Entropy and Temperature of a Static Granular Assembly: An *Ab Initio* Approach

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We construct a statistical framework for static assemblies of deformable grains which parallels that of equilibrium statistical mechanics but with a conservation principle based on the mechanical stress tensor. We define a state function that has all the attributes of entropy. In particular, maximizing this function leads to a well-defined granular temperature and the equivalent of the Boltzman distribution for ensembles of grain packings. Predictions of the ensemble are verified against simulated packings of frictionless, deformable disks.

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Grains are small but macroscopic objects whose interactions are dissipative and whose collective behavior determines properties such as flow and mechanical strength of granular matter [1,2]. The dissipative nature of granular materials makes them explicitly nonequilibrium: energy has to be supplied to the system to maintain a steady state. If the energy supply is turned off, granular materials relax to a static, mechanically stable packing (a blocked state) through the dissipation of energy. Given a fixed set of macroscopic parameters, e.g., volume and number of grains, many such states are possible. The statistical properties of this ensemble of blocked states determines collective phenomena such as the phase behavior and response of weakly driven granular matter. A natural question that arises is whether there are fundamental principles that predict the statistical weights of the different blocked states [3–5]. In this Letter we establish a statistical theory of blocked states starting from a conservation law and a maximum entropy postulate. We demonstrate that packings of frictionless grains, generated through dissipative dynamics, obey the statistical weights predicted by this theory.

Our approach for predicting probability distributions of blocked states parallels that of equilibrium statistical mechanics: we (i) identify a conservation principle associated with the internal virial [6], Γ; (ii) define an entropy function that depends on Γ, volume, and the number of particles; (iii) postulate entropy maximization to introduce a ''granular temperature;'' and (iv) construct a probability distribution involving the inverse granular temperature, α. This granular temperature is distinct from earlier definitions [4,7] but is shown to have the property most commonly associated with temperature, i.e., it is equal in all parts of a packing in granular equilibrium. We also demonstrate that the entropy is indeed the logarithm of the density of states, providing strong support for the microcanonical ansatz that all blocked states with the same Γ are equally likely. The Edwards ensemble for incompressible grains is based on equal probability of blocked states with the same volume [3,4].

Conservation principle.— Every grain in a blocked state satisfies constraints of force and torque balance, leading to the macroscopic conditions of a symmetric and divergence-free stress tensor, $\hat{\sigma}$ [8]. The divergence-free property implies that $\hat{\Sigma} = V\hat{\sigma}$, where V is the volume of the packing, is left invariant by grain rearrangements that do not involve the boundary. This conservation principle can be explicitly demonstrated for two-dimensional packings.

For planar packings of grains interacting through contact forces, the force and torque-balance constraints can be incorporated through a mapping to a set of auxiliary (height) variables defined on the dual network of the voids surrounded by grains [9,10]. Choosing the center of an arbitrary void as the zero of the height field, the height vectors are constructed iteratively through $\vec{h}_\nu = \vec{F}_{ij} + \vec{h}_\mu$, where ij is the contact traversed in going from the center of the void μ to that of ν (cf. Fig. 1). Since the $\vec{F}_{ij}$'s around a grain sum to zero, the mapping of forces to heights is one to one up to an arbitrary choice of the origin (O in Fig. 1). This mapping satisfies Newton's third law and enforces the force-balance constraint. The constraint of torque balance imposes a divergenceless condition on the height field [9,10]. The microscopic stress tensor for grain i is defined as [8]

$$\hat{\sigma}_i = \sum_{j=1}^{z_i} \vec{d}_{ij}\vec{F}_{ij}, \tag{1}$$

where the $\vec{d}_{ij}$ are the vectors connecting the grain center to its contact points, the $\vec{F}_{ij}$ are the contact forces and z_i is the number of contacts for grain i. In terms of the height field [9], $\hat{\sigma}_i = \sum_{\mu=1}^{z_i}(\vec{r}_{\mu 1} + \vec{r}_{\mu 2})\vec{h}_\mu$, where the $\vec{r}_{\mu 1}$ and $\vec{r}_{\mu 2}$ are the vectors linking the two contact points associated with the void μ (cf. Fig. 1). The grain area is defined as the area enclosed by the $\vec{r}_\mu$-vectors and tesselate the plane (cf. Fig. 1). The macroscopic stress tensor $\hat{\sigma}$ is $\hat{\sigma}_A = \frac{1}{A}\sum_{i\in A}\hat{\sigma}_i$, where the summation is over a connected cluster of grains and the area A is the combined grain area of all grains in the cluster. In the summation over grains in $\hat{\sigma}_A$,

