it has a simple interpretation depicted in Fig. 1a.

The Voronoi construction is additive and successfully tiles the total volume. Prior to this result, there was no analytical formula to calculate the Voronoi volume in terms of the contact network \( r_{ij} \). A further simplification arises when we consider isotropic systems. Then the volume function reduces to the orientation volume, without the average over \( \hat{s} \). We define the reduced free orientational volume function as

\[
\mathcal{w}^s = \mathcal{w}^s_i - V_g,
\]

with \( \mathcal{w}^s_i = V_g \left( \frac{1}{2\pi} \min_{\hat{s}: \hat{s} \cdot \vec{r}_{ij} > 0} \left( \frac{R_{ij}}{2\hat{s} \cdot \vec{r}_{ij}} \right) \right)^3 \), see Fig. 1a (\( V_g \) is the particle volume). This equation allows theoretical analysis in the V-ensemble since it reduces the complicated definition (3) to a more amenable “one-dimensional” volume which can be treated analytically.

The next step is to develop a theory of volume fluctuations to coarse grain \( \mathcal{w}^s_i \) over a mesoscopic length scale. We call this the quasi-particle approximation. It could be considered as well as a mean-field approximation, although mean field is supposed to be exact in infinite dimensions. The approximations used in the present theory are supposed to get better as the dimension increases, but we cannot claim that the theory is exact in large dimensions. Thus, we prefer to call our approximation “quasi-particle” in the spirit of Landau and the quasiparticles as “coordinons”.

The coarsening reduces the degrees of freedom to one variable, the coordination number of each grain, and defines an average volume function which is more amenable to statistical calculations than Eq. (3) as shown in [16]:

\[
w(z) = \langle w^s \rangle_i = \frac{2\sqrt{3}}{z},
\]

valid for monodisperse hard spheres where \( z \) is the geometrical coordination number. For now on we assume \( V_g = 1 \) for simplicity. The available volume per grain is inversely proportional with the coordination number, in agreement with the X-ray tomography experiments (see Fig. 6 in [17] where the volume fraction is \( \phi^{-1} = w + 1 \)).

III. DEFINITION OF JAMMING VIA \( \Theta_{\text{jam}} \): ISOSTATIC ENSEMBLE

The definition of the constraint function \( \Theta_{\text{jam}} \) is intimately related to the proper definition of a jammed state, with a minimum requirement of mechanical equilibrium. In an attempt to define the jammed states in a rigorous mathematical
way, Torquato and coworkers have proposed three categories of jamming [18]: locally jammed, collectively jammed and strictly jammed based on geometrical constraints. Unfortunately this definition cannot be easily extended to frictional systems since it is based on geometry and does not include the contact forces. Other approaches based on minima of the potential energy landscape also fail since such a potential does not exist for frictional grains due to their path-dependency.

Then we define an alternative approach to characterize jamming for the general case of frictional granular matter. In [16] we propose the isostatic condition [19, 20] as a possible formulation of jamming. The isostatic condition implies a mechanical coordination number to be \( Z = 2d \), where \( d \) is the dimension, for frictionless spherical particles and \( Z = d + 1 \) for infinitely rough particles (with interparticle friction coefficient \( \mu \to \infty \)). Numerical simulations [21, 22], experiments [23] and theoretical work [20] suggest that at the jamming transition the system becomes exactly isostatic. However, no rigorous proof of this statement exist. It should be noted that experiments [23] and theoretical work [20] suggest that at the jamming transition the system becomes exactly isostatic. Thus, for shear cycling protocols, a unique relation may not be expected between \( Z \) and \( \mu \); the coordination number smoothly varies between \( Z(\mu = 0) = 6 \) and \( Z(\mu \to \infty) \to 4 \) [24, 16].

