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Citation: [AIP Conference Proceedings](#) **1542**, 1186 (2013); doi: 10.1063/1.4812149

View online: <http://dx.doi.org/10.1063/1.4812149>

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Granular Statistical Mechanics: Volume-Stress Phase Space, Equipartition and Equations of State

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Abstract. This paper first reviews a recent report[1], showing that the volume and stress ensembles, often used separately in the statistical mechanics of stable granular systems, are interdependent and must both be used to compute expectation values. A reformulation of the combined partition function in 2D allows us to calculate exactly a number of structural and stress-related expectation values. It is shown that structural measureables may depend on the angoricity and stress-based quantities on the compactivity, demonstrating that the compactivity and angoricity are not conjugate variables of volume and force moment, as commonly believed. We review a derivation of an equipartition principle, which makes it possible to determine the compactivity experimentally. We conclude by deriving an equation of state.

Keywords: granular systems, statistical mechanics, equipartition, equations of state
PACS: 64.30.+t, 45.70.-n 45.70.Cc

INTRODUCTION

Formulating statistical mechanics for granular materials[2, 3, 4] was expected to lead to derivation of macroscopic equations of state and constitutive relations, but we are still far from this goal. This is due to: uncertainty over the identities and number of degrees of freedom (DoF), the difficulty to conceive an analog of a thermometer - a 'compactometer', the lack of ergodicity, the difficulty in measuring the compactivity experimentally and recent suggestions of absence of an equipartition principle[5, 6] in agitated systems. Here we review a recent argument that the phase space for static systems must include both structural DoF (SDF)[7] and force DoF (FDF) and a derivation of an equipartition principle in 2D. This makes possible to estimate the compactivity by macroscopic measurements. We use these to derive an equation of state.

The entropy-based statistical mechanical of Edwards and collaborators was based on replacing the conventional Hamiltonian by a volume function W , such that for similarly generated mechanically stable packs of $N(\gg 1)$ grains and a mean coordination number \bar{z} , the partition function is[2],

$$Z_v = \int e^{-\frac{W}{X_0}} d\{\text{all SDF}\} \quad (1)$$

where X_0 is the compactivity, quantifying configurational fluctuations. The SDF of such systems are the position vectors of the intergranular contacts, better described by their differences - the vectors \vec{r}^i defined below[8].

However, it was argued that Z_v does not specify completely the macroscopic state of the system because it does not account for the entropy due to different stress

states. These stress 'microstates' were described by a separate partition function, Z_f [9, 10, 11],

$$Z_f = \int e^{-\sum_{\alpha\beta} X_{\alpha\beta} \frac{1}{x_{\alpha\beta}} \mathcal{F}_{\alpha\beta}} d\{\text{all boundary forces}\} \quad (2)$$

where α, β are components x, y and $\mathcal{F}_{\alpha\beta}$ is a force moment function (from which the stress $\sigma_{\alpha\beta}$ is derived),

$$\mathcal{F}_{\alpha\beta} = \sum_g V^g \sigma^g = \sum_{gg'} \bar{F}_{\alpha}^{gg'} \mathcal{R}_{\beta}^{gg'} \quad (3)$$

The sum is over pairs of grains gg' , in contact at $\mathcal{R}^{gg'}$ as measured from the centroid of grain g , $\bar{F}_{\alpha}^{gg'}$ is the force that g' applies to g and V^g is the volume associated with grain g . The tensor $X_{\alpha\beta} = \partial \mathcal{F}_{\alpha\beta} / \partial S$ is the 'angoricity' - an analogue of the temperature and the compactivity[9, 13, 14], where S is the entropy. In the following, S is the log of the total number of both structural configurations and stress states. This partition function is based on the postulate that every structural configuration can support an ensemble of such microstates. Seeming support for this idea came from numerical simulations[11, 12].

