Statistical Mechanics of Granular Systems

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Abstract: This work is a review that deals with the possibility of application of statistical mechanics into granular systems. Some modifications of statistical mechanics concepts are introduced in order to apply statistical methods to these systems. The quadron method is proposed to determine correctly the degrees of freedom of granular systems. The total partition function is computed, and it is shown that it gives rise to an equipartition principle for granular systems. In section IV, the failure in the description of granular matter with the volume function, and a reformulation aimed at overcoming such problems is proposed. Section V discuss the possibility of using the above result in the Jamming transition problem. Finally, a personal perspective is given on this topic.

I. INTRODUCTION

Granular matter is a conglomeration of a large number of solid macroscopic particles, with thermal motion fluctuations being irrelevant. Thus, the predominant forces on these systems are frictional. The importance of these systems is obvious: granular matter is present in our everyday experience. Some examples of granular matter are sand, rice, salt, coffee, etc. The size of a particle that constitutes a granular system can range from μm up to m.

This kind of matter is very important in industry. The second most manufactured class of materials, after water, are in the form of granular matter. As a matter of fact, more than 1/10 of the total energy consumption in the whole world is spent in processing granular materials.

Due to the high rate of collisions between grains, these systems are highly dissipative. Therefore, unless the presence of an external force, these systems rapidly achieve mechanical equilibrium. Another important feature is that depending on the density of the system, granular matter will behave as a fluid (low density) or as a solid (high density).

For many decades, scientific research has been done in order to fully understand the unusual behavior of granular systems.

In this work we discuss and review recent work aimed at applying statistical physics techniques to the study of granular matter.

II. STATISTICAL PHYSICS OF GRANULAR MATTER

Thermodynamics is the branch of physics that describes the macroscopic behavior of a system. Using probability theory, statistical physics deals with the same systems and describes their macroscopic behavior in terms of its microscopic constituents. For example, the equation of state of an ideal gas, $PV = nRT$, can be obtained by using statistical physics methods, considering that the gas is constituted of N independent, non-interacting particles, with kinetic energy, $p^2/2m$, where $\vec{p}$ is the linear momentum of each particle.

In principle, statistical mechanics methods could apply to granular systems in order to describe their macroscopic behavior in terms of its constituents and its interactions [5]. In order to use statistical physics to study thermal systems, we must make two assumptions: firstly, assume that it is possible to project the state of the system described by a large number of macroscopic variables $(\vec{q}, \vec{p})$ on a small set of parameters, determining the macroscopic degrees of freedom (DoF). Secondly, the *equal a priori probability postulate* which means that the system can be found, with the same probability, in any of its accessible micro-states (of equal energy). In thermal systems, the total energy is described by the Hamiltonian, $\mathcal{H}$. Fluctuations are a direct manifestation of the temperature, T, of the system.

In granular systems, the potential energy involved in moving a grain of size l, $\sim mgl$, is much larger than the thermal energy, $k_B T$. Thus, granular matter can be considered to be at *zero temperature*. In addition, these systems are in a metastable state, since any external perturbation would change the configuration of the grains.

In granular statistical mechanics, (GSM), we must consider that there are two kinds of DoF, structural and stress, that define the phase space. The original idea proposed in [1] was to replace the Hamiltonian by a volume function $\mathcal{W}$ that depends on the structural DoF. In the volume ensemble, the analogue of the temperature is a scalar parameter called *compactivity*, X_0. If $X_0 = 0$, the system is in the most compact possible state, whereas $X_0 = \infty$, corresponds to the least compact one. In the corresponding stress ensemble, the analogue of the temperature is a tensor, called *angoricity*, X_{ij}.

By analogy with the usual thermodynamic expression for temperature, $T = \partial\langle\varepsilon\rangle/\partial S$, ($\langle\varepsilon\rangle$ is the mean value of the internal energy of a thermal system and S is the entropy) in the two ensembles we can write the com-

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pactivity and the angoricity as:

$$X = \frac{\partial \langle \mathcal{W} \rangle}{\partial S}, \tag{1}$$

$$X_{ij} = \frac{\partial \langle \mathcal{F}_{ij} \rangle}{\partial S}, \tag{2}$$

where $\mathcal{W}$ is the volume function and $\mathcal{F}_{ij}$ is the force-moment tensor.