We notice that while the relationship between friction and \( Z \) may not be unique, the theory is only based on \( Z \). Thus, given the mechanical coordination number we predict the state of the packing with the compactivity. Additionally, we conjecture that \( \mu \) determines \( Z(\mu) \) if we follow certain protocols as discussed in [16]. These protocols imply compression of a packing from an unjammed state to jamming by following one single continuous path. That is, the path dependent shear forces are not reset by a sudden change in the preparation path. It should be stated that there are other protocols, like shear cycling, that start with a given \( Z \) and can produce packings that continuously compactify until RCP (and even beyond). This is done by effectively changing the path followed by the shear forces at every cycle. Thus, for shear cycling protocols, a unique relation may not be expected between \( Z \) and \( \mu \). However, the theoretical results as derived below are still valid in shear cycling experiment since they concern the relation between \( Z \) and volume. In fact, a shear experiment may be the easiest way to obtain the packings at the RLP line as explained below.

Assuming that a system of hard spheres is isostatic at the jamming transition, Eq. (2) can be written in terms of \( Z \) and the mean-field Eq. (5) can be used in the single-particle (or more precisely quasi-particle) partition function:

\[
\mathcal{Z}_{\text{iso}}(X) = \int_Z e^{-w(z)/X} g(z)dz. \tag{6}
\]

We notice that in principle the coordination number of each particle takes only integer values. However, the coordination number in (6) implies a coarse graining over several particles, and therefore can take non-integer values. Thus the use of an integral in (6) instead of a sum is justified.

This ensemble is referred to as the *Isostatic-ensemble*. Note that the upper limit of integration is \( z = 6 \) [16]. This implies that only disordered packings are included. The solution of such a partition function for monodisperse hard spheres has been done in [16] revealing the phase diagram depicted in Fig. 1b.

This phase diagram predicts a series of important results, such as the value of RCP at \( X = 0 \),

\[
\phi_{\text{RCP}} = 6/(6 + 2\sqrt{3}), \tag{7}
\]

and the lowest density of the RLP at \( X = \infty \),

\[
\phi_{\text{RLP}} = 4/(4 + 2\sqrt{3}), \tag{8}
\]

in close agreement with experiments. The diagram restricts the possible packings to the yellow triangle in Fig. 1b, ranging from frictionless systems with \( Z = 6 \), to infinitely rough grains in the \( Z = 4 \) granular line or G-line.
FIGURE 1. (a) Schematics of the Voronoi volume and the orientational volume associated with particle \( i \). The boundary of the Voronoi cell (shown in two-dimensions for simplicity) corresponds to the irregular pentagon in black which defines \( W_{\text{vor}}^i \). The limit of the Voronoi cell of particle \( i \) in the direction \( \hat{s} \) is the minimum of \( r_{ij} / 2 \cos \theta_{ij} \) over all the particles in the packing, as indicated. This defines the orientational volume \( W_{\text{s}}^i \) which is the volume of the sphere of radius \( r_{ij} / 2 \cos \theta_{ij} \) defined by the dash red circle in the figure. (b) Phase diagram of jamming in the hard sphere plane under the isostatic assumption. All the disordered packings fall within the yellow triangle demarcated by the RCP and RLP lines and the G-line. The isocompactivity lines are in color. (c) Generalization of the phase diagram to the space \((Z, \phi, p)\).

IV. DENSITY OF STATES

A difficult problem is the determination of the density of states \( g(W) \) in Eq. (2). For the simplest case of the Isoensemble from Eq (6), the density of states reduces to

\[
g(z) = (h_\text{z})^z, \tag{9}\]

where \( h_\text{z} \) is a small microscopic constant arising due to the discrete volume space of configurations [16]. The situation is analogous to the discreteness of the configuration space imposed by the Heisenberg uncertainty principle in quantum mechanics. The formula is analogous to the factor \( h^{-d} \) for the density of states in equilibrium statistical mechanics. While the degrees of freedom \( \{p_i, q_i\} \) are continuous, the uncertainty principle imposes the discreteness \( (\Delta p, \Delta q) \) in the configurational space given by \( \Delta p \Delta q \sim h \). This consideration allows for the approximate solution explained in the above section and depicted in the phase diagram of Fig. 1b.

