Rapid Communications

Direct measurement of force configurational entropy in jamming

James D. Sartor* and Eric I. Corwin†

Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403, USA

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Thermal fluctuations are not large enough to lead to state changes in granular materials. However, in many cases, such materials do achieve reproducible bulk properties, suggesting that they are controlled by an underlying statistical mechanics analogous to thermodynamics. While themodynamic descriptions of granular materials have been explored, they have not yet been concretely connected to their underlying statistical mechanics. We make this connection concrete by providing a first-principles derivation of the multiplicity and thus the entropy of the force networks in granular packings. We directly measure the multiplicity of force networks using a protocol based on the phase space volume of allowed force configurations. Analogous to Planck's constant, we find a scale factor, h_f, that discretizes this phase space volume into a multiplicity. To determine this scale factor, we measure angoricity over a wide range of pressures using the method of overlapping histograms and find that in the absence of a fundamental quantum scale it is set solely by the system size and dimensionality. This concretely links thermodynamic approaches of angoricity with the microscopic multiplicity of the force network ensemble.

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Introduction. Thermodynamics connects abstract and difficult to measure details, such as entropy, with more easily measured bulk properties, such as temperature. In granular systems, for which the thermal energy scale is irrelevantly small, similar connections have been proposed for the volume ensemble [1,2] using compactivity as a temperature analog and also for the force network ensemble [2,3] using angoricity. While these quantities are measurable [4,5], they are not physically meaningful unless they (1) are shown to have temperaturelike properties, such as following the zeroth law and (2) can be rigorously linked to a first-principles definition of microscopic entropy [6]. Entropy itself was initially an empirical quantity until Sackur and Tetrode placed it on firm footing for the ideal gas with the discretization of phase space into quantum-mechanical states [6,7]. The length scale of the discretization depends both on properties of the system and the universal constant $\hbar$, whose value cannot be inferred from bulk properties of the ideal gas alone. Angoricity holds promise as a temperature analog, as it has been shown to follow the zeroth law, while compactivity fails to do so [2,4,8]. However, before the thermodynamic approach of angoricity can be considered to be on solid ground, the nature of the entropy of jammed systems must first be understood.

When the density of an overjammed packing increases, force networks are affected in two ways: (1) force magnitudes, and thus pressure, increase, and (2) new contacts between particles form, increasing the number of contact forces in the network. Both of these changes increase the entropy of the force networks. While the effect on entropy from pressure changes is well understood [5,9], the effect from changes in the contact network is not. To decouple these effects, we propose an extension to the force network ensemble in which changes in the contact network are allowed. This leads us to identify a critical number of excess contacts, δz_c, describing the transition from a regime in which entropy is dominated by changes in pressure to one in which it is dominated by changes in the contact network.

The temperature analog angoricity is defined as the derivative of entropy with respect to the stress tensor [3]. In isotropic systems this tensor quantity can be simplified to a scalar derivative of entropy with respect to pressure. Just as temperature of an ideal gas can be measured from the velocity distribution, angoricity can be measured from the distribution of local pressures [5]. As a derivative, angoricity provides information about the difference in entropy between two systems but not the absolute values. Previous theoretical and experimental work has identified an inverse scaling of angoricity with pressure in the near jamming limit for two-dimensional (2D) soft spheres [5,9]. However, these studies do not systematically explore the effect of changing the contact network, which remains static in the near jamming limit. In our computational study, we explore the system by varying the spatial dimension, pressure, and number of particles over ranges much larger than would be feasible in a physical experiment.