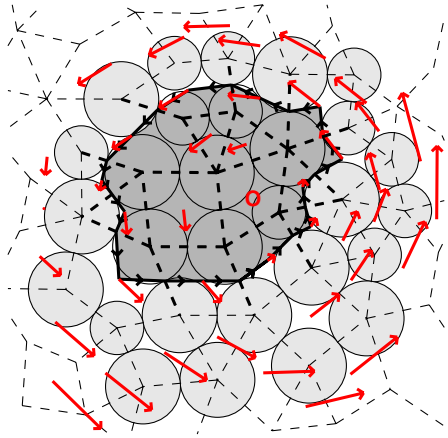

FIG. 1 (color online). Height map: A height map with its origin at **O** in the interior of a packing obtained from simulations. The height vectors $\vec{h}_\mu$ [gray (red) arrows] are shown along with the boundary vectors $\vec{r}_{\mu 1}$, $\vec{r}_{\mu 2}$ (dark arrows) entering Eq. (2). The dashed lines denote intergrain contacts and the ones included in $\hat{\sigma}_A$ for a cluster with $m = 8$ grains occupying the shaded region with area v_m, are in bold.

the terms related to voids fully inside the area A add up to zero and, as illustrated in Fig. 1, we are left with a sum over the voids at the boundary of A:

$$\hat{\sigma}_A = \frac{1}{A} \sum_{\mu \in \text{boundary}} (\vec{r}_{\mu 1} + \vec{r}_{\mu 2}) \vec{h}_\mu. \tag{2}$$

It follows that the extensive quantity, $\hat{\Sigma} = A\hat{\sigma}_A$, is left invariant by local rearrangements not involving the boundary. Different packings with the same value of $\hat{\Sigma}$ can be related to each other through such rearrangements. An example is provided by the "wheel moves" in a triangular lattice [11].

For packings in higher dimensions, the loops around grains cannot be defined unambiguously and, therefore, the height map cannot be constructed. Nevertheless, the divergence-free property of the macroscopic stress tensor $\hat{\sigma}$ implies that a differential form of Stokes' theorem [12] can be used to establish the same conservation principle.

In general, the full tensor $\hat{\Sigma}$ is needed to characterize a system. For frictionless isotropic systems, however, the only independent quantity is the trace Γ, which is nothing but the internal virial [6]. In this case, since packings with different values of $\Gamma = \sum_{ij} d_{ij} F_{ij}$ [cf. Eq. (1)] cannot be transformed into one another through purely internal rearrangements, the space of blocked states can be divided into sectors labeled by Γ. The density of states $\Omega(\Gamma, V, N)$ can, therefore, be defined unambiguously and Γ becomes the analog of energy in thermal systems. The function $S = \ln\Omega(\Gamma, V, N)$ is the analog of the Boltzman entropy [13]. Assuming an entropy maximization principle for granular equilibrium implies equalization of the granular temperature [13,14] $(1/\alpha)$: $\alpha = \partial S/\partial\Gamma|_{V,N}$. A constant-$\alpha$ canonical ensemble [13] follows with the probability of finding a blocked state ν being given by: $P_\nu = \exp(-\alpha\Gamma_\nu)/Z(\alpha, V, N)$. This treatment can be easily generalized to nonisotropic systems or systems with friction by considering the full stress tensor, and a tensorial granular temperature.