V. GEOMETRICAL VERSUS MECHANICAL COORDINATION NUMBER

It is important to note that the derivation of the volume function in Section II implies nothing about the value of the contact forces; the volume function represents the contribution arising purely from the geometry of the packing. Thus, the coordination number \( z \) appearing in Eq. (5) is the geometrical coordination number related to volume, which is different from the mechanical coordination number \( Z \) that counts the number of contacts per particle with non-zero force related to the isostatic condition and force network.

Having acknowledged a difference between the geometrical coordination number \( z \) in Eq. (5) and the mechanical coordination number \( Z \) which counts only the contacts with non-zero forces, below we discuss the bounds of \( z \) and how to measure it.

Since some geometrical contacts may carry no force, then we have:

\[
Z \leq z. \tag{10}\]

To show this, imagine a packing of infinitely rough \((\mu \to \infty)\) spheres with volume fraction close to 0.64. There must be \( z = 6 \) nearest neighbors around each particle on the average. However, the mechanical balance law requires only \( Z = 4 \) contacts per particle on average, implying that 2 contacts have zero force and do not contribute to the contact force network.

Such a situation is possible as shown in Fig. 2: starting with the contact network of an isostatic packing of frictionless spheres having \( Z = 6 \) and all contacts carrying forces (then \( z = 6 \) also as shown in Fig. 2a), we simply allow the existence of tangential forces between the particles and switch the friction coefficient to infinity. Subsequently, we solve the force and torque balance equations again for this modified packing of infinitely rough spheres but same
Isostatic packing

\( z = 6 \)

\( \mu = 0 \)

\( Z = 6 \)

\( \mu = \infty \)

\( z = 6 \)

\( Z = 4 \)

**FIGURE 2.** (a) Consider a frictionless packing at the isostatic limit with \( z = 6 \). In this case the isostatic condition implies also \( Z = 6 \) mechanical forces from the surrounding particles. (b) If we now switch on the tangential forces using the same packing as in (a) by setting \( \mu \to \infty \), the particle requires only \( Z = 4 \) contacts to be rigid. Such a solution is guaranteed by the isostatic condition for \( \mu \to \infty \). Thus, the particle still have \( z = 6 \) geometrical neighbors but only \( Z = 4 \) mechanical ones.

geometrical network, as shown in Fig. 2b [Notice that the shear force is composed of an elastic Mindlin component plus the Coulomb condition determined by \( \mu \). Thus when \( \mu \to \infty \), the elastic Mindlin component still remains].

The resulting packing is mechanically stable and is obtained by setting to zero the forces of two contacts per ball, on average, to satisfy the new force and torque balance condition for the additional tangential force at the contact. Such a solution is guaranteed to exist due to the isostatic condition: at \( Z = 4 \) the number of equations equals the number of force variables. Despite mechanical equilibrium, giving \( Z = 4 \), there are still \( z = 6 \) geometrical contacts contributing to the volume function.

Therefore, we identify two types of coordination number: the geometrical coordination number, \( z \), contributing to the volume function and the mechanical coordination number, \( Z \), measuring the contacts that carry forces only. This distinction is crucial to understand the sum over the states and the bounds in the partition function.

We have established a lower bound of the geometrical coordination in Eq. (10). The upper bound arises from considering the constraints in the positions of the rigid hard spheres. For hard spheres, the \( Nd \) positions of the particles are constrained by the \( Nz/2 \) geometrical constraints, \( \| \vec{r}_{ij} \| = 2R \), of rigidity. Here \( d \) is the dimension. Thus, the number of contacts satisfies \( Nz/2 \leq Nd \), and \( z \) is bounded by:

\[
  z \leq 2d. \tag{11}
\]

Notice that this upper bound applies to the geometrical coordination, \( z \) and not to the mechanical one, \( Z \), and it is valid for any system irrespective of the friction coefficient, from \( \mu = 0 \to \infty \).