ENSEMBLES INTERDEPENDENCE

Consequently, the volume and stress ensembles are considered independent in the literature, implying that the total partition function is $Z = Z_v Z_f$, and results have been derived from the statistics of one ensemble or the other. Three arguments have been presented against this picture. Firstly, the volume ensemble alone cannot represent all the entropy because it implies different con-

figurations under the exact same boundary forces. Yet no many-grain experiment can reproduce the same precise forces on every boundary grain - only the global boundary stresses can be controlled. Thus, to predict experimental measurements, the statistics of the boundary forces must be taken into consideration. Secondly, the stress ensemble alone also cannot represent all the entropy because this ensemble presumes a fixed structural configuration, to which the ensemble of boundary forces is applied. Yet, such a many-grain such a system can be realised only possibly in numerical simulations, not in real experiments. Thirdly, the two ensembles are interdependent, $Z \neq Z_v Z_f$. This is both a result of the above two arguments and of an inspection of the stress partition function - any expectation value computed from (2) would remain a function of the SDF unless integrated over all possible structural configurations.

While these arguments hold in any space dimension, it is in 2D that this can be used to derive explicit analytic results. These results illustrate the impact of the arguments and provide new significant insight into the physics of granular systems in general. Let us define an ensemble of all the configurations that a collection of $N(\gg 1)$ 2D grains can make in mechanical equilibrium. The ensemble is constrained to be under the same M external compressive forces, acting on the boundary grains, and to have a fixed mean contact number \bar{z} . We disregard body forces, in the absence of which ‘rattlers’ can also be ignored, as they do not affect the stress states.

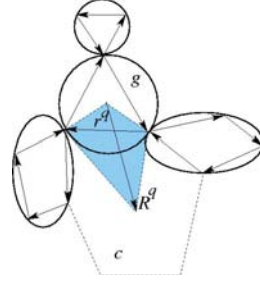


FIGURE 1. The vectors \vec{r}^q connect contacts around grain g . The vectors \vec{R}^q extend from grain centroids to cell centroid. These vectors are the diagonals of quadrangle q (blue).

We use the quadron-based formulation of [7, 10, 15]. The quadrons are elementary volumes tessellating the granular space. In 2D, a quadron is generically a quadrilateral whose two diagonals are vectors: \vec{r}^q connects contact points around the grain (clockwise) and \vec{R}^q extends from the centroid of the grain contacts to the centroid of the contacts around a neighbour cell (Fig. 1). The volume function is the sum of all the quadron volumes, $W = \sum_q v^q = \frac{1}{2} |\vec{r}^q \times \vec{R}^q|$ in 2D (summation over repeated indices implied). It is important to identify correctly the phase space of SDF, which consists of a subset of $N\bar{z}/2$

\vec{r}^q -vectors. This follows [7], who have shown that the \vec{R}^q -vectors depend linearly on the \vec{r}^q 's and that only $N\bar{z}/2$ of the latter are independent due to the loops they close [8, 10]. Hence, $N_{sdf} = N\bar{z}$. It is therefore convenient to define the vector $\vec{\rho} \equiv (r_x^1, r_x^2, \dots, r_x^{N\bar{z}/2}, r_y^1, r_y^2, \dots, r_y^{N\bar{z}/2})$, in terms of which W is quadratic and the volume partition function is explicitly

$$Z_v = \int e^{-\frac{1}{2X_0} a_{\alpha\beta}^{qp} r_{\alpha}^q r_{\beta}^p} \prod_{n=1}^{N\bar{z}/2} \prod_{i=1}^2 dr_i^q = \int e^{-\frac{1}{2} \vec{\rho} \cdot A \cdot \vec{\rho}} d^{N\bar{z}} \vec{\rho} \quad (4)$$

Here p, q run over quadrons, α, β run over vector components x, y and A is a matrix whose elements are

$$(A)_{\alpha\beta}^{qp} = \frac{1}{X_0} \begin{cases} a_{xx}^{qp} & q, p \leq N\bar{z}/2 \\ a_{xy}^{qp} & q \leq N\bar{z}/2, p > N\bar{z}/2 \\ a_{yx}^{qp} & p \leq N\bar{z}/2, q > N\bar{z}/2 \\ a_{yy}^{qp} & q, p > N\bar{z}/2 \end{cases}$$

