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# Statistical mechanics for static granular media: open questions

Massimo Pica Ciamarra <sup>\*</sup>   Patrick Richard <sup>†</sup>   Matthias Schröter <sup>‡</sup>  
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## Abstract

The theoretical description of granular materials, or assemblies of macroscopic particles, is a formidable task. Not only are granular materials out of thermal equilibrium, but they are also characterized by dissipative interactions and by static friction. Following a suggestion by S. F. Edwards, researchers have investigated the possible existence of a statistical mechanics of static granular systems, which would permit the description of macroscopic properties of mechanically stable granular assemblies from just a few parameters. The formulation and the validity of such an approach is still a matter of debate. This “emerging area” focuses on three important questions concerning such a statistical mechanics approach. First, we consider how the phase space of interest is affected by the requirement of mechanical stability. Second, we explore how the intensive parameters analogous to temperature can be determined from experimental or numerical data. Finally, we contrast different ways to express the granular counterpart to the classical Hamiltonian, known as the volume function.

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# 1 Introduction

Describing the properties and the behaviour of granular materials is a problem of great interest, as granular materials are widely used in industrial processes and found in a number of natural phenomena. How can we characterize the disordered structure of a granular pack? Can we deduce from such a characterization the response (evolution of the packing fraction, of the force network...) of a granular material submitted to mechanical perturbations or stresses? There is not yet a theoretical framework that permits such a description. From the theoretical point of view, the challenge is that of describing a disordered out-of-equilibrium many-particle system, as granular particles are so heavy that their thermal motion is negligible. The problem is further complicated by dissipation and static friction in the interparticle interaction, both of which arise due to the macroscopic size of the particles.

More than 20 years ago, S.F. Edwards and co-workers proposed that the methods of statistical mechanics could be extended to dense disordered granular assemblies.<sup>1,2</sup> Such a statistical mechanics of granular matter, if valid, would permit granular systems to be described with just a few parameters, and would represent a breakthrough in the field of granular media. Edwards' original suggestion has been the subject of intense research, both theoretically and experimentally. The statistical mechanics proposed by Edwards is specifically geared towards static granular materials, where 'static' indicates that the phase-space of interest is restricted to mechanically stable configurations.

Granular media are often static. Grains under gravity naturally settle down in a mechanically stable state, which is a local energy minimum in the absence of driving. Stable states in mechanical equilibrium can also be prepared without gravity by imposing a confining stress. In either case, grain scale deformations under typical conditions are extremely small; hence one might expect that elastic energy plays a marginal role in static granular systems, and no role at all in the limit of hard spheres in the absence of gravity. Motivated by this, Edwards<sup>3</sup> suggested that in a granular statistical mechanics, the conventional Hamiltonian should be replaced with a volume function  $W$  that expresses the volume of the system as a function of the degrees of freedom of

the system  $\mathbf{q}$ . In strict analogy with equilibrium statistical mechanics, one assumes that all microstates (mechanically stable states) of given volume occur with the same probability. One then derives the partition function of the system,

$$Z(\chi) = \int \exp(-W(\mathbf{q})/\chi) \Theta(\mathbf{q}) d\mathbf{q},$$

where  $\chi$  is termed *compactivity*, a Lagrange parameter analogous to the temperature, and  $\Theta(\mathbf{q})$  imposes the condition of mechanical stability, including a finite bulk and shear modulus.<sup>4</sup> At a given compactivity  $\chi$ , the equiprobability condition leads to the minimization of the granular free energy  $F(\phi) = W - \chi S$ , where we have introduced the granular entropy  $S(W) = \log(\Omega(W))$ ,  $\Omega(W)$  being the number of mechanically stable states of volume  $W$ . The inverse compactivity  $\chi^{-1} = \partial S / \partial V$  is therefore related to the volume dependence of the entropy. If one considers not only the number of ways the grains can occupy the volume  $V$  but also the number of ways the grains support the boundary stresses  $\sigma$ , the partition function becomes

$$Z(\chi, \alpha_{ij}) = \int \exp(-W(\mathbf{q})/\chi - \Gamma_{ij}(\mathbf{q})/\alpha_{ij}) \Theta(\mathbf{q}) d\mathbf{q}, \quad (1)$$

where  $\Gamma_{ij}$  and  $\alpha_{ij}$  are the virial and the tensorial angoricity, which reduce to scalars  $\Gamma$  and  $\alpha$  for systems loaded isotropically. Similarly to the compactivity, the angoricity is related to the pressure dependence of the entropy  $S(\sigma)$ , which is now a measure of the number of mechanically stable states supporting a given stress  $\sigma$ . From this partition function, as for conventional statistical mechanics, many quantities can be obtained – in principle. As we shall show, doing so remains challenging.