In conclusion, the mechanical coordination number, \( Z \), ranges from 4 to 6 as a function of \( \mu \), and provides a lower bound to the geometrical coordination number, while the upper bound is \( 2d \). A granular system is specified by the interparticle friction which determines the average mechanical coordination at which the system is equilibrated, \( Z(\mu) \).

The possible microstates in the ensemble available for this system follow a Boltzmann distribution Eq. (2) for states satisfying the following bounds:

\[
  Z(\mu) \leq z \leq 2d = 6. \tag{12}
\]

**V.A. How to measure the geometrical coordination number**

Measuring the geometrical coordination number can be a tricky task, in principle. At the onset, it is the coordination number of a single quasiparticle. What we measure in a real packing (numerically or experimentally generated) is an ensemble average of many quasiparticles according to the partition function Eq. (6). Thus, rigorously speaking, it is not possible to isolate a quasi-particle and measure its properties in a real packing. Beyond this caustic and somehow pessimistic remark, yet rigorous, below we offer light at the end of the tunnel by using the theoretical predictions to define an approximative, yet accurate, way to measure the geometrical coordination.

Figure 3 summarizes the predictions of the theory regarding the behaviour of \( z \) and \( Z \) for the packings in the phase diagram. First, we can think that the quasiparticle behaviour is revealed when the system has infinite compactivity and
implying that there are many particles almost touching. We introduce a modified radial distribution function (RDF) coordination. Indeed, it is known that the radial distribution function in contact (giving rise to a zero force) may be close enough to be considered as contributing to the geometrical coordination number.

This result is explained with the analysis offered in Fig. 2 and explained above. The conclusion is that the packings followed up paper in cond-mat.

B. For the limiting case of the RCP line, the contact number should be constant and equal to the maximum coordination, which produces the minimum Voronoi volume: $z = 6$. At the same time, the mechanical coordination number varies from 4 to 6 as we reduce friction to zero.

This result is explained with the analysis offered in Fig. 2 and explained above. The conclusion is that the packings along the RCP line are geometrically the same (with $z = 6$ all of them) but they differ in the value of the forces between the particles as $Z$ varies from 6 to 4. This prediction can be also applied to other packings with lower $Z$ but different $Z$ from 4 to the maximum $Z$ given by the RLP line.

Using this theoretical result, it is easy then to define the geometrical coordination number for real packings and propose a clear way to measure it. The idea is to inflate the particles infinitesimally by a $\Delta r$ value and measure the contacting particles. By setting $\Delta r = 0$, we clearly measure the mechanical coordination. By considering an infinitesimally small $\Delta r$ we should measure the geometrical one. The question is to know what value of $\Delta r$ to use. Here is where the theory comes handy. We know that along the RCP line the packings are the same geometrically. So, whatever the definition of coordination number we use, it should satisfy that after a given $\Delta r$, we should find the same packing structure for the packings along the RCP line and below the given $\Delta r$, the structure should change reflecting the different values of $Z$ for different packings in the RCP line.

Using these considerations, we identify the geometrical coordination as follows. Two particles that may not be in contact (giving rise to a zero force) may be close enough to be considered as contributing to the geometrical coordination. Indeed, it is known that the radial distribution function $g(r)$ has a singularity, $g(r) \sim (r - 0.5)^{-0.5}$ [24], implying that there are many particles almost touching. We introduce a modified radial distribution function (RDF)

![FIGURE 3. Summary of the theoretical findings regarding the range of $z$ and $Z$ along the different iso-$z$, iso-$Z$, and iso-$X$ lines and the J, C, and L-points in the phase diagram.](image-url)
the center of a given ball. When one is obtained for a small value in Supplementary Information Section of \[16\] contains a typo. The correct definition is Eq. (13).

\[
\Theta = \begin{cases} 0 & \text{if } r < R \\ 1 & \text{if } r \geq R \end{cases}
\]