Assuming a uniform measure of the SDF and that the contribution of very large \vec{r} magnitudes is negligible, Z_v can be calculated explicitly

$$Z_v = \sqrt{\frac{(2\pi)^{N\bar{z}}}{\det A}} \quad (5)$$

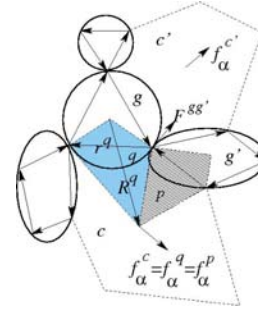


FIGURE 2. f_{α}^q is the α component of the loop force \vec{f}^c , which contains the quadron q (shaded blue). The loop forces of c and c' give the inter granular force at the contact point that they share, $\vec{F}^{gg'} = \vec{f}^c - \vec{f}^{c'}$ [15]. Quadron p (striped) shares the same loop as q and hence also the same loop force.

The stress states result from all the possible combinations of compressive forces on the boundary grains, \vec{g}^m ($m = 1, 2, \dots, M$), subject to the constraint that the total stress on the boundary is fixed [13, 8, 14]. Only boundary forces that do not drive the system out of its fixed mechanically stable configuration are allowed. A key to the explicit derivation in [1] is the equivalent representation of the force moment function [15, 7],

$$\mathcal{F}_{\alpha\beta} = \sum_{gc} f_{\alpha}^q r_{\beta}^q \quad (6)$$

where f_α^q is the α component of a loop force of the cell containing the quadron q (Fig. 2). The loop forces are defined in terms of the contact forces[15], e.g. $\vec{F}^{ss'} = \vec{f}^c - \vec{f}^{c'}$ in Fig. 2. Their advantage is that they automatically satisfy force balance conditions on every grain and are determined only by the torque balance conditions[15]. For clarity, we specialise the discussion to isostatic systems ($\bar{z} = 3$); extension to hyperstatic assemblies ($\bar{z} > 3$) is possible. Using (6) in (2) we need to integrate over all boundary forces \vec{g}^m

$$dZ_f = e^{-\frac{1}{X_{\alpha\beta}} f_{\alpha\beta}^q} \prod_{m=1}^M d\vec{g}^m \quad (7)$$

Quadrons sharing the same cell have the same loop force (Fig. 2), which means that only $N/2$ of the $N\bar{z}$ quadron forces are independent. These forces depend linearly on the M boundary forces. Defining then a loop forces vector $\vec{\phi} \equiv (f_x^1, f_x^2, \dots, f_x^{N/2}, f_y^1, f_y^2, \dots, f_y^{N/2})$, the solution for $\vec{\phi}$ in terms of the boundary forces is

$$\phi_\alpha^c = C_{\alpha\beta}^{qm} g_\beta^m \quad (8)$$

where $\alpha, \beta = x, y$, $c = 1, 2, \dots, N/2$ runs over all cells, $m = 1, 2, \dots, M$ runs over all boundary forces and C is $N \times 2M$ matrix. In terms of these, $\vec{f}^q = E\vec{\phi}$, where E is a $N\bar{z} \times N$ matrix. Defining $B_{\alpha\beta}^{qp} = X_{\alpha\beta}^{-1} \delta_{qp}$, with δ_{qp} being the delta function, gives

$$dZ_f = e^{-\vec{\phi} \cdot E^T \cdot B \cdot \vec{\rho}} \prod_{m=1}^M d^2 \vec{g}^m = e^{-\vec{g} \cdot C^T \cdot E^T \cdot B \cdot \vec{\rho}} \prod_{m=1}^M d^2 \vec{g}^m \quad (9)$$