In the following three sections we will discuss recent developments and open questions regarding three key ingredients of eqn (1): first, how does the requirement of mechanical stability, represented by  $\Theta(\mathbf{q})$ , shape the explored phase space? Second, how can the intensive parameters  $\chi$  and  $\alpha$  be determined from experimental or numerical data? And finally, what is the right way to compute the equivalent to the classical Hamiltonian,  $W$ ?

## 2 The phase space of mechanically stable configurations and its exploration

The function  $\Theta(\mathbf{q})$  limits the integration in eqn 1 to the mechanically stable configurations of grains \*. This raises two questions: what is the range in volume fraction  $\phi$  (the fraction of the total volume occupied by grains) and confining pressure for which mechanically stable configurations exist? And how does the system explore this phase space?

### 2.1 The condition of mechanical stability

For a better understanding of the role of  $\Theta$  it is helpful to contrast the Edwards' approach with the hard sphere gas. In the latter we only request that the particles do not overlap. Consequently, the phase space volume of configurations where any two particles touch is of measure zero. In contrast, imposing mechanical stability requires sufficient permanent contacts to constrain all rotational and translational degrees of freedom – there can be no zero energy (“floppy”) modes.<sup>5</sup> Absent geometric degeneracies such as crystallinity, mechanically stable frictional sphere packings must have an average coordination number  $Z \geq 4$ , the so-called frictional isostatic contact number.<sup>6,7</sup>

A second important reference point is the jamming paradigm for *frictionless* soft particulate systems such as foams, colloids and emulsions.<sup>5</sup> Mechanically stable packings of frictionless spherical particles exist only above the so-called point J with  $\phi_J \approx 0.64$ . In frictionless packings both the packing fraction and the contact number display scaling with distance to point J, and both in turn are controlled by the pressure – unjamming corresponds to zero pressure. The presence of nonzero surface friction  $\mu$  renders granular materials qualitatively distinct from foams, emulsions, etc.. Friction allows for tangential contact forces, which permit frictional packings to support loads in ways unavailable to frictionless materials.<sup>8</sup> For various confining pressures, there are mechanically stable packings over a range of volume fractions.<sup>9</sup> Moreover, even for a given combination of  $\phi$  and  $p$ , the average contact number can depend on the

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\*In the following we will exclusively discuss spherical grains

preparation history.<sup>10</sup>

The empirical fact that mechanically stable packings of spheres can only be prepared in a finite range of  $\phi$  was first established by Scott<sup>11</sup> and Bernal.<sup>12</sup> The apparent absence of crystallinity earned the upper and lower bounds the names Random Loose Packing (RLP) and Random Close Packing (RCP), respectively. From a statistical mechanics perspective, one expects that these two bounds should be related to a configurational entropy  $S$  corresponding to the logarithm of the phase space volume of all mechanically stable configurations at a given volume fraction compatible with the mechanical boundary conditions. It is then natural to ask what features characterize  $S(\phi_{\text{RLP}})$  and  $S(\phi_{\text{RCP}})$ . We shall consider RLP first.

One possible interpretation of RLP is that below  $\phi_{\text{RLP}}$  the entropy is zero.<sup>†</sup> This is suggested by the observation from numerics that loose packings approach the isostatic value  $Z = 4$  in the large friction limit. Provided lowering  $\phi$  lowers  $Z$  – an assumption supported by numerics – then  $S$  must be zero below loose packing. By considering the fraction of “fully mobilized” contacts, which saturate the Coulomb inequality, Shundyak et al.<sup>13</sup> showed that packings with finite friction approach an “isostatic line” connecting frictionless and frictional isostatic states (Fig. 1a). In this sense even packings at finite  $\mu$  are isostatic, at least in numerics. By the same reasoning as above, one would then expect  $S$  to vanish at RLP for any value of  $\mu$ .