This factor is not crucial for our analysis (as the main constraint is that when \(R = 0\)). Following the definition of Eq. (13), we should get \(Z = 1\) as explained below, but we argue that it is useful since we need to properly normalize by the fact that we are inflating the balls. Please notice that Eq. (29) in Supplementary Information Section of \[16\] contains a typo. The correct definition is Eq. (13).

\[
g_z(r) = \frac{1}{N} \frac{R^2}{r^2} \sum_{i \neq j}^{N} \Theta \left( \frac{r_{ij}}{r - R} - 1 \right) \Theta \left( \frac{r + R}{r_{ij}} - 1 \right), \quad r > R
\]

where \(R\) is the radius of particle, \(N\) is the number of particles, \(r_{ij}\) is the distance of two particle’s centers, \(r_{ij} = |\vec{r}_i - \vec{r}_j|\), and \(\Theta\) is the Heaviside step function. The RDF describes the average value of the number of grains in contact with a virtual particle which has been inflated up to a radius \(r \geq R\), and the factor of \(R^2/r^2\) is the ratio of a real sphere’s area and the virtual one’s. Without the normalization factor \(R^2/r^2\), Eq. (13) is the same definition of coordination as used by Torquato and Zamponi in their analysis of infinite pressure jammed hard sphere glasses \([26, 27]\). This factor is not crucial for our analysis (as the main constraint is that when \(r = R\) we should get \(Z\)) as explained below, but we argue that it is useful since we need to properly normalize by the fact that we are inflating the balls. Please notice that Eq. (29) in Supplementary Information Section of \[16\] contains a typo. The correct definition is Eq. (13).

\[
g_z(r) = \frac{1}{N} \frac{R^2}{r^2} \sum_{i \neq j}^{N} \Theta \left( \frac{r_{ij}}{r - R} - 1 \right) \Theta \left( \frac{r + R}{r_{ij}} - 1 \right), \quad r > R
\]

\(g_z(r)\) measures the number of balls with their volume intersecting the surface of a sphere of radius \(r\) measured from the center of a given ball. When \(r = R\) in (13) we obtain the mechanical coordination number while the geometrical one is obtained for a small value \(\Delta r = \frac{r - R}{2R} \neq 0\) for which we distinctly find a signature from computer simulations, unambiguously defining it at \(\Delta r = 0.04\) for the system size used by following the packings along the RCP line.

Figures 4 and 5 plot the \(g_z(\Delta r)\) of packings with various friction coefficient \(\mu\) along the RCP and RLP lines respectively. Following the definition of Eq. (13), \(g_z\) with \(\Delta r = 0\), should be directly equal to the mechanical coordination number, \(Z\), and should range from 4 to 6 along both RCP and RLP (if \(h_c \ll 1\) lines which is confirmed by our numerical simulations in Figs. 4 and 5, respectively.

More importantly, as shown in the figures, we find that \(g_z(\Delta r)\) along the RCP line is exactly the same for all the packings when \(\Delta r > 0.04\) as shown in Fig. 4. For \(\Delta r < 0.04\), Fig. 4 shows that the packings have different mechanical coordination numbers from 4 to 6. This is exactly what the theory predicted. All these packings have actually the same
geometrical structure evidenced when $\Delta r > 0.04$ but with different mechanical coordinations which appears only in a difference observed for $\Delta r < 0.04$. Based on this analysis, we then define the geometrical coordination number as the one appearing at $\Delta r = 0.04$. We identify the geometrical coordination number as $z = \Delta z(0.04)$ under the accuracy of the simulations and for this particular system size $N = 10,000$ (we notice though that this value may depend on system size).