Testing the equality of granular temperature.—To test the predictions of our statistical framework, we generate blocked states of bidisperse deformable disks that interact via purely repulsive linear spring interactions, for $N = 1024$ and $N = 4096$ disks. The mixtures are 50:50 by number and the diameter ratio between large and small disks is 1.4. For each N we study several packing fractions from around random close packing $\phi = 0.84$ to more than 20% above this value. To create the packings, we initialize the disks with random initial conditions at a specified packing fraction and then implement conjugate gradient energy minimization at fixed volume to find the nearest local energy minimum [15]. Near random close packing, the packings typically have some grains with no contacts ("rattlers"). In all of our analyses, these rattlers have been excluded since the rattlers are not in contact with the rest of the system and cannot achieve granular equilibrium. In the simulations, lengths are measured in units of the large-particle diameter and energy is measured in units of the characteristic interaction strength [15]. This renders Γ dimensionless and the contact force is numerically equal to the magnitude of the disk overlap. Each packing is characterized by Γ_N, the total value of Γ for the N-grain packing and by $\langle z \rangle$, the average value of the number of contacts in the packing.

The above dynamics is an alternative to the shaking mechanism [3] for exploring the space of blocked states. If the blocked states generated through this dynamics achieve granular equilibrium, then all subregions of a packing (p) should have the same granular temperature α_p, and the values of Γ_m for m-grain clusters inside packing p should be distributed according to

$$\begin{aligned} P_{m,p}(\Gamma_m) &= \sum_\nu e^{-\alpha_p \Gamma_\nu} \delta(\Gamma_\nu - \Gamma_m) \\ &= \Omega(\Gamma_m, m) \exp(-\alpha_p \Gamma_m)/Z_m(\alpha_p), \end{aligned} \tag{3}$$

where $Z_m(\alpha_p)$ is the partition function, and $\Omega(\Gamma_m, m)$ is an effective density of states arising from combining clusters with the same Γ_m, but different values of v_m. We measure $P_{m,p}$ and $P_{m,q}$ of two different packings p and q at pairs of Γ's, Γ_m and Γ'_m, to construct the ratio

$$\begin{aligned} r_{p,q} &\equiv \log\left(\frac{P_{m,p}(\Gamma_m) P_{m,q}(\Gamma'_m)}{P_{m,p}(\Gamma'_m) P_{m,q}(\Gamma_m)}\right) \\ &= -(\alpha_p - \alpha_q)(\Gamma_m - \Gamma'_m). \end{aligned} \tag{4}$$

The last equality follows if the packings p and q are close enough in ϕ to neglect the dependence of Ω on the overall volume.

Sample packings with $N = 4096$ in two narrow packing fraction ranges are shown in the first column of Fig. 2. We

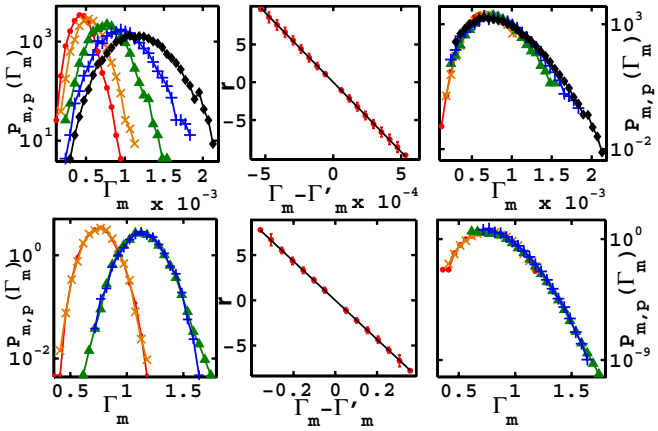

FIG. 2 (color online). Numerical test of the equality of α: Row 1: Sample results from packings with $N = 4096$, $m = 8$ and $\phi = 0.838$–0.844. Row 2: Same for $\phi = 0.95$ and 1.0. First column shows $P_{m,p}(\Gamma_m)$; second column is $r_{p,q}$ vs $\Gamma_m - \Gamma'_m$ for a sample pair (p, q), and a linear fit. The points represent mean and spread of a scatter plot of $r_{p,q}$ obtained for different values of Γ_m and Γ'_m. The third column shows the scaling of $P_{m,p}(\Gamma_m)$ using the $\alpha_{p,q}$ obtained from fit, according to Eq. (5).

find that for pairs (p, q) of packings in the low (0.838–0.844) packing fraction range and in the range (0.95, 1.00), $r_{p,q}$ is indeed a linear function of $\Gamma_m - \Gamma'_m$, establishing that α is equal for all parts of a grain packing. An example of the linear correlation is shown in column 2 of Fig. 2. A further test of the equality of α inside a packing is to verify that for a pair (p, q) with negligible differences in ϕ,

$$P_{m,q}(\Gamma_m)\exp[-(\alpha_p - \alpha_q)\Gamma_m] = P_{m,p}(\Gamma_m), \qquad (5)$$

if both distributions are normalized to unity. The third column in Fig. 2 demonstrates the scaling of packings with an arbitrary packing chosen as the reference p.