The total partition function comprises the phase space of both SDF and FDF, $dZ = dZ_v dZ_f$

$$Z = \int e^{-\frac{1}{2} \vec{\rho} \cdot A \cdot \vec{\rho} - \vec{g} \cdot Q^T \cdot \vec{\rho}} (d^{N\bar{z}} \vec{\rho}) (d^{2M} \vec{g}) \quad (10)$$

with the abbreviated notation, $Q = B^T \cdot E \cdot C$. As mentioned above, the dependence of dZ_f on the SDF $\vec{\rho}$'s shows that $Z \neq Z_v Z_f$. The quadratic form in $\vec{\rho}$ leads to a Gaussian integral, making it possible to integrate (10) analytically. Changing variables to $\vec{\rho} = \rho + A^{-1} Q \vec{g}$ separates the variables in the exponent, giving $\frac{1}{2} \vec{\rho} A \vec{\rho} + \vec{g} Q^T \vec{\rho} = \frac{1}{2} \vec{\rho} A \vec{\rho} - \frac{1}{2} \vec{g} P \vec{g}$, where, for brevity, $P = Q^T \cdot A^{-1} \cdot Q$.

EQUIPARTITION

Expression (10) can be used to calculate expectation values. An important one is the mean volume,

$$\langle V \rangle = \frac{X_0}{2Z} \cdot \int (\vec{\rho} A \vec{\rho} + \vec{g} P \vec{g}) e^{\frac{1}{2} (-\vec{\rho} A \vec{\rho} + \vec{g} P \vec{g})} (d^{N\bar{z}} \vec{\rho}) (d^{2M} \vec{g}) \quad (11)$$

which separates into two Gaussian integrals, giving

$$\langle V \rangle = \frac{\bar{z}N + 2M}{2} X_0 \quad (12)$$

This result is significant: (i) it is independent of the details of the connectivity matrix A and of the particular stress state; (ii) it is an equipartition principle - the mean volume is shared equally amongst the $\bar{z}N$ SDF and the $2M$ FDF, with each getting on average $X_0/2$, analogously to the mean energy of $3k_B T/2$ per DoF in thermal systems; (iii) it provides a way to measure the compactivity X_0 from the experimentally measurable mean volume.

Other relevant expectation values can also be calculated by expressing them in terms of $\vec{\rho}$ and \vec{g} . Such calculations are straightforward due to the Gaussian form of the integrals. For example, after a little algebra

$$\langle \mathcal{F}_{\alpha\beta} \rangle = -\frac{\partial \ln Z}{\partial (1/X_{\alpha\beta})} = \sum_i \frac{2M R_{ii}^{\alpha\beta}}{p_i} \quad (13)$$

$$\langle \vec{\rho} \cdot \vec{\rho} \rangle = -\frac{\partial \ln Z}{\partial A_{ii}} = Tr\{A^{-1}\} + \sum_i \frac{2M T_{ii}}{p_i} \quad (14)$$

$$\langle \vec{f} \cdot \vec{f} \rangle = -\eta_{ij} \frac{\partial \ln Z}{\partial P_{ij}} = \sum_i \frac{2M U_{ii}}{p_i} \quad (15)$$

again with abbreviated notations: $R = Y^T \cdot C^T \cdot E^T \otimes A^{-1} \cdot Q \cdot Y$, $T = Y^T \cdot Q^T \cdot A^{-1} \cdot A^{-1} \cdot Q \cdot Y$, $U = Y^T \cdot C^T \cdot E^T \cdot E \cdot C \cdot Y$, Y is the matrix that diagonalises P , p_i are the eigenvalues of P , and η_{ij} are straightforward functions of E and C . Relations (12) and (15) are measurable experimentally[16, 17], demonstrating the usefulness of this approach. Furthermore, these results show that, contrary to expectations, structural measurable quantities may depend on the angoricity and stress-based quantities on the compactivity. For example, the purely structural quantity $\langle \vec{\rho} \cdot \vec{\rho} \rangle$ is both proportional to X_0 and depends on the $X_{\alpha\beta}$'s. Another surprising example is the dependence of $\langle \vec{f} \cdot \vec{f} \rangle$, the mean square inter-granular force magnitude, on both a homogeneous function of order 2 of the $X_{\alpha\beta}$'s and on $1/X_0$. These are a direct consequence of the interdependence of the structural and stress subspaces.