A. The canonical volume ensemble

In the canonical ensemble, the system is in thermal equilibrium with an external bath at a constant temperature, T. The probability of finding the system with an energy E_r is

$$P(E_r) = \frac{1}{\mathcal{Z}} e^{-\beta E_r}, \quad \text{with } \beta = 1/k_B T. \tag{3}$$

$\mathcal{Z}$ is the partition function of the system and is expressed as follows:

$$\mathcal{Z} = \sum_r e^{-\beta E_r}. \tag{4}$$

In granular systems, we can assume that the total system acts as a "thermal bath", so we can write the probability, p_n of finding the granular system in a specific configuration, with volume v_n, as

$$p_n = \frac{1}{\mathcal{Z}_v} e^{-\frac{v_n}{X}}, \tag{5}$$

where the denominator of (5) is the *volume partition function* and it is defined as

$$\mathcal{Z}_v = \int e^{-\frac{\mathcal{W}(u)}{X}} d\left\{u\right\}, \tag{6}$$

where $\{u\}$ are the structural DoF. Then, the mean value of any observable, A, in this canonical ensemble is given by

$$\langle A \rangle = \frac{1}{\mathcal{Z}_v} \int A\left(\{u\}\right) e^{-\frac{\mathcal{W}(\{u\})}{X}} d\left(\{u\}\right). \tag{7}$$

In particular, the mean volume and the volume fluctuations can be expressed in the following form:

$$\langle V \rangle = \frac{1}{\mathcal{Z}_v} \sum_q V_q e^{-V_q/X} = -\frac{\partial \ln \mathcal{Z}_v}{\partial(1/X)}, \tag{8}$$

$$\langle V^2 \rangle - \langle V \rangle^2 = -\frac{\partial^2 \ln \mathcal{Z}_v}{\partial(1/X)^2}. \tag{9}$$

It is clear that (8) and (9) are the analogues of the mean energy and energy fluctuations in the canonical thermal systems.

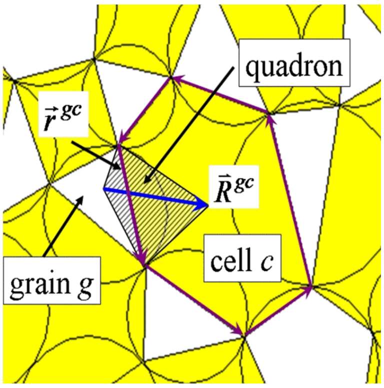

FIG. 1: The quadron is shaded and is constructed with the two vectors $\vec{r}^{gc}$ and $\vec{R}^{gc}$.

III. STRUCTURAL DESCRIPTION OF GRANULAR MATTER

In order to analyze the structure of 2-D granular packing, we introduce the *quadron* method [4]. We consider an N-grain system, each grain with the same coordination number, $\bar{z}$, defined as the mean number of contact points with neighbouring grains.

A. Quadron method

Quadrons are space-tessellating quadrilateral elements in 2-D [3]. To construct a quadron, we must follow four steps:

1. Connect the contact points of each grain, g, with vectors $\vec{r}^{gc}$ that circulate in the clockwise direction
2. Define the centroid of each grain
3. Define the centroid of the surrounding cell, c
4. Connect the centroid of grain g with the centroid of c by a vector $\vec{R}^{gc}$

The quadron is the quadrilateral formed by the two vectors $\vec{r}^{gc}$ and $\vec{R}^{gc}$. Fig. 1 is an illustration of the quadron method. For brevity, we define $\vec{r}^q \equiv \vec{r}^{gc}$ and $\vec{R}^q \equiv \vec{R}^{gc}$.