For packings with $\phi \sim 0.84$, it is possible to find overlapping distributions, $P_{m,p}(\Gamma_m)$ over a range of Γ_N extending from $\simeq 10^{-5}$–10^{-3}. In this range, we determine α up to an arbitrary constant C by extracting the differences $\alpha_p - \alpha_q$ between packings and summing them starting from an arbitrary reference configuration. Since we expect that $1/\alpha \to \infty$ as $\Gamma_N \to \infty$, we choose C, accordingly. Figure 3 shows the resulting values of $1/\alpha$ as a function of Γ_N. For $m > 2$, we find that over 2 orders of magnitude in Γ_N, the results are independent of m and

$$\alpha = aN/\Gamma_N \qquad (6)$$

with a numerically evaluated coefficient of $1/a = 0.489$.

Density of states.—Since α is defined by the derivative of the entropy with respect to Γ, Eq. (6) implies a specific form of the density of states: $\Omega(\Gamma, V, N) = e^S \sim \Gamma^{Na}$, with $a \simeq 2$, independent of ϕ, for packings with $\phi \simeq 0.84$. Combining this relation with the functional form of $\alpha(\Gamma)$, it is straightforward to show that the distribution of Γ_m in a packing [cf. Eq. (3)] is a function only of $x = N\Gamma_m/\Gamma_N$:

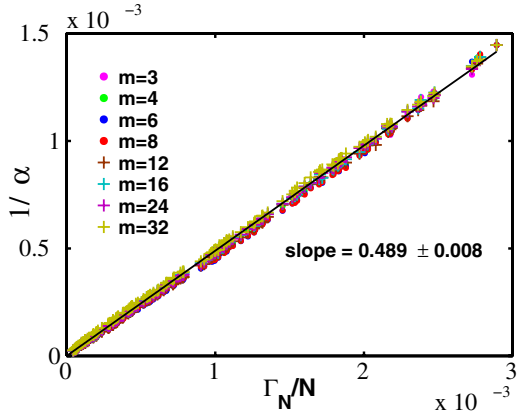

FIG. 3 (color online). Granular temperature: $1/\alpha$ as a function of Γ_N/N obtained from 118 $N = 4096$ packings, showing m independence. The relation is linear over 2 orders of magnitude in Γ_N/N.

$$P_{m,p}(\Gamma_m) \equiv P_m(x) = Cx^{ma}\exp(-ax). \qquad (7)$$

The scaling of the distributions, obtained from multiple packings with $\phi \sim 0.84$, is illustrated in Fig. 4(a) for $m = 24$ and verifies that S is indeed proportional to $\ln\Omega$ in this regime.

For packings with $\phi \geq 0.85$, we found that the distributions obtained from different packings no longer scale with $x = N\Gamma_m/\Gamma_N$, but depend explicitly on ϕ; becoming narrower with increasing ϕ. We know from the simulation data and previous work [15] that the average number of contacts, $\langle z\rangle$, is a strongly increasing function of the packing fraction ϕ and that, in the low packing fraction regime, $\langle z\rangle \to z_{\rm iso} = 4$ (for frictionless disks the isostatic packing has $2d$ contacts where d is the spatial dimension [16,17]). It is also clear from Eq. (7) that $1/a$ is proportional to the width of the rescaled distributions. Based on these observations we hypothesize that the distributions are still de-