An alternative viewpoint holds that RLP corresponds to a maximum in  $S$ ,<sup>14,15</sup> as outlined in Fig. 1 b. This explanation is supported by the observation that the experimental and numerical protocols used to build RLP packings are all gentle deposition protocols, which aim to avoid disturbing the already existing structure.<sup>14,16,17</sup> If  $S(\phi_{\text{RLP}})$  is a maximum, either  $S$  drops discontinuously to zero below  $\phi_{\text{RLP}}$ , or there is another, lower packing fraction where  $S$  goes to zero. Pica Ciamarra et al. termed this Random Very Loose Packing (RVLP),<sup>14</sup> and showed that states below RLP can be prepared numerically with carefully chosen initial conditions (Fig. 1b). If RVLP exists, one must explain why it is not observed in experiments. One such explanation is dynamical. During preparation the system explores the much larger phase space of

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<sup>†</sup>States below RLP might still exist, but their number would have to grow subextensively with volume.

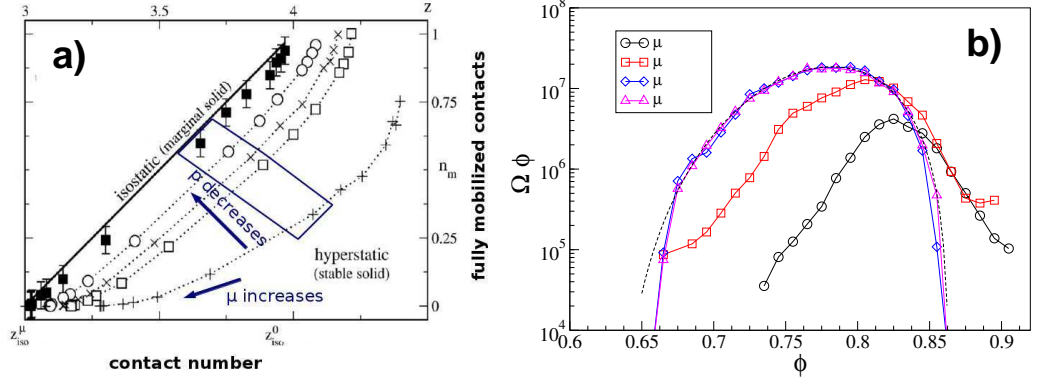


Figure 1: Numerical results on frictional disc packings. (a) Taking into account the number of fully mobilized contacts (where the tangential force is just at the coulomb threshold) slowly prepared packing approach the isostatic limit for vanishing pressure. From Shundyak *et al.*<sup>13</sup> (b) The lower bound of the configurational entropy of two-dimensional disc packings is below the RLP value ( $\approx 0.77$ ) for the same system. From Pica Ciamarra *et al.*<sup>14</sup>

non-overlapping hard sphere states before it settles down in a static configuration. The probability ending up in a particular configuration will depend on the phase space volume of the basin of attraction leading to this state. The apparent absence of very loose packings in the experiment could be simply due to their very small basins of attraction. This in turn leads to the question of ergodicity, which we revisit below.

We now return to Random Close Packing. Similar to loose packing, RCP is primarily a phenomenological fact: multiple protocols, including tapping<sup>18</sup> and flow pulses,<sup>19</sup> slow down asymptotically when  $\phi$  approaches 0.64. Under other protocols, like cyclic shear, no peculiar changes in dynamical properties occur at  $\phi \simeq 0.64$ .<sup>20</sup> However, all protocols that cross RCP observe the onset of some crystalline order. While these facts seem uncontroversial, their interpretation is not. It has been proposed that RCP is a first order phase transition<sup>21,22</sup> between the amorphous and the crystalline state; this would imply that  $S$  is still finite at RCP. An alternative viewpoint holds that it is the endpoint of the amorphous branch of the hard sphere fluid,<sup>23</sup> corresponding to a vanishing  $S$  at RCP. Yet another possibility is that RCP corresponds to a local minima of the curve  $S$  versus  $\phi$ ; the physical mechanism behind RCP is then explained by geometrical properties like the maximum frequency of polytetrahedral structures.<sup>24</sup> Clearly more work is needed.