In this Rapid Communication, we present a first-principles derivation of the entropy for the force networks of granular packings. We measure this entropy up to a multiplicative constant, h_f, in the near jamming limit by directly measuring the volume of the space of allowed force configurations. Analogous to Planck's constant in the Sackur-Tetrode equation, h_f discretizes the space of force configurations into an integer number of accessible states. We then use the method of overlapping histograms to measure angoricity as a function

*jsartor7@uoregon.edu
†ecorwin@uoregon.edu

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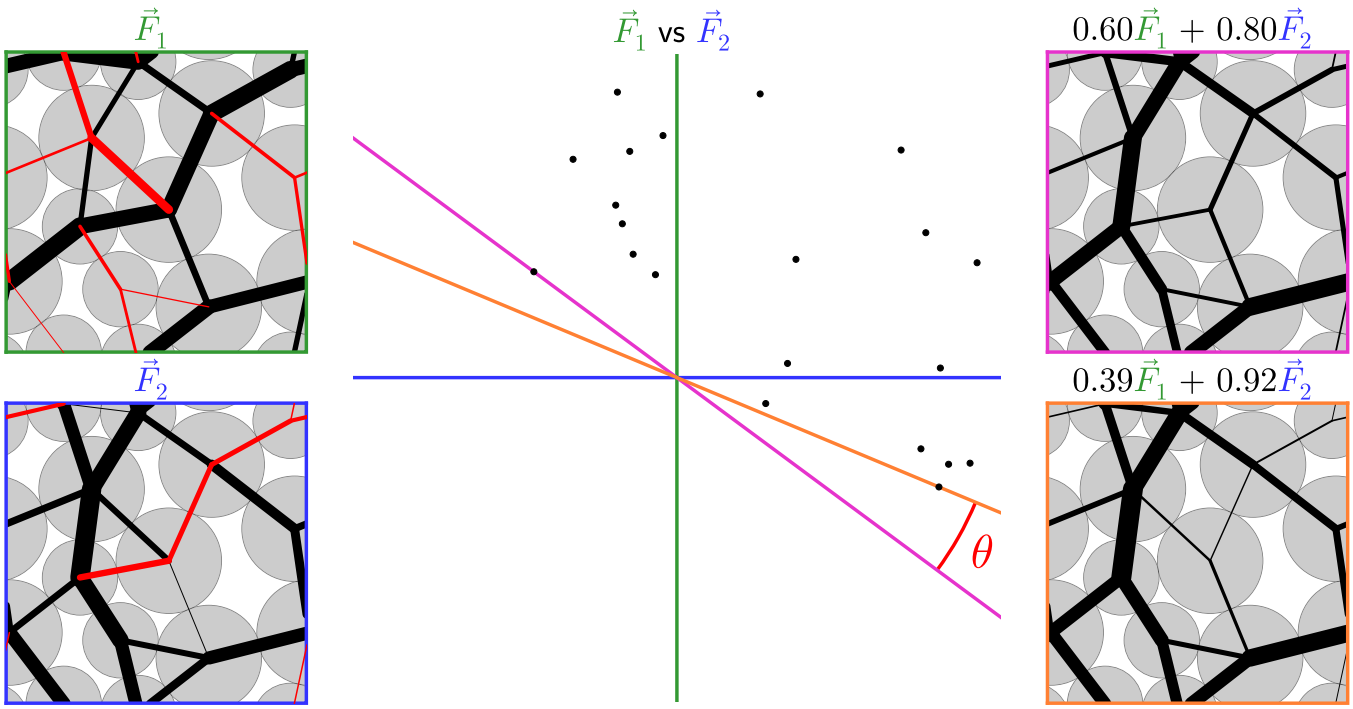

FIG. 1. Force volume measurement for a system with one excess contact. Left: The two independent states of self stress, F_1 and F_2. Black lines between particles represent positive (compressive) forces; red lines represent negative (tensile) forces. Center: A scatter plot of F_1 vs F_2 for each pair of particles. Linear combinations of F_1 and F_2 are represented graphically by drawing a sloped line through the origin and measuring the distance to each point. Any sloped line for which all of the points fall into the same half-space corresponds to a positive-definite linear combination. The set of lines which allow for such solutions is the force space volume, indicated by the angle θ. Note that in a system with ΔZ excess contacts, this volume is a ΔZ-dimensional quantity. Right: The two extremal positive-definite linear combinations at the edge of this region are shown. Each has one force brought to precisely zero.

of pressure, and compare with our force volume measure to solve for h_f. This concretely connects the bulk nature of angoricity with the microscopic multiplicity of the force network Ensemble.