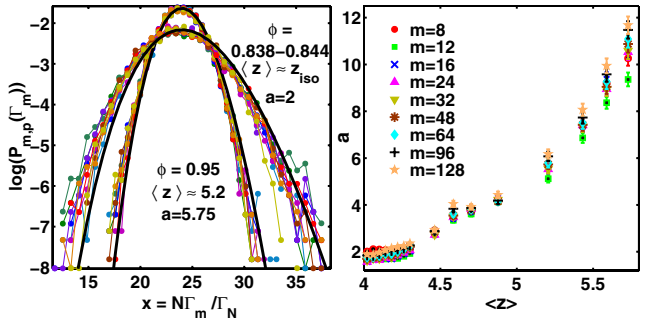

FIG. 4 (color online). Test of Eq. (7): (a) Distributions for $N = 4096$ and $m = 24$ plotted as a function of $x = N\Gamma_m/\Gamma_N$. For $\phi = 0.838$ to $\phi = 0.844$, distributions are compared to Eq. (7) with $a = 2$ (solid line). For $\phi = 0.95$, with $\langle z\rangle$ in the range 5.207 ± 0.06, Eq. (7) with $a = 5.75$ (solid line) best describes the data. (b) Fitting parameter a obtained from distributions of $N = 1024$ grain packings with different values of the average number of contacts, $\langle z\rangle$.

scribed by Eq. (7) but with $a = 2 + f(\langle z\rangle - z_{\rm iso})$ and $f(0) = 0$. The number 2 is consistent with the numerically obtained value (Fig. 3) and is suggestive of the dimension of the packing [18]. A test of the hypothesized form of a is presented in Fig. 4(a). For packings with $\phi = 0.95$, the measured $\langle z\rangle \approx 5.2$ and the best fit to Eq. (7) yields $a = 5.75$. For smaller systems, with $N = 1024$, we performed numerical fits to the distributions over a wide range of $\langle z\rangle$. Figure 4(b) shows the numerical values of a for a discrete set of $\langle z\rangle$ values and for $8 \leq m \leq 128$. It is clear that a increases with $\langle z\rangle$ and approaches 2 for $\langle z\rangle \to 4$. Combining the above results yields an equation of state $\alpha = Na(\langle z\rangle)/\Gamma_N$ that is the analog of an equation of state relating energy, temperature, and density in a thermal system.

For all the packings studied, with α spanning 4 orders of magnitude, we have established that different subregions of a packing have the same value of α. Moreover, α is independent of m and a unique function of Γ_N. These results establish α as an intensive variable which is the granular equivalent of inverse temperature [14].

As $\Gamma \to 0$, the compression of the grains approaches zero and $\Gamma \to \sum_{ij} d_{ij} F_{ij} \equiv F$. Since $\langle z\rangle \to z_{\rm iso}$ in this limit and a tends to a constant, the geometry decouples from Γ. The density of states becomes $\Omega(\Gamma, V, N) \sim \Gamma^{2N} \propto F^{2N}$ and the equation of state is $\alpha \propto 2N/F$. In the incompressible limit, the conservation of Γ reduces to a conservation of F [19], and we recover a Edwards microcanonical ensemble [3] in force space [19,20]. In recent work, based on an entropy maximization principle, the same equation of state was derived by assuming a decoupling of forces and contact geometry and independent contact forces at $\langle z\rangle = z_{\rm iso}$ [21], implying that the contact forces become independent variables.

The numerical data analyzed in this Letter were obtained from a fairly generic dynamical algorithm with no *a priori* information about the ensemble and, therefore, we expect that the results have broad applicability. An interesting question that we have been able to explore in only a limited fashion is that of history independence of the density of states. We have established that configurations with the same value of Γ_N, but obtained from different packing fractions (this is quite likely in the low packing fraction regime) have the same value of the granular temperature $1/\alpha$ and the same distribution $P_{m,p}(\Gamma_m)$.

The full richness of granular statistical mechanics, which is founded on a conserved tensor, not a scalar, can be explored only in systems with friction. Our tests of the statistical ensemble so far have been confined to numerical simulations of frictionless disks because the verification required extensive statistical sampling. We are extending the verification of the statistical ensemble to experimental packings of grains with friction.

In conclusion, we have established a statistical framework for investigating collective properties of granular packings. The constant α ensemble has been used by two of us [10] to formulate a theory of the jamming transition and some of the theoretical predictions have been verified experimentally [22]. The demonstration that equilibrium concepts such as temperature can be extended to granular assemblies opens up new avenues for understanding the intriguing properties of granular matter.

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