## 2.2 Exploring the phase space

Besides establishing the range of  $\phi$  where disordered mechanically stable states exist, we also need to consider how the system explores these states. A basic assumption of classical statistical mechanics is that all configurations are realized with equal probability. As pointed out above, due to their dissipative and macroscopic nature, granular materials cannot explore their phase space *via* thermal fluctuations. An external, macroscopic perturbation like shearing or tapping will always be needed to move the system from one mechanical stable configuration to another. Consequently, we must allow for the possibility, indeed likelihood, that the probability of visiting a microstate depends on the chosen protocol and preparation history. There is ample experimental evidence for such protocol dependence. For example, the force chains in a granular pile differ if it is poured from a single point source or through a wide sieve.<sup>25</sup>

For at least two experimental driving protocols – shaking<sup>18,26</sup> and flow pulses<sup>19</sup> – the existence of history-independent steady states has been established. While this does not guarantee equiprobability of the microstates, it at least assures the existence of an effective heat bath with time-independent probabilities. Moreover, numerical simulations of frictional particles driven *via* flow pulses<sup>27</sup> are compatible with an equivalence between time and ensemble averages, suggesting that this protocol allows to uniformly sample the phase space.

The only direct experimental test (with matching numerics) of the equiprobability hypothesis involved a complete enumeration of all mechanically stable configurations of 7 frictionless discs in a two dimensional box,<sup>28</sup> generated by tapping or slow compression. Here it was found that the probabilities of creating individual configurations differed by orders of magnitude. This can again be understood by looking at the dynamic part of the evolution towards these static state: the large probability differences of these states reflects a large size disparity in the volumes of their respective basins of attraction (assuming the preparation protocol adds no bias). However, the phase space volume of mechanically stable configurations of frictional particles is much larger than its frictionless counterpart. This means that the frictionless system will have passed through many states that would have been mechanically stable in the presence of fric-



tion. Unfortunately, no results on the probability distribution of frictional particles are available.

On a more general note, it is not clear how much a statistical mechanics of granular media will require the equiprobability assumption. One could imagine, *e.g.*, a partition function including a protocol-dependent degeneracy function,<sup>29</sup> which accounts for the different probabilities. Also it has been shown that equiprobability is not a necessary condition for the existence of intensive thermodynamic parameters like compactivity.<sup>30</sup> Again, more work is needed.

### 3 Measuring intensive thermodynamic parameters

Any canonical ensemble is characterized by one or more intensive thermodynamic parameters, *e.g.* the inverse temperature  $\beta = 1/k_B T$  in equilibrium statistical mechanics. In the usual thermodynamics the temperature is measured introducing a thermometer, a calibrated probe that acquires the temperature of the system of interest when the two equilibrate at constant energy, *i.e.* in the microcanonical ensemble. In the simplest form of a granular statistical mechanics, the counterpart to  $\beta$  is a scalar  $\chi$  conjugate to the packing's volume  $V$ , termed “compactivity,” or a scalar  $\alpha$ , the “angoricity,” conjugate to the product of pressure and volume  $\Gamma = pV$ .  $\Gamma$  is an extensive stress-related quantity known variously as the virial, force moment, or extensive pressure. How to measure these intensive parameters in the granular case is not so obvious, because there is no natural dynamical process by which two systems in contact can exchange volume (or force moment) and thus come to equilibrium, *i.e.* there is not a microcanonical ensemble. The analogy between compactivity (or angoricity) and the temperature must therefore be regarded as an assumption of Edwards' theory.

It is natural to ask how to measure these intensive parameters, and which aspects of Edwards's theory – if any – are tested by these measurements. This is the goal of the present section which focuses mainly on the “overlapping histograms” method and discusses some aspects of the Edwards' theory that remain to be tested. In the discussion below, there is no intrinsic difference between measurements of  $\chi$  and  $\alpha$ ; the reader

can freely exchange the conjugate pairs  $(\chi, V)$  and  $(\alpha, \Gamma)$ .