Computational methods. We use pyCudaPacking [10], a GPU-based simulation engine, to generate energy minimized soft sphere packings at specified pressures in periodic boundary conditions. We do so for number of particles, N, spanning from 256 to 4096, and dimension, d, from 2 to 5. The particles are monodispersed, except in 2D in which we use equal numbers of bidispersed particles at a size ratio of 1.4:1 to prevent crystallization. Particles interact through a harmonic contact potential as defined in [10], and the system's energy is minimized using the FIRE minimization algorithm [11].

Starting with random initial positions, we minimize energy and then adjust overall density by uniformly scaling particle radii to achieve a pressure P of 10^{-2} in natural units, as defined in [12]. This pressure is chosen to prevent crystallization artifacts from high density packings. From there, we iteratively adjust the density both up and down to achieve specific values of pressure. We do this efficiently by exploiting the known linear scaling of pressure with density above jamming for a harmonic potential [13]. For each targeted pressure, we ensure that the actual pressure is accurate to a factor of 10^{-5}. We sample 100 logarithmically spaced steps per decade of pressure to ensure sufficient overlap between the distributions of local pressure for neighboring systems, as is needed for the method of overlapping histograms.

Rigidity. To understand the behavior of packings close to the jamming transition we examine the geometric mechanisms necessary for rigidity by constructing an unstressed spring network with the geometry of the packing. The rigidity matrix [14–16], $\mathcal{R}$, describes this spring network by encoding the normalized contact force vectors from the packing, n_{ij}, between pairs of particles i and j as

$$\mathcal{R}^{k\alpha}_{\langle ij\rangle} = (\delta_{jk} - \delta_{ik}) n^{\alpha}_{ij}, \tag{1}$$

where k indexes contacts and α indexes spatial dimensions. For a system with N_{stable} stable particles and N_{contact} contacts, this will be an N_{contact} by $N_{\text{stable}}d$ matrix. The singular value decomposition of this matrix yields two sets of singular vectors, analogous to eigenvectors for a square matrix. The right singular vectors describe the normal modes of position displacements, and the left singular vectors describe the normal modes of force displacements. The left singular vectors corresponding to zero eigenvalues represent mechanically stable force configurations, termed states of self-stress. These vectors need not be positive definite, and therefore are not necessarily valid force configurations for the underlying packing.

The magnitude of each contact force can be considered as a degree of freedom while the requirement for mechanical stability introduces d constraints for each particle. Balancing these constraints requires a minimum number of contacts to ensure stability, which in systems with periodic boundary

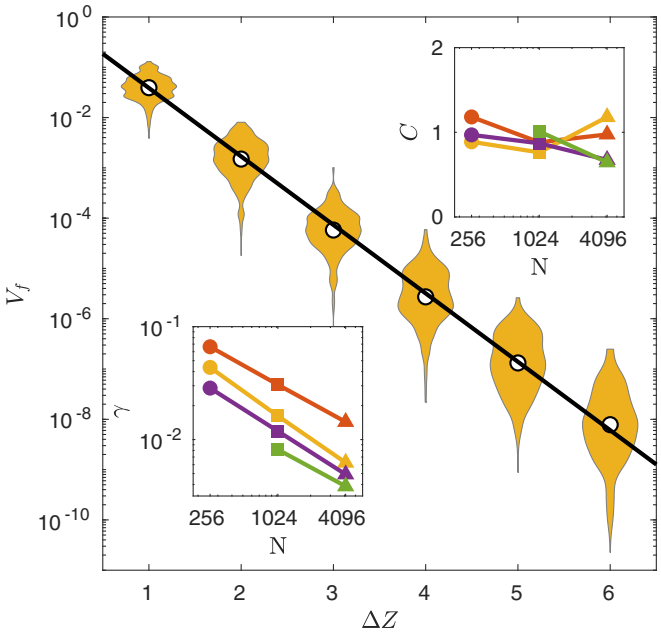

FIG. 2. Representative exponential scaling of the force volume, V_f, with number of excess contacts, ΔZ, for $N = 1024$, $d = 3$. The median of the distribution for each ΔZ is shown as a white circle, surrounded by the full distribution in yellow. The black line shows the exponential fitting form, with exponential base γ. Inset (bottom left): γ for each N and d. Inset (top right): The scale, C, of the exponential. Inset data is presented for $d = 2$ (red), 3 (yellow), 4 (purple), and 5 (green), and $N = 256$ (circles), 1024 (squares), and 4096 (triangles).