We evaluate the shape of the quadron from the following tensorial product,

$$C^q = \vec{r}^q \otimes \vec{R}^q. \tag{10}$$

The volume function, in terms of $\vec{r}^q$ and $\vec{R}^q$, can be expressed as,

$$\mathcal{W} = \sum_q v^q = \frac{1}{2} |\vec{r}^q \times \vec{R}^q| \tag{11}$$

Then, the partition function is given by

$$\mathcal{Z}_v = \int e^{-\frac{1}{2X_0}|\vec{r}^q \times \vec{R}^q|} \prod_{q=1}^{N_{sdf}/2} dr_x^q dr_y^q, \tag{12}$$

where N_{sdf} are the structural DoF (SDFs).

Having fixed the coordination number for each grain, the number of contacts of each grain is $N_{contacts} = N\bar{z}/2$. Thus, the number of independent variables, in 2-D is $N_{indep} = N\bar{z}$. So, the number of structural DoF is equal to the number of independent variables of the system, $N_{sdf} = N\bar{z}$.

If the vector $\vec{\rho} \equiv \left(r_x^1, r_x^2, ...r_x^{N\bar{z}/2}, r_y^1, r_y^2, ..., r_y^{N\bar{z}/2} \right)$ is defined, the volume function $\mathcal{W}$ becomes quadratic, and therefore, the partition function can be written as,

$$Z_v = \int e^{-\frac{1}{2X_0} a_{\alpha\beta}^{qp} r_\alpha^q r_\beta^p} \prod_{q=1}^{N\bar{z}/2} \prod_{i=1}^{2} dr_i^q = \int e^{-\frac{1}{2}\vec{\rho}\cdot A \cdot \vec{\rho}} d^{N\bar{z}} \vec{\rho}, \tag{13}$$

where $a_{\alpha\beta}^{qp}$ is a matrix that represents the area of the quadrilateral, $\frac{1}{2}|\vec{r}^q \times \vec{R}^q|$, α and β run over the Cartesian components, and x, y and p, q run over quadrons.

In view of this discussion, we can understand the quadrons as the quasi-particles of the volume ensemble. As grain volumes are constituted by small volume elements, it is reasonable to think that quadrons are the quasi-particles of the volume ensemble.

B. The canonical stress ensemble

Consider that the granular system is subjected to M boundary forces, $\vec{g}^m$ $(m = 1, 2, ..., M)$, acting on the boundary grains. As the system is static, its state will be defined solely by these boundary forces. Thus, the stress DoF will correspond to these $\vec{g}^m$ forces. The partition function will be given by combinations of these boundary forces acting on the boundary grains, with the constrain that these boundary forces are fixed.

Then, we can write the canonical partition function of the stress ensemble as follows,

$$Z_f = \int e^{-\frac{1}{X_{\alpha\beta}}\mathcal{F}_{\alpha\beta}} \prod_{m=1}^{M} d\vec{g}^m, \tag{14}$$

where $X_{\alpha\beta}$ is the angoricity, $\mathcal{F}_{\alpha\beta}$ is the force moment function, and $\vec{g}^m$ are the independent boundary forces.

The force moment function can be expressed in terms of the *loop forces* of the cell containing the quadron, q:

$$\mathcal{F}_{\alpha\beta} = \sum_{gc} f_\alpha^q r_\beta^q, \tag{15}$$

where f_α^q is the α component of the loop force containing the quadron q, and r_β^q is the r vector of quadron q. As quadrons sharing the same cell have the same loop force, only $N/2$ of the $N\bar{z}$ loop forces are independent. So, we define the loop force vector, $\vec{\phi} = (f_x^1, f_x^2, ..., f_x^{N/2}, f_y^1, f_y^2, ..., f_y^{N/2})$ as is done in the volume ensemble.

Taking into account that the stress DoF are the boundary forces, we must express the loop forces in terms of these boundary forces [2]. To do that, the $N\bar{z}/2$ intergranular forces must be expressed in terms of the M boundary forces and then, using the definition of loop forces, in terms of the contact forces. The result is,

$$\phi_\alpha^c = C_{\alpha\beta}^{qm} g_\beta^m, \tag{16}$$

where $\alpha, \beta = x, y$, $c = 1, 2, ..., N/2$ runs over all cells, $m = 1, 2, ..., M$ runs over all boundary forces and C is an $N \times 2M$ matrix.