Several methods exist to measure intensive parameters like compactivity. Among them are the “specific heat” method,<sup>26</sup> which consists in measuring the compactivity from the fluctuations around the mean volume of a granular packing, just as the specific heat of a thermal system can be determined from its energy fluctuations. This method has been used widely for granular packings undergoing compaction.<sup>18,19,26,31</sup> However, the interpretation of the measured quantity as a granular analog of temperature relies on the assumptions built into the Edwards’ approach; hence the method cannot test their validity. The compactivity can also be determined from the probability distribution of the volume of cells tessellating the granular packing.<sup>32</sup>

Here, we will focus on a third way: the “overlapping histograms method,” proposed by Dean and Lefèvre<sup>33</sup> and applied to granular systems by Henkes et al.<sup>34</sup> and McNamara et al.<sup>35</sup> It has the advantage of allowing one to probe system size dependence from one ensemble of packings. Moreover it does not require detailed knowledge of the entropy and is a relevant test of the theory. We describe the method as a *Gedankenexperiment*, though of course ref.<sup>34</sup> and<sup>35</sup> have implemented it in numerics. Imagine sampling  $m$ -grain clusters from a packing of  $N \gg m$  grains, labeled packing 1. The force moment  $\Gamma$  on each cluster can be measured and in this way the histogram or frequency distribution  $P_m^{(1)}(\Gamma)$  can be built up. If the system is statistically homogeneous and if it is entropy maximizing, then packing 1 can be seen, in the framework of Edwards’ theory, as the analog of a thermal bath characterized by an intensive parameter  $\alpha_1$ . All other parameters  $P_m$  can potentially depend on, *e.g.* packing fraction, friction coefficient, particle shape, *etc.* and will be summarized in  $\mathbf{x}$ . In this case the distribution we have sampled is the stationary probability distribution  $P_m^{(1)}(\Gamma) = \rho_m(\Gamma; \mathbf{x}, \alpha_1)$ :

$$\rho_m(\Gamma; \mathbf{x}, \alpha) = \frac{\Omega_m(\Gamma; \mathbf{x}) e^{-\alpha\Gamma}}{Z(\alpha)}, \text{ with } Z = \int \Omega_m(\Gamma; \mathbf{x}) e^{-\alpha\Gamma} d\Gamma. \quad (2)$$

where  $Z$  is the partition function, which normalizes  $\rho_m$ . Eqn (2) lacks predictive power because we do not know  $\Omega_m(\Gamma; \mathbf{x})$ , the density of states of  $m$ -grain clusters. Continuing

the thought experiment, we prepare a second packing and label it 2. Care is taken to hold the parameters  $\mathbf{x}$  fixed, but we admit the possibility that in constructing packing 2 it equilibrates in a state characterized by an intensive parameter  $\alpha_2$  different from packing 1<sup>‡</sup>. Of course naïvely one expects that  $\alpha^{-1}$  will bear some relation to the mean pressure in the bath  $\Gamma_{\text{bath}}/N$ . As before we collect  $m$ -grain clusters and sample the frequency distribution  $P_m^{(2)}(\Gamma)$ .

With malice aforethought we construct the ratio  $r_m(\Gamma, \Gamma')$  from the sampled distributions:

$$r_m(\Gamma, \Gamma') := \ln \frac{P_m^{(1)}(\Gamma) P_m^{(2)}(\Gamma')}{P_m^{(1)}(\Gamma') P_m^{(2)}(\Gamma)}. \quad (3)$$

If the system is entropy maximizing, eqn (2) holds and

$$r_m(\Gamma, \Gamma') = -(\alpha_1 - \alpha_2)(\Gamma - \Gamma'). \quad (4)$$

The unknown density of states  $\Omega_m$  has dropped out, so that the ratio is linear in  $\Gamma - \Gamma'$ , with decay constant given by  $\alpha_1 - \alpha_2$ .

A method for determining  $\alpha$  (or  $\chi$ ) thus emerges: one constructs a family of packings at fixed  $\mathbf{x}$ , sample distributions of  $\Gamma$  (or  $V$ ) on clusters of grains, and compares them pairwise *via* eqn (3). Obviously the method requires adequate statistics to make a comparison. It is also necessary to prepare enough packings so that for each packing  $i$  there is another  $j$  such that the histograms  $P_m^{(i)}$  and  $P_m^{(j)}$  have sufficient overlap to construct the ratio  $r_m$  — hence the name of the method. Note that the intensive parameter can only be determined up to an offset, which can be fixed assuming that RLP has infinite compactivity. The aforementioned *Gedankenexperiments* had been applied to 2D numerical simulations by Henkes et al.<sup>34</sup> and to 3D experiments and numerical simulations by McNamara et al.<sup>35</sup> An example, extracted from the former work, is given in Fig. 2.