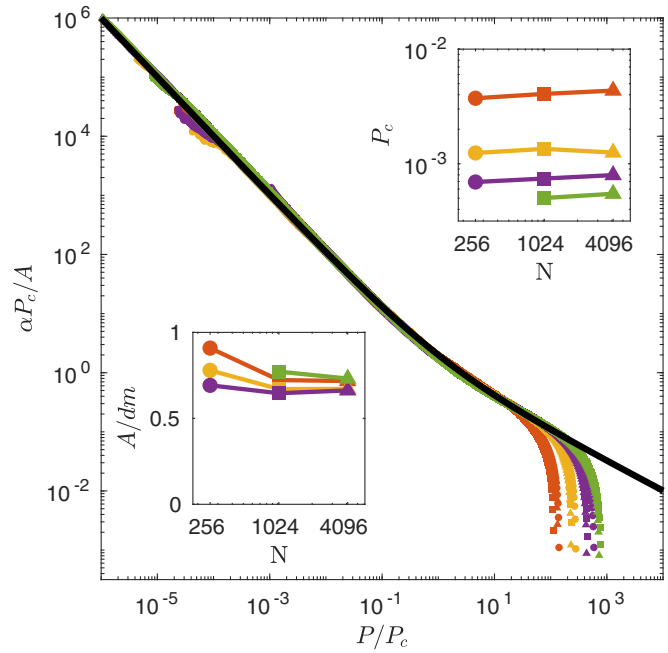

FIG. 3. Scaled angoricity, $\alpha P_c/A$, for all N and d, collapses onto Eq. (8) (black line) when plotted against scaled pressure, P/P_c, until high pressure deviations caused by second-nearest-neighbor interactions. Inset (top right): The crossover pressure P_c. Inset (bottom left): A/dm is approximately 0.7. Colors denote dimensions from 2 to 5 and symbols denote number of particles as in Fig. 2.

conditions is given by [17,18]

$$N_{\text{contact}}^{\min} = d(N_{\text{stable}} - 1) + 1. \tag{2}$$

A system with this minimum number of contacts has exactly one state of self-stress, and each additional contact formed imparts an additional independent state of self-stress. Thus, we define the number of excess contacts, ΔZ, as

$$\Delta Z = N_{\text{contact}} - N_{\text{contact}}^{\min}, \tag{3}$$

making the number of independent states of self-stress $\Delta Z + 1$. We define the number of excess contacts per particle,

$$\delta z = 2\Delta Z/N, \tag{4}$$

where the 2 reflects that each excess contact is shared between two particles. These independent states of self-stress form a basis for the $(\Delta Z + 1)$-dimensional space of all mechanically stable force configurations of the spring network. However, imposing a normalization condition restricts this to a ΔZ-dimensional subspace.

Force volume. The force network ensemble samples all valid force networks in the spring representation of a packing with equal probability [19–21]. To determine the force volume, we calculate the normalized independent states of self-stress where F_μ^q is the contact force on contact q in the state of self-stress μ. The set of all possible repulsive contact forces is defined by linear combinations that satisfy

$$\sum_\mu \lambda_\mu F_\mu^q \geqslant 0 \tag{5}$$

for all contacts q, where $\{\lambda_\mu\}$ are coefficients subject to the normalization condition $\sum_\mu \lambda_\mu^2 = 1$. We define the force volume V_f to be the volume of the space of λ_μ coefficients that satisfy this rule as illustrated in Fig. 1.