Two definitions are introduced now. Firstly, $\vec{f^q} = E\vec{\phi}$, where E is an $N\bar{z} \times N$ matrix. Secondly, $B_{\alpha\beta}^{qp} \equiv X_{\alpha\beta}^{-1}\delta qp$. With these definitions, we have now all the ingredients needed to compute the stress partition function, $\mathcal{Z}_f$. The expression is,

$$\mathcal{Z}_f = \int e^{-\vec{\phi}\cdot E^T \cdot B \cdot \vec{\rho}} \prod_{m=1}^{M} d^2\vec{g}^m = \int e^{-\vec{g}\cdot C^T \cdot E^T \cdot B \cdot \vec{\rho}} \prod_{m=1}^{M} d^2\vec{g}^m. \tag{17}$$

C. Total partition function

In order to compute the total partition function, we must integrate over all the phase space, $dZ = dZ_v dZ_f$. Defining $Q \equiv B^T \cdot E \cdot C$, the total partition function will be given by,

$$Z = \int e^{-\frac{1}{2}\vec{\rho}\cdot A \cdot \vec{\rho} - \vec{g}\cdot Q^T \cdot \vec{\rho}} (d^{N\bar{z}}\vec{\rho})(d^{2M}\vec{g}). \tag{18}$$

This last equation shows that the volume ensemble and the stress ensembles are inter-dependent, as the stress ensemble has in the exponential a linear term in $\vec{\rho}$.

In order to separate the variables in the exponential, we change the variables to $\tilde{\vec{\rho}} = \vec{\rho} + A^{-1}Q\vec{g}$. Then, the partition function becomes:

$$\mathcal{Z} = \int e^{\frac{1}{2}(-\tilde{\vec{\rho}}A\tilde{\vec{\rho}} + \vec{g}P\vec{g})} (d^{N\bar{z}}\tilde{\vec{\rho}})(d^{2M}\vec{g}). \tag{19}$$

The calculation of the partition function allows us to estimate the mean volume as,

$$\langle V \rangle = \frac{X_0}{2\mathcal{Z}} \int (\tilde{\vec{\rho}}A\tilde{\vec{\rho}} + \vec{g}P\vec{g}) e^{\frac{1}{2}(-\tilde{\vec{\rho}}A\tilde{\vec{\rho}} + \vec{g}P\vec{g})} (d^{N\bar{z}}\tilde{\vec{\rho}})(d^{2M}\vec{g}). \tag{20}$$

This expression can be split into two gaussians, which gives the surprising result:

$$\langle V \rangle = \frac{N\bar{z} + 2M}{2} X_0. \tag{21}$$

This result plays the role of the equipartition principle of granular statistical mechanics. In thermal systems, the kinetic energy of a particle with mass m and velocity $\vec{v} = (v_x, v_y, v_z)$ is equally shared $k_B T/2$ times among the DoF. In granular systems, the mean volume is distributed equally among the volume, $(N\bar{z})$, and stress, $(2M)$, DoF, each of them having a contribution of $X_0/2$ to the mean volume of the granular system.

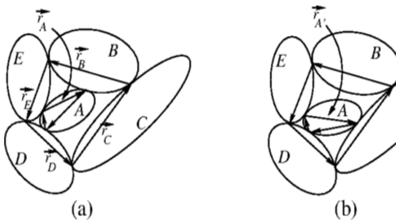

FIG. 2: The volume function in Eq. (23) can not distinguish between the configurations of (a) and (b).