By verifying the linearity of the ratio of two overlapping histograms, the present method has been used to successfully test Edwards' theory.<sup>34,35</sup> However, new exper-

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<sup>‡</sup>In fact equilibrating a new packing may produce fluctuations in some parameters, *e.g.* packing fraction (in an stress ensemble) or pressure (in a volume ensemble). One hopes that  $\Omega_m$  depends on these parameters sufficiently weakly that eqn (4) can still be used.

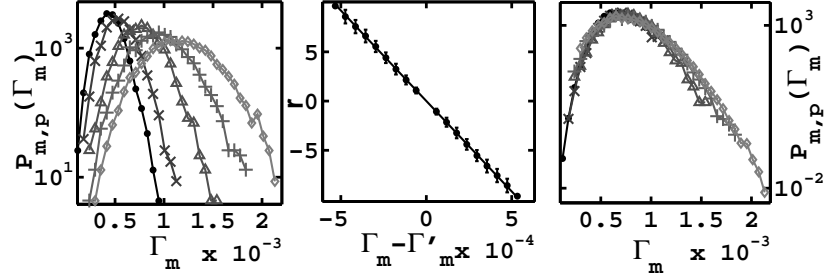


Figure 2: The method of overlapping histograms. (a)  $P_m(\Gamma)$  of  $m = 8$ -grain clusters sampled from packings with  $N = 4096$  grains. The symbols correspond to runs with different packing fractions. (b) The ratio  $r_m$  of eqn 3. (c) Distributions of (a) rescaled according to the values of  $\alpha$  extracted from (b). From *Phys. Rev. Lett.* **99**, 038002; Copyright (2007) by the American Physical Society.

imental protocols must be proposed to test the microscopic details of the theory, such as equipartition (see the discussion in section 2.2). Moreover, a rigorous justification of the validity of the canonical assumption in the context of granular media (eqn 2) remains an open question.

## 4 Expressing the partition function

The interest in the statistical mechanics of granular media originates from the possibility of predicting the properties of granular assemblies by solving the partition function, eqn 1. Such a task can only be accomplished if one is able to express in terms of the degrees of freedom  $\mathbf{q}$  the partition function, namely the projector operator  $\Theta(\mathbf{q}) = 0, 1$  and the volume function  $W(\mathbf{q})$ . While this is easily done in lattice models, where one can solve the partition function using standard statistical mechanics tools,<sup>36</sup> how to express  $\Theta$  and  $W$  on the continuum in a manageable form is not obvious.

We restrict the discussion in this section to hard sphere states. Hard spheres have no intrinsic stress scale and hence the magnitude of the confining pressure is arbitrary, analogous to temperature in thermal hard spheres. A treatment of deformable particles must keep track of the imposed stress as well as the imposed volume, as in the partition function of eqn (1). There is a growing literature focusing on stress-based ensemble approaches to granular statistical mechanics, see ref.<sup>8</sup> and <sup>37</sup> for details.

The function  $\Theta$  weights mechanically stable states. As discussed above, there are similarities to the hard-sphere Hamiltonian  $H_{\text{hs}}$ , which gives zero statistical weight to all states with particle overlaps. By writing  $W_{\text{ms}} = -\log \Theta$  and assuming equiprobability, one may relate  $\Theta$  to a volume function  $W_{\text{ms}} = 0$ , and  $\infty$  for mechanically stable and unstable states, respectively. However, while  $H_{\text{hs}}$  can be expressed as a sum of two body contributions,  $W_{\text{ms}}$  results from an  $N$  body interaction,  $N$  being the number of grains of the system. Formally, linear stability can be imposed in conservative systems by demanding that the system's Hessian have a positive definite spectrum (excluding rigid body modes);<sup>4</sup> extensions to dissipative systems are also possible.<sup>38,39</sup> Practically, however, such constraints are too complicated to include in the partition function. Some authors approximate them with global constraints on the connectivity<sup>40</sup> or moments of the stress.<sup>41–43</sup>