We measure this force volume with the following protocol:

(1) Recast F_μ^q into a set, $\{\vec{C}^q\}$, of N_{contacts} vectors containing the value of the force on contact q in each of the $\Delta Z + 1$ states of self-stress.

(2) Planes which pass through the origin and place all of the $\{\vec{C}^q\}$ into a single half-space satisfy inequality (5). We compute the extremal values of such planes as the facets of the convex hull [22] of $\{\vec{C}^q, \vec{0}\}$. The normal vector to each facet is the $\{\lambda_\mu\}$ which defines a vertex of the allowed space of coefficients and corresponds to a linear combination of the independent states of self-stress in which exactly ΔZ forces are precisely 0.

(3) To respect the normalization requirement we calculate V_f as the ΔZ-dimensional solid angle subtended by the volume defined by these vertices in coefficient space.

We convert this volume into a pure number of configurations by discretizing it into hypercubes of side length h_f, named to emphasize the parallelism with Planck's constant h used in the enumeration of phase space states in the Sackur-Tetrode equation. Because the pressure sets the scale of the average force, we then multiply this enumeration by the pressure, as has been shown in previous theoretical

and experimental work [5,9,23]. Putting these considerations together, we arrive at an ansatz relating the microscopic force volume to the multiplicity, and thus the entropy:

$$\Omega = P\frac{V_f}{(h_f)^{\Delta Z}} \implies S = \ln P + \ln V_f - \Delta Z \ln h_f. \tag{6}$$

Although pressure and number of excess contacts both appear in the entropy, they are not independent variables but related in the thermodynamic limit by [12,13]

$$\Delta Z = B(d)N\sqrt{P}, \tag{7}$$

where B is some function of dimension only. We find values of B of approximately 2.1, 6.0, 12.5, and 23 in dimensions two, three, four, and five. These values are roughly consistent with previous studies for two- and three-dimensional spheres [12,18].

Angoricity [3], α, is derived as

$$\alpha \equiv \frac{\partial S}{\partial P} = \frac{1}{P} + \frac{\partial}{\partial P}\ln V_f - \frac{1}{2}\frac{BN}{\sqrt{P}}\ln h_f. \tag{8}$$

First, we measure the volume of force space V_f and explore how it scales with the number of excess contacts. Second, we measure bulk angoricity to confirm our prediction in Eq. (8) and measure the microscopic constant h_f.

Results. As shown in Fig. 2, the measured force volume scales exponentially with the number of excess contacts:

$$V_f = C\gamma^{\Delta Z}. \tag{9}$$

We find C to be well approximated by 1, as shown in the top inset. The lower inset shows that γ decreases with increasing N and d.

We can simplify the expression for angoricity by combining the preceding three equations to find

$$\alpha = \frac{1}{P} + \frac{1}{\sqrt{P_c P}}, \tag{10}$$

where the crossover pressure between the two power laws is

$$P_c = \left[\frac{BN}{2}\ln\left(\frac{\gamma}{h_f}\right)\right]^{-2}. \tag{11}$$

We use the method of overlapping histograms of local pressures [5,24,25] to measure angoricity and determine the value of P_c and therefore h_f. For each system, we measure the local pressure for many random samples of a particle with its $m = 50$ nearest neighbors. The choice of m controls the sharpness of the local pressure distribution and so induces a trivial prefactor A, shown in the inset to Fig. 3 to be proportional to dm. We then compute the angoricity by comparing these local pressure distributions as in Ref. [5]. We fit the angoricity curve to the power law in Eq. (10) with prefactor A and an additive offset. As shown in Fig. 3, all data collapse onto Eq. (10). We extract the crossover pressures, P_c, shown in the upper inset of Fig. 3, and find that they are insensitive to N, but decrease with increasing d.