IV. FAILURE OF THE VOLUME FUNCTION IN GRANULAR STATISTICAL MECHANICS

In thermal statistical mechanics, the Hamiltonian, H, describes the total energy of the system in terms of all the DoF. Any derivative of H respect to a DoF must be different from a derivative respect to another DoF. If the derivatives are equal, the Hamiltonian does not describe properly the energy of the system, leading to a miscounting of the microstates, and therefore, a wrong calculation of the entropy of the system. Within this viewpoint, it has been shown [6], that the volume function, $\mathcal{W}$, does not depend on all the structural DoF, and a reformulation must be done in order to have a good estimation of the entropy.

Consider the system of grains as represented in Fig. 2. The volume function of Fig. 2(a) is

$$\mathcal{W} = \frac{1}{2}\left(|\vec{r}_B \times \vec{r}_C| + |\left(\vec{r}_B + \vec{r}_C\right) \times \vec{r}_D|\right). \tag{22}$$

Changing the position of grain A in Fig. 2(b), we obtain the same volume function as in the (a) configuration. Therefore, $\mathcal{W}$ can not discriminate the two configurations. Following the argument at the beginning of this section, and taking the derivative of $\mathcal{W}$ with respect to $\vec{r}_A$ and $\vec{r'}_A$, we obtain

$$\frac{\partial \mathcal{W}}{\partial \vec{r}_A} = \frac{\partial \mathcal{W}}{\partial \vec{r'}_A} = 0. \tag{23}$$

Thus, $\mathcal{W}$ does not depend on all the DoFs. Therefore, it is not a good analogue of the Hamiltonian.

The *connectivity function*, $\mathcal{C}$ is now introduced in order to have a good analogue of the Hamiltonian that includes a dependence on *all* the DoFs. It is defined as follows:

$$\mathcal{C} = \sum_{q,p=1}^{n\bar{z}} \sum_{\alpha,\beta=1}^{d} b_{qp;\alpha\beta} r_{q\alpha} r_{p\beta} \tag{24}$$

where $b_{qp;\alpha\beta}$ are coefficients that are discussed below and the sum runs over all the vectors, $\vec{r}$, of the system. The *contacture* is the replacement of the compactivity, X_0, and is defined as

$$\tau = \frac{\partial\langle\mathcal{C}\rangle}{\partial S}, \tag{25}$$

where S is the entropy of the system. As temperature is related to energy fluctuations in thermal systems, the contacture is a measure of the fluctuations of the connectivity function in granular systems. With this definition, the exponential term of Eq. (13), $\mathcal{W}/X_0$, must be replaced by $\mathcal{C}/\tau$.

In order to compute the coefficients $b_{qp;\alpha\beta}$, it must be assumed that $\mathcal{C}$ is additive. This fact implies that $b_{qp;\alpha\beta}$ do not have cross terms, and thus, that is independent of p and q. $\mathcal{C}$ must be independent of the orientation of the coordinate system as well, defining $b_{qp;\alpha\beta}$ as a scalar times the unit matrix. Dividing τ by the constant parameter, $\mathcal{W}$ is then expressed as follows,

$$\mathcal{C} = \sum_{q=1}^{N\bar{z}} \vec{r}_q \cdot \vec{r}_q = \sum_{n=1}^{d} \vec{R}^{(n)} \cdot \vec{R}^{(n)}, \tag{26}$$

where the vector $\vec{R}^{(n)} \equiv (r_{1x_n}, r_{2x_n}, ...)$ contains all the x_n components of the $\vec{r}$ vectors of the system.

V. JAMMING

An interesting problem where the previous formalism could be applied is the problem of Jamming [7]. A granular system is jammed when it is at zero temperature, zero shear stress and high density. Jamming is the transition from a flowing to a rigid state. Note however that Jamming does not mean crystallization. Crystallization is the process where a group of atoms are ordered in a defined structure forming a solid. Instead, in the Jamming state the grains that form the solid do not present any kind of order.

Consider an ideal spheres model at zero temperature and zero shear stress, that interact via a pairwise potential of the form:

$$V\left(r_{ij}\right) = \begin{cases} \frac{\varepsilon}{\alpha}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^{\alpha} & r_{ij} < \sigma_{ij} \\ 0 & r_{ij} \geq \sigma_{ij} \end{cases} \tag{27}$$

where ε is the repulsion energy, σ_{ij} is the average diameter between two spheres and r_{ij} is the distance between centers of two spheres. Special cases of interest correspond to $\alpha = 2$ (harmonic), $\alpha = 5/2$ (Hertzian in 3-D) and $\alpha = 0$ (hard-spheres).