Since the volume is an extensive quantity, the general approach to estimate  $W$  consists in tessellating the whole medium into  $N$  non-overlapping elements and associate to them a volume function  $W_i$  (which can be seen, for example, as the free volume available per grain) such that  $W = \sum_i W_i$ . Blumenfeld and collaborators proposed a way to determine the volume function  $W_i$ . First introduced for 2D systems,<sup>44,45</sup> this method consists in partitioning the system into voids defined from the grain contacts, and the voids into quadrilaterals defined from the centers of the grains and the contact points (Fig. 3). This method can be generalized to 3D granular systems and also to cellular media. The description has several advantages: (i) it allows a quantitative description of the structure at any arbitrary point within the material; (ii) the shape tensor is a constitutive property; and (iii) all the basic elements are octahedra, allowing a unique tensorial description. One of the drawbacks is that this approach may ill-tessellate non-convex voids<sup>46</sup> and so overestimate their volumes. The importance of these non-convex voids, and the amount by which they overestimate volume remain a matter of debate.<sup>47</sup> Another drawback is that, while formally elegant, the volume function is a complicated object which is difficult to handle. Indeed, this volume function has never been used in conjunction with an estimation of the projector  $\Theta$  to solve the partition function, and to predict properties of granular assemblies.

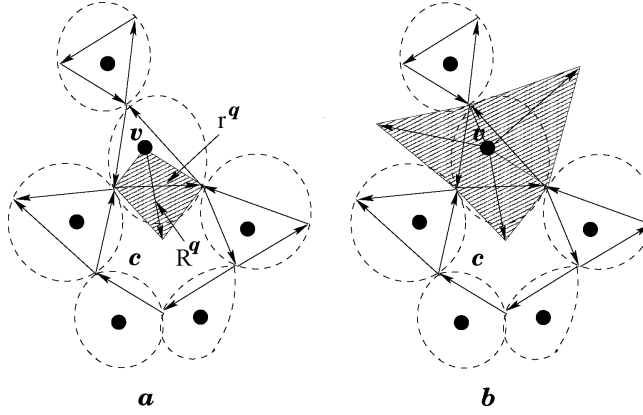


Figure 3: The geometric construction around grain  $v$  in 2D. The vectors  $\mathbf{r}^q$  connect contact points anticlockwise around each grain (and clockwise around each cell  $c$ ). The vectors  $\mathbf{R}^q$  connect from grain centroids to centroids of neighboring cells. (a) The quadrilateral, or quadron, associated with grain  $v$  and cell  $c$  is shown shaded. (b) The sum of the areas of all the quadrilaterals around grain  $v$  constitute the area associated with this grain. The sum of all these areas is the area of the entire system (reprinted with permission from *J. Chem. Phys. B* **113**, 3982. Copyright 2009 American Chemical Society).

As an alternative approach, a natural way to partition space is the well known Voronoï tessellation,<sup>48</sup> which is purely geometric and not tied to the connectivity of the contact network.<sup>49</sup> From this tessellation the theoretical derivation of the volume function is not straightforward, and no analytical formula exists. An approximation of this volume function has been introduced by Song et al.,<sup>40</sup> which expressed  $W_i$  as a function of just one parameter, the local coordination number  $z_i$ :  $W_i/V_i = 2\sqrt{3}/z_i$ , where  $V_i$  is the volume of a grain. Here  $z_i$  refers to geometric contacts, *i.e.* it includes contacts that bear no force. Song et al. predict  $\phi_{RCP} \approx 6/(6 + 2\sqrt{3}) = 0.634$ . We stress that the calculation is not exact, but an analytical expression of an approximate value.

Song et al.<sup>40</sup> used their approximate  $W_i$  to solve the partition function, in conjunction with an approximation for  $\Theta$ . By hypothesizing that  $\Theta$  restricts the ensemble to isostatic packings, they numerically determined the function  $\phi(\chi, Z)$ , where  $Z \leq z$  denotes the mean number of load-bearing contacts. Isocompactivity lines can then be plotted as part of a phase diagram in  $(Z, \phi)$ ; see Fig. 4. This diagram is made of (i) a random loose packing (RLP line), corresponding to  $\chi \rightarrow \infty$  and  $\phi_{RLP} \approx 4/(4 + 2\sqrt{3})$ ; (ii) a random close packing line (RCP line) corresponding to  $\chi = 0$  and  $\phi_{RCP} \approx 6/(6 + 2\sqrt{3})$ ,

deduced from the theory; (iii) a granular-line (horizontal G-line) corresponding to an infinite grain-grain friction coefficient ( $\mu$ ); and (iv) a jamming point (J point) corresponding to  $Z = Z_{\text{iso}}^0, \mu = 0, \phi = \phi_{\text{RCP}}$ .

