

Experimental Demonstration of Nonuniform Frequency Distributions of Granular Packings

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We developed a novel experimental technique to generate mechanically stable (MS) packings of *frictionless* granular disks. We performed a series of coordinated experiments and numerical simulations to enumerate the MS packings in small 2D systems composed of bidisperse disks. We find that frictionless MS packings occur as discrete, well-separated points in configuration space and obtain excellent quantitative agreement between MS packings generated in experiments and simulations. In addition, we observe that MS packing probabilities can vary by many orders of magnitude and are robust with respect to the packing-generation procedure. These results suggest that the most frequent MS packings may dominate the structural and mechanical properties of granular systems. We argue that these results for small systems represent a crucial first-step in constructing a statistical description for large granular systems from the ‘bottom-up’.

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The power of equilibrium statistical mechanics is that it enables the evaluation of macroscopic state variables (such as temperature and pressure) of a macroscopic system in thermal equilibrium simply by counting microstates. A number of recent studies have applied similar statistical methods to describe dense granular materials [1, 2, 3]. For example, Edwards-ensemble descriptions are based on an assumption that all mechanically stable (or ‘jammed’) configurations of a granular system under a given set of macroscopic constraints are equally likely. The Edwards’ theory also implies the existence of a temperature-like variable—the compactivity χ [4].

Despite the fact that granular media are dissipative and require external driving forces (not thermal fluctuations) to explore configuration space, there has been surprising success in describing these materials using statistical methods based on the Edwards’ assumption [5]. For example, simulations of slowly sheared granular systems have shown that χ can be used to quantify effective ‘thermal’ equilibrium, since different tracer particles achieve the same χ [6] and several equilibrium measures of temperature all agree [7]. However, statistical mechanics approaches for dense granular materials have been applied without directly testing the underlying fundamental assumptions. In particular, the assumption of equal microstate probability has not been tested explicitly, and the relevant microstates have not been clearly defined. We advocate a novel ‘bottom-up’ approach to constructing statistical mechanics descriptions of dense granular materials—one where we enumerate the microstates and accurately measure the probabilities with which they occur.

To do this, we performed a coordinated set of experimental and computational studies of mechanically stable (MS) packings in small 2D granular systems undergoing vertical vibrations. To enable enumeration of MS packings (i.e., microstates), we focused on small systems with no frictional forces. We show that in the absence of frictional forces, the set of MS packings is *discrete*; thus packing probabilities can be directly evaluated by counting the frequency with which

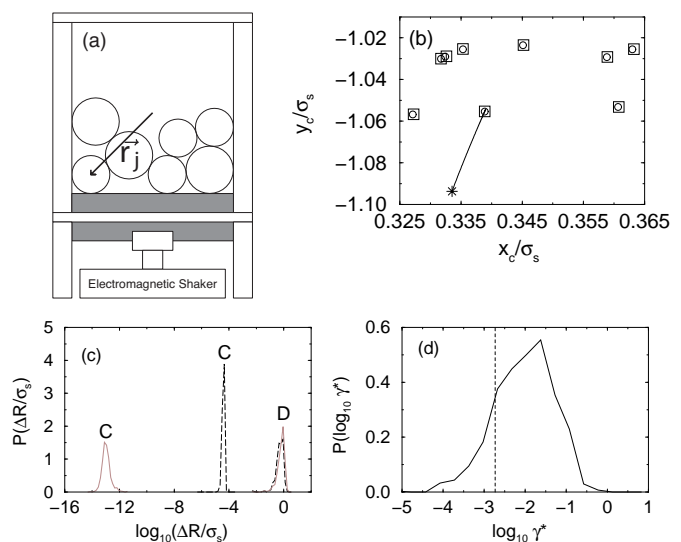


FIG. 1: (a) Schematic of experiment. (b) Coordinates (x_c, y_c) of the centroids of several $N = 7$ MS packings from experiments on plastic (squares) and simulations for γ_{plastic} (circles). The solid line shows the location of one of the centroids for $10^{-7} \leq \gamma \leq \gamma^*$, where γ^* is the value at which the MS packing becomes unstable. The star indicates the location of the centroid at γ^* . (c) Probability distributions of the separation ΔR in configuration space between distinct MS packings (D) and between a given MS packing and the packing furthest away with the same contact network (C) for experiments (dashed lines) and simulations (solid lines). (d) Probability distribution for γ^* from simulations. The vertical line indicates $\gamma = \gamma_{\text{plastic}}$.

they occur in a long sequence of independent trials. In contrast, frictional MS packings [8] form continuous families, and therefore packing probabilities cannot be uniquely determined without first defining an appropriate probability measure. To generate frictionless packings in our experiments, we have developed a novel technique where frictional forces are relaxed using small-amplitude, high-frequency vibrations.

In both experiments and simulations we find the following four key results concerning the microstate distributions of

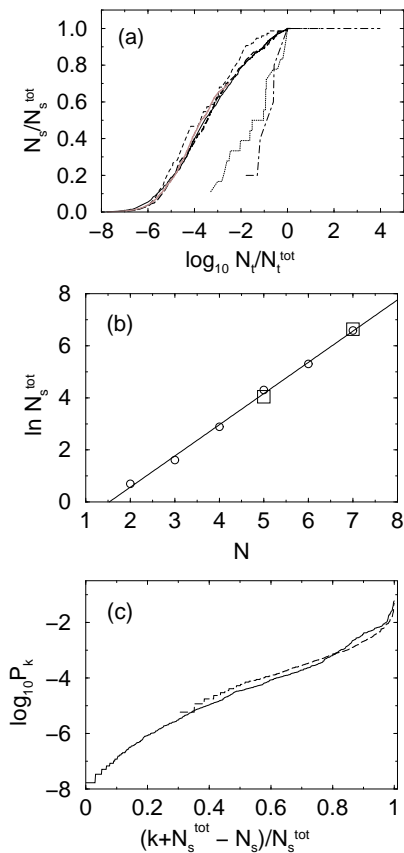


FIG. 2: (a) Number of distinct states N_s found in N_t trials for experiments on plastic (gray solid line) and $N = 3$ (dot dashed), 4 (dotted), 5 (dashed), 6 (long dashed), and 7 (solid) simulations at $\gamma = \gamma_{\text{plastic}}$. The horizontal (vertical) axis is scaled by the total number of MS packings N_s^{tot} (trials, N_t^{tot}) at saturation. The experimental curve was obtained by fitting N_s^{tot} and N_t^{tot} to simulations. (b) N_s^{tot} vs. N from simulations (circles) and experiments (squares). The solid line has slope 1.2. (c) Sorted probability P_k of MS packings for $N = 7$ vs. index $(k + N_s^{\text{tot}} - N_s)/N_s^{\text{tot}}$ for simulations (solid) and experiments (dashed). $N_s/N_s^{\text{tot}} \approx 0.695$ for experiments was determined from (a).

granular packings in the zero-friction limit: 1) There exist a finite number of discrete MS packings that grows exponentially with system size. 2) The frequency with which these packings occur is highly *nonuniform*. 3) The sets of packings found in experiments and simulations of model granular media are very similar. 4) The packing frequency is relatively insensitive to the packing preparation protocol. We argue that the above important new results need to be incorporated into statistical descriptions of dense granular media.

Experiments A schematic of the apparatus used to generate MS frictionless disk packings is shown in Fig. 1(a). A mixture of thin disks of thickness 3.175 ± 0.003 mm and two different diameters σ_s and σ_l were confined between two glass plates separated by 3.20 ± 0.01 mm and rested on a thin plunger connected to an electromagnetic shaker through a slot in the bottom of the cell. The shaker enabled us to apply vertical vibrations at variable amplitude and frequency to repeatedly generate static particle packings.

The particle mixtures consisted of $(N + 1)/2$ small and $(N - 1)/2$ large particles, with $N = 5$ and 7. For these systems we enumerated the majority of frictionless MS packings by performing $N_t = 1.8 \times 10^5$ ($N = 7$) and 1.2×10^4 ($N = 5$) independent trials using the protocol described below. The ratio of disk diameters was $d = \sigma_l/\sigma_s = 1.2520 \pm 0.0003$, and the ratio of the cell width L to the small particle diameter was $\lambda = L/\sigma_s = 4.25314 \pm 0.00001$ (2.65 ± 0.02) for $N = 7$ (5). We used bidisperse systems to prevent ordering.

The degree to which our particles behave as hard disks can be estimated using the dimensionless stiffness parameter $\gamma = m_s g/k\sigma_s$, where g is the gravitational acceleration, m_s is the mass of a small particle, and k is the effective spring constant of the elastic interparticle interaction. By measuring the deformation of single plastic (steel) disks under gravity, we estimate $\gamma_{\text{plastic}} \approx 1.85 \times 10^{-3}$ ($\gamma_{\text{steel}} \approx 3 \times 10^{-7}$), which implies that the deviation of the particle packings from hard-disk behavior is small (cf., Figs. 1(b) and 1(d)).

To generate an ensemble of frictionless MS packings, we repeatedly performed the following protocol: The plunger was first oscillated at high amplitude and low frequency (50 Hz) for 100 ms to randomize particle positions. The system was allowed to relax under gravity with the shaker turned off for 400 ms. We then applied a low-amplitude, high-frequency (400 Hz) oscillation for 500 ms, which excites particle rotation and relaxes frictional particle-particle and particle-wall interactions. Finally, the oscillations were turned off and positions of particle centers were determined to an accuracy of $\Delta/\sigma_s = 6 \times 10^{-6}$ using a digital camera and particle-tracking software. The MS packings in experiments were identified using the set of particle positions $\vec{R}_i = \{\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\}$ for each configuration i , where \vec{r}_j are the x - and y -coordinates of the N particles. (See Fig. 1(a).)

Computer Simulations We also performed molecular dynamics simulations of gravitational deposition of bidisperse frictionless disks. Our goal was to determine how key features of MS packing distributions depend on the particle-deposition process, and to identify which features are robust, i.e., do not depend on specific details of the dynamics. Thus, in the simulations we do not exactly mimic the packing-preparation process in experiments. In particular, we do not model frictional contact forces, but instead we use velocity-dependent resistance forces to dissipate energy. However, geometrically similar sets of MS packings are needed for a detailed comparison of the probability distributions. Thus, we closely match the cell width λ , particle size distribution, gravitational force, and elastic interactions in simulations and experiments to obtain very similar sets of MS packings.

We assume that the disks interact via a finite-range, purely repulsive linear spring force

$$\vec{F}^r(r_{ij}) = \frac{\varepsilon}{\sigma_{ij}} \delta_{ij} \Theta(-\delta_{ij}) \hat{r}_{ij}, \quad (1)$$

which mimics elastic interparticle repulsion. ε is the characteristic energy scale, r_{ij} is the separation between particles i and j , $\sigma_{ij} = (\sigma_i + \sigma_j)/2$ is the average diameter, $\delta_{ij} = r_{ij} - \sigma_{ij}$

is the interparticle overlap, \hat{r}_{ij} is the unit vector connecting particle centers, and $\Theta(x)$ is the Heaviside step function.

To create each MS packing, we randomly place particles in a square cell of size L , with no particle overlaps. We then allow initially stationary particles, interacting via elastic repulsive forces (1) and dissipative forces proportional to relative particle velocities, to fall under gravity. The system evolves according to Newton's equations of motion

$$m_i \vec{a}_i = -m_i g \hat{y} + \sum_{j \neq i}^N \left[\vec{F}^r(r_{ij}) - b \theta(-\delta_{ij}) \vec{v}_{ij} \cdot \hat{r}_{ij} \right] \hat{r}_{ij} + F_i^w, \quad (2)$$

where \vec{a}_i is the acceleration of particle i , \vec{v}_{ij} is the relative velocity of particles i and j , and b is the damping coefficient. The particle-wall interaction force F^w has an analogous form to the particle-particle interaction (2), with energy scale $\epsilon^w = 2\epsilon$. We set the dimensionless damping coefficient to $\bar{b} = \sigma_s b / \sqrt{m_s \epsilon} = 0.25$. The simulations are terminated when the total force \vec{F}_{tot} on each particle is vanishingly small. (In most simulations we used the threshold $F_{\text{tot}} < F_{\text{max}} = 10^{-14}$).

To determine which of the relaxed configurations are mechanically stable, we calculated the eigenvalues of the dynamical matrix [9]. The MS packings possess $2N'$ positive eigenvalues, where $N' = N - N_r$, and N_r is the number of ‘rattler’ particles. Rattlers have fewer than three contacts (including wall contacts) and if present typically rest on the bottom. In the simulations, we distinguish distinct MS packings by comparing the eigenvalue lists. The eigenvalues are considered to be equal if they differ by less than the noise threshold 10^{-6} . Less than 1% of the distinct MS packings contain rattlers. In these configurations, we ignore the translational degeneracy of the rattlers—two configurations with the same contact networks of non-rattler particles are treated as the same. To compare simulation and experimental data in configuration space, we omit the rattler particles, and consider only positions of particles forming the contact network. To enumerate all MS packings and accurately measure their frequencies, we considered small systems in the range $N = 2$ to 7 particles. Systems with an even number of particles contained equal numbers of large and small particles, while systems with an odd number contained one additional small particle.

Results We find that MS packings in frictionless granular systems occur as discrete points in configuration space [14]. In Fig. 1(b) we display the coordinates (x_c, y_c) of the centroids of MS packings in a small region containing several microstates for $N = 7$ (plastic discs in experiments and particles with γ_{plastic} in simulations). The results show that the MS packing centroids are indeed distinct and well-separated. Moreover, the experimental and simulation points agree. Our simulations do not involve static frictional forces, thus this agreement indicates that our novel experimental technique is able to generate mechanically stable frictionless packings.

Fig 1(c) shows that the experimental and numerical scatter in the MS packing centroids is several orders of magnitude smaller than the average separation between discrete MS packings in configuration space. We find that the average dis-

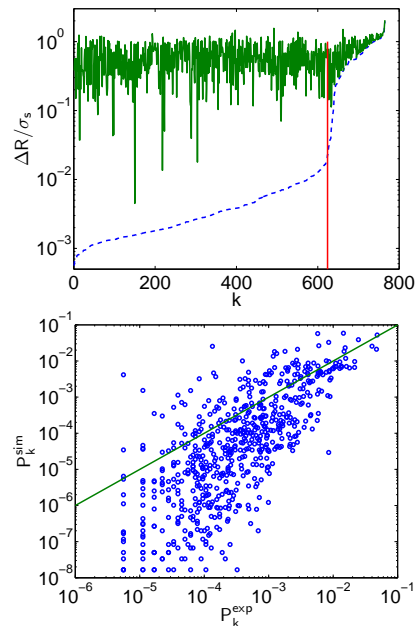


FIG. 3: (a) Distance ΔR_n and ΔR_{nn} between each MS packing from experiments on plastic disks and the nearest (dotted) and next-nearest (solid) MS packing from simulations at γ_{plastic} vs. index k for the experimental MS packings sorted in order of increasing ΔR_n . The vertical line at $k = 618$ separates matched MS packings to the left from those that are unmatched. (b) The probability with which MS packings occurred in experiments, P_k^{exp} versus probability of the matching state in simulations P_k^{sim} . The solid line has slope one.

tance between distinct MS packings in configuration space is approximately $10^{-1}\sigma_s$, whereas the maximum size of the scatter is $10^{-12}\sigma_s$ in simulations and $10^{-5}\sigma_s$ in experiments. Based on this observation, in our analysis of experimental data, two packings \vec{R}_i and \vec{R}_j are considered to be the same microstate if $\Delta R = |\vec{R}_i - \vec{R}_j|/\sigma_s < \Delta R^* = 0.01$.

To determine if particles in our system can be treated as hard disks, we tested the sensitivity of the numerically generated MS packings to variation in the stiffness parameter γ . The solid line in Fig. 1(b) shows the change of position of the centroid of a MS packing when γ is increased from 10^{-7} to the critical value γ^* where a sudden change in the particle contacts occurs ($\gamma^* = 0.06$ for this particular packing). While the overall variation of the position of the centroid is significant, the position of the centroid for $\gamma = \gamma_{\text{plastic}}$ is essentially indistinguishable from the position in the hard-disk limit $\gamma \rightarrow 0$. The distribution of the critical parameters γ^* for the set of all simulation MS packings is depicted in 1(d). These results indicate that most of the hard sphere packings remain stable even when the stiffness parameter is increased above γ_{plastic} .

In simulations, we are able to perform an extremely large number of trials and find nearly all MS packings in small systems. In Fig. 2(a), we show the number of distinct states N_s as a function of the number of trials N_t for systems with $N = 3$ through 7 particles. In all cases (except $N = 7$), we saturate the packing-generation process in the sense that we do not generate new MS packings when the number of trials

is increased by a factor of 10 beyond N_t^{tot} . In experiments we followed a similar procedure, but we were unable to fully saturate the curves because of insufficient number of trials. Fig. 2(b) shows that in experiments and simulations the total number of MS packings grows exponentially with the system size, $N_s^{\text{tot}} \sim e^{aN}$. The exponent $a \approx 1.2$ is the same as found for periodic systems [14]; however, the prefactor is larger by roughly an order of magnitude. The number of trials required to reach saturation of the simulation packing-generation algorithm (cf., Fig. 2(a)) also grows exponentially with N , but with a larger exponent. Since N_t^{tot} grows rapidly with system size, enumeration of $N_s^{\text{tot}} \approx 728$ MS packings for $N = 7$ requires $N_t^{\text{tot}} \sim 10^9$ trials. This large number of trials stems from the extremely nonuniform packing probability distribution.

The frequency distributions for MS packings are extremely nonuniform in both simulations and experiments. As depicted in Fig. 2(c) the MS packing probabilities vary by many orders of magnitude. In addition, we find quantitative agreement in the shape of the frequency distributions, which implies that frequencies of the MS packings are only weakly sensitive to the dynamics used to generate them.

To make a quantitative comparison between MS packings found in experiments and simulations, we calculated the distance in configuration space ΔR between each MS packing generated in experiments and the nearest and next nearest MS packings found in simulations. In Fig. 3(a), we show the nearest-neighbor and next-nearest neighbor separations ΔR_n and ΔR_{nn} for experiments with $N = 7$ plastic disks and the corresponding simulations at γ_{plastic} versus index k sorted by increasing ΔR_n . For approximately 80% of the packings the nearest-neighbor and next-nearest-neighbor distances are well separated, with ΔR_n much smaller than the average distance between packings shown in Fig. 1(c). This separation of length scales in configuration space allows an unambiguous match between packings found in experiments and simulations. At $k \approx k^* = 618$ the distance ΔR_n rapidly increases, and packings with $k > k^*$ are unmatched.

We find that $n = 110$ ($m = 146$) MS packings from simulations at γ_{plastic} (experiments on plastic disks) are unmatched for $N = 7$. However, approximately 70% of the unmatched experimental packings are unstable when used as initial conditions in the simulations. (In experiments, these packings are likely stabilized by residual frictional forces or small inaccuracies in the numerical representation of the experiment.) For example, the results shown in Fig. 1(d) indicate that stability of some packings may depend on the stiffness parameter near $\gamma \approx \gamma_{\text{plastic}}$. The unmatched MS packings from simulation most likely result from insufficient experimental statistics.

To determine the sensitivity of packing probability distributions on the particle deposition process, in Fig. 3(b) we compare the experimental probabilities P_k^{exp} with the probabilities found in simulations P_k^{sim} for the set of matched states. We demonstrate a strong correlation between P_k^{exp} and P_k^{sim} : likely packings in experiments tend to be likely in simulations, and rare packings in experiments tend to be rare in simulations

(although there is also a significant scatter). In fact, we calculate that the rms deviation in the probabilities of matched packings in simulations and experiments is only 8% of the probability of the most frequent MS packing. Since the dynamics in experiments and simulations is quite different, this is an important result, which implies that properties of static frictionless packings are weakly dependent on the packing-preparation protocol.

Conclusions We introduced a novel experimental method to generate frictionless MS packings of granular materials. This method is crucial for studies aimed at differentiating the effects of geometrical constraints and friction on the structural and mechanical properties of jammed granular systems. We performed coordinated experimental and computational studies of frictionless MS packings in small systems, which showed that MS packing probabilities are extremely nonuniform and relatively insensitive to the procedure used to prepare them. In future studies, we will investigate the consequences of our present results for