In order to have a representation of the jamming transition, the Jamming phase diagram (Fig. 3) is introduced. When the density of the system is very low, the particles are free to move, they do not overlap each other. The system behaves as a fluid. At high density, overlapping between particles occurs, and then, the system is in the jammed state. At a critical density, φ_c, the system is between the jammed and unjammed state. As the transition between the two states is discontinuous, it has a first-order nature. Point J represents the critical point in the ideal spheres model. The location of the critical point is at $\varphi = \varphi_c$, $T = 0$ and $\sigma = 0$.

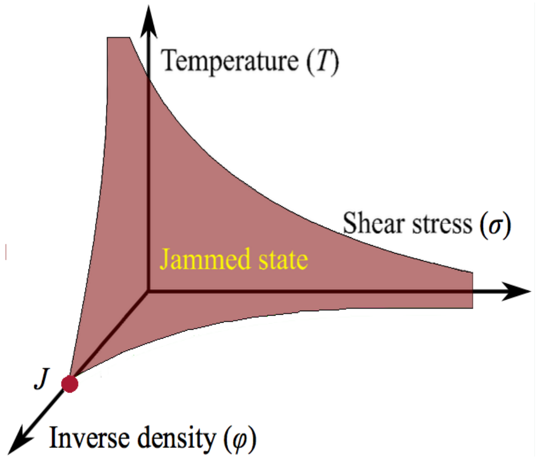

FIG. 3: Jamming phase diagram. At high density values, low temperature and low shear stress, the system is in the jammed state. Point J represents the transition for the ideal spheres model at $T = 0$ and $\sigma = 0$.

The order parameter of this transition is Z, the average number of overlaps of a particle with its neighbors. $Z = 0$ corresponds to a very low packing fraction of the system, ϕ. The density is very small, so that there is no overlapping between particles. At a critical packing fraction value, ϕ_c, Z jumps from 0 to the critical transition value, Z_c.

In order to apply statistical mechanics formalism of granular matter to the jammed state, we suggest to establish an order parameter based on the quadron concept introduced previously. Firstly, construct the quadron of the system in the jammed state. As the coordination number of the grains in the jammed state is different from that of the unjammed state, the quadron will not be the same for the two states. It is clear that this order parameter is closely related to the usual order parameter Z. Indeed, this order parameter will take zero value in the unjammed state and non-zero value in the jammed state. Notice that the volume function, $\mathcal{W}$, will be different in both states. We expect that its calculation allows us to compute the total partition function, $\mathcal{Z}$, and then, the mean volume, $\langle V \rangle$, of the jammed state.

VI. CONCLUSIONS

Since the first attempt of applying statistical physics methods to granular systems done by Edwards in 1988 [1], a lot of theoretical and computational research have been done during all of these years. Unless the efforts of many physicists trying to elaborate a theory that describes the behavior of granular systems, some issues remain open up to date.

Firstly, no equation of state has been written yet. This fact points out some misconceptions in applying the concepts of statistical physics in granular systems. Secondly, the lack of ergodicity in granular systems, that imposes a difficulty in order to describe the dynamics of these systems from static partition functions.

However, some surprising results have been achieved, such as, finding an equipartition theorem for granular systems (21), the fact that the stress and volume ensemble are coupled and the reformulation of the volume function in terms of all the DoF, opening the door to a possible equation of state for granular matter.

The jamming transition could be an interesting problem to test the theoretical framework that has been developed in this work. Moreover, this phase transition contributes to close the circle of the different behaviors that granular matter present under certain conditions.

The field of granular matter physics is still open. Great discoveries have been found, but some issues remain open. Ideas are required in order to elaborate a general theory of granular matter that can be confirmed with experiments.

Acknowledgments

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