Discussion. From Eq. (11) and our measured values of γ and P_c we compute h_f, shown in the inset to Fig. 4. A complete expression for entropy can now be written as

$$S = \ln P + \Delta Z \ln\left(\frac{\gamma}{h_f}\right). \tag{12}$$

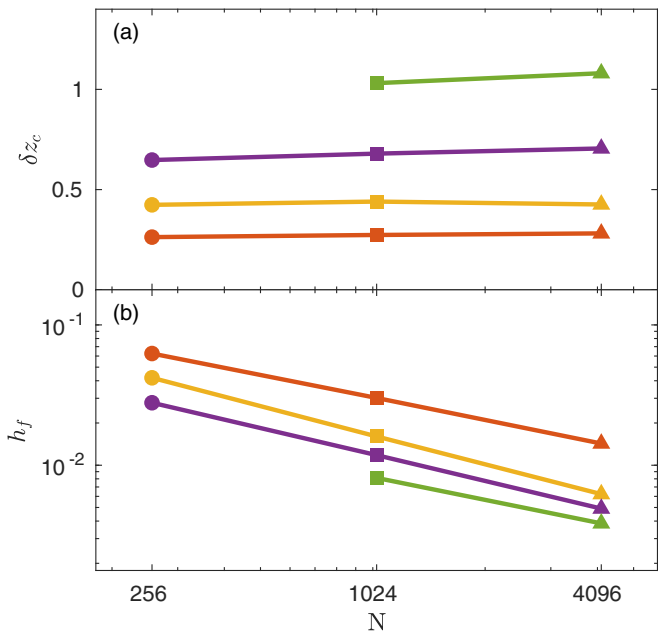

FIG. 4. (a) Scaling of δz_c with N and d. (b) Scaling of h_f, with N and d, calculated from P_c by inverting Eq. (11). Colors denote dimensions from 2 to 5 and symbols denote number of particles as in Fig. 2.

This can be recast into a natural form using Eqs. (7) and (10) by expressing the ratio of γ and h_f as a critical number of excess contacts per particle,

$$\delta z_c = 2B\sqrt{P_c} = \frac{2}{N\ln\left(\frac{\gamma}{h_f}\right)}, \tag{13}$$

$$S = \ln P + \frac{\delta z}{\delta z_c}. \tag{14}$$

Thus, the entropy is dependent on two intensive thermodynamic variables, P and δz, and a constant δz_c for each dimension. While h_f is observed to decrease with N and expected to vanish in the thermodynamic limit, we find δz_c to be intensive with system size, as shown in Fig. 4.

The first term in Eq. (14) describes the entropy increasing from the absolute pressure scale, whereas the second describes the entropy increasing from the number of contacts increasing. Sufficiently close to jamming the first term will dominate as there will be few changes in the contact network even as the pressure changes dramatically. Further from jamming the second term will dominate, reflecting the primacy of changes in the contact network. Note that while this equation may be rewritten as a function of pressure using Eq. (7), for any particular finite packing the integer number of excess contacts is required to calculate the entropy precisely.

Conclusion. We have demonstrated that the force network ensemble framework can be used to directly compute the multiplicity of the force configurations in packings close to the critical jamming point. We have presented an ansatz linking the volume of the force configurational space associated with a packing to the entropy of the packing. This entropy can be expressed as a function of pressure and is independently confirmed by measurements of the angoricity over approximately

seven orders of magnitude of pressure. We have combined these two approaches of measuring entropy in order to extract the fundamental scales governing the discretization of phase space that allows for enumeration. We discover a crossover value for the excess contacts per particle, δz_c, below which the entropy is governed primarily by changes in pressure at fixed contact network and above which the entropy is governed primarily by the creation of new contact forces.

This work places angoricity on a firm footing as a thermodynamic quantity that controls the behavior of overjammed systems. By tracing this entropy all the way down to an enumeration of states we discover that, perhaps unsurprisingly, Planck's constant does not set the fundamental scale of discretization h_f. In a purely classical model such as this, the discretization can only depend on the finite-size effects of the system which are determined by N and d. Thus, in the thermodynamic limit, while h_f vanishes, the behavoir of the system is controlled by δz_c and thus P_c which do obtain fixed values. This full expression for entropy provides the first concrete linking of the microscopic force network ensemble to the thermodynamic description of granular materials and offers a complete description for the thermodynamics of the force networks in overjammed systems.

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