EQUATION OF STATE

We next use this formalism to derive what is arguably the most coveted result of the statistical mechanics of granular matter - equations of state. An equation of state is a relation between measurable macroscopic properties, i.e. between expectation values derived from the partition function. Such a relation is also expected to contain a variable that quantifies the fluctuations, e.g. the temperature in thermal systems. One equation of state is that

relating the mean square of the boundary forces, $\langle \vec{g} \cdot \vec{g} \rangle$ and the mean volume $\langle V \rangle$. To obtain such a relation we first note that $\langle \vec{g} \cdot \vec{g} \rangle = 2 \frac{\partial \ln Z}{\partial P_i}$ and that, from its definition, $P_{ij} = h_{i\alpha\beta\gamma\epsilon j} \frac{X_0}{X_{\alpha\beta\gamma\epsilon}}$, where $h_{i\alpha\beta\gamma\epsilon j}$ is independent of both the compactivity and the angoricity. It follows that $\langle \vec{g} \cdot \vec{g} \rangle = 2J(\{X_{ij}\})/X_0$, where $J(\{X_{ij}\})$ is a homogeneous function of order two in the angoricity components, $J(\{\lambda X_{ij}\}) = \lambda^2 J(\{X_{ij}\})$. Using now the equipartition principle we obtain the equation of state

$$\langle \vec{g} \cdot \vec{g} \rangle \langle V \rangle = (Nz + 2M)J(\{X_{ij}\}) \quad (16)$$

As required, this equation relates the macroscopically measurable quantities on the left hand side to the measure of the fluctuations - the angoricity components.

To conclude, we have reviewed several recent results and derived a new one. The volume and stress ensembles cannot be considered independent in the statistical mechanics of granular matter - the phase space must consist of both structural and force DoF. Accordingly, the entropy, which is the log of all the microstates, is not simply the sum of the configurational and stress entropies. This calls into question a large body of work obtained from either ensemble alone. This conclusion holds in any dimension. The combined partition function and an exact description of the volume function in 2D have been used to obtain analytic expressions for a number of expectation values: the mean volume, the force moment, the correlation between distances between intra-grain contact points, and the square magnitude of the contact force. Interestingly, structural properties may depend on the angoricity and stress-based quantities may depend on the compactivity, demonstrating clearly that the commonly believed conjugation of the compactivity with structure / volume and of angoricity with stress is misplaced. Indeed, the natural variable is $\bar{\rho}$, whose conjugate is an involved combination of the compactivity and angoricity. We reviewed the derivation of an equipartition principle for 2D static granular materials - every degree of freedom, whether SDF or FDF, shares a mean volume of $X_0/2$. This result opens again the discussion about the relation between the ensemble statistics and the dynamics of dense granular matter, where an equipartition principle has been shown to be absent, at least in the conventional phase space of positions and momenta[5, 6]. However, since static granular systems are the equivalent of 'zero temperature' granular fluids, our result gives hope that an equipartition principle may be found for dense dynamic systems by considering a larger phase space that includes SDF and FDF. The equipartition principle makes it possible to compute the elusive compactivity from macroscopic measurables and the mean coordination number.

Furthermore, we have outlined how to use these results to obtain equations of state and derived explicitly an

experimentally measurable equation of state relating the boundary loading, the mean volume the angoricity components. We are looking forward to experimental tests of this result. Since the interdependence of the structural and stress ensembles holds in any dimension, it is important to extend the analysis to 3D. Although analytic calculations are difficult due to the cubic form of the volume function in 3D, it should be possible to establish equivalent results using numerical calculations.

ACKNOWLEDGMENTS

JFJ acknowledges support by EPSRC grant - EP/H051716/1

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