It is important to note that in terms of the radial distribution function, $g(r)$, nothing really happens at $\Delta r = 0.04$: that is, there is no peak in $g(r)$ at 0.04 and the second peak after the first coordination shell appears for larger $\Delta r$ in $g(r)$. On the other hand, we clearly see a peak in Fig. 4 at this value. We point out that the peak at 0.04 is the byproduct of the normalization factor $R^2/\rho^2$ in Eq. (13). This factor is suggested since we need to renormalize by the area of the virtual sphere. However, other factors, for instance $R^3/\rho^3$ in Eq. (13) would produce a peak in Fig. 4 located in another position. The important fact is not the location of the peak, but the fact that above 0.04 all the functions in Fig. 4 coincide. This is the basis of the definition of 0.04 as the location to define the geometrical coordination number. At this position, there is no peak in the $g(r)$. Indeed, the second peak in $g(r)$ beyond the first coordination shell appears much further around $\Delta r \approx 1$ and are indeed also identified by $g_z(\Delta r)$ as can be seen in Fig. 4 and Fig. 5 as well. Therefore the peak associated with the geometrical coordination number is not revealed from the structure in $g(r)$. It has a more subtle meaning as explained above.

It is also important to note that in experiments there is always an uncertainty in measuring the position of the particles. According to our analysis an small uncertainty of a few percent will render the mechanical coordination into the geometrical one. Thus experiments will be very difficult to differentiate between $z$ and $Z$. A possible solution to this problem is to use complementary fluorescent techniques [23, 28, 29] to obtained a signal when the particles are carrying a force and not to rely on geometrical reconstruction of index-matched images or X-ray tomography. Another route would be to obtain approximate coordinates from experiments and then use them as input into a Molecular Dynamics simulations to obtain the exact force balance for each particle. This last approach may provide the final way to accurately measure the coordinations of the particles with accuracy. In our website http://www.jamlab.org we offer the computer codes to perform MD simulations with Hertz-Mindlin forces as well the code to calculate the entropy of the packings.

The theoretical analysis is also confirmed in the RLP packings. Along the RLP line, Fig. 5, we find that the geometrical coordination number as extracted from $g_z(0.04)$ is very close to the mechanical one. Since the RLP line is at $X \rightarrow \infty$ and $h_z \ll 1$, all the states along RLP have $z \approx Z$ as we move along the line varying the friction coefficient. Thus, the numerical results confirm the theory.

In conclusion, a prescription to measure the geometrical coordination is the following: First we identify a theoretical way to define it. For instance, here we use the theoretical prediction that all the packings along RCP have the same $z$. With the proper definition of coordination number for an inflated particle, Eq. (13), we calculate the coordination as a function of $\Delta r$. This identifies $\Delta r = 0.04$ as the position to obtain the geometrical $z$. We then explore any packing (not only at RCP line) and apply Eq. (13) at $\Delta r = 0.04$ and obtain $z$. Figure 3 summarizes the theoretical predictions of values of $z$ and $Z$ for all the packings in the phase diagram. If the reader still has doubts about the difference between $z$ and $Z$ we offer a final more vivid way to understand it in terms of the famous kissing number conjecture from Newton and Gregory due to a remark of A. Coniglio (private communication): a mechanical contact is like a French kiss while a geometrical contact is any other inconsequential kiss.

VI. CONCLUSIONS

In conclusion, using Edwards statistical mechanics we have elucidated some aspects of RLP and RCP in the disordered spherical packing problem. The phase diagram introduced here serves as a beginning to understand how random packings fill space in three dimensions. The comparative advantage of the present approach over extensive work done in the past, is in the classification of all packings through $X$, $Z$ and $\phi$ in the theoretical phase diagram from where these studies could be systematically performed. This classification guides the search for indications of jamming from a systematic point of view, through the exploration of all jammed states from $\mu = 0$ to $\mu \rightarrow \infty$. Our results not only apply to packings at the jamming transition in the limit of hard spheres, but may also be extended to a general phase diagram as sketched in Fig. 1c to include states with finite nonzero pressure. Such states are described by an angoricity in addition to the compactivity as developed here. Extensions to other dimensions, polydisperse systems and other shapes of particles like ellipsoids and spherocylinders are being worked out with the goal of developing a unifying thermodynamic view of the physics of packings.
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