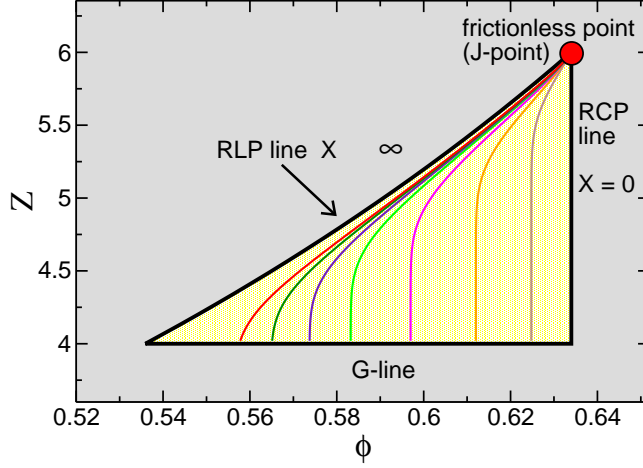


Figure 4: Phase diagram of jamming obtained from the theory exposed in ref.<sup>40</sup> All disordered packings lie within the yellow triangle demarcated by the RCP line, RLP line and granular line. Iso-compatibility lines are in color.

The validity of this theory is controversial. While there is reasonable agreement with some experiments<sup>50</sup> and simulations,<sup>40</sup> recent X-ray tomography experiments display significant differences with the prediction  $W_i/V_I = 2\sqrt{3}/z_i$ . For a given packing fraction, the difference between the number of contacts measured and the theoretical prediction can be as much as 15%.<sup>51</sup> Further, simulations show that  $\phi_{\text{RCP}}$  decreases monotonically on increasing the dimensionality;<sup>52</sup> the approach by Song et al. does not reproduce this dependence. Finally, all packings in the tomographic experiments were hyperstatic (*i.e.* grains possess a number of contacts in excess of that which would uniquely determine the contact forces from mechanical equilibrium), contrary to the assumption that  $\Theta(\mathbf{q})$  restricts packings to isostatic states.<sup>40</sup> This suggests that the discrepancy between the prediction and the observed behaviors originates from the identification of the isostatic condition with the ensemble of jammed configurations, *i.e.* the approximation used to deal with the projector operator  $\Theta$ . In addition, since this approach resorts on an approximation of the volume function that neglects the contact network, it cannot be used to investigate the geometrical and the mechanical

properties of granular systems.

More work is clearly needed in this direction. The objective is to find approximations for  $\Theta$  and  $W$  that are simple enough to allow analytical and/or numerical calculations, and which also give access to the calculations of properties of granular systems one could be interested in, such as the fabric tensor, fixed by the contact network.

## 5 Conclusion

The statistical mechanics of static granular systems is a theoretical effort towards the description of many particle systems out of thermal equilibrium. Here we have shown that there are a number of experimental and conceptual challenges that stand in the way of a predictive theoretical formalism. From the experimental viewpoint, the main problem is that of devising protocols that can uniformly sample the phase space of interest. From the theoretical viewpoint, apart from the difficulties related to measuring the intensive parameters and to identifying the bounds on volume fraction, the main open problem is to express the volume fraction and the projector on the mechanically stable states in terms of the particles coordinates. In particular, the condition of mechanical stability, which imposes that the forces and the torques acting on each grain sum to zero, is expected to introduce correlations which have been neglected so far. A refined theory would find applications not only in granular media but also in other quenched, amorphous materials. Indeed, methods similar to those described here have also been applied to structural<sup>53</sup> and spin glasses,<sup>54,55</sup> to polymer and other elastic networks,<sup>56</sup> and to crumpling of sheets of paper.<sup>57–60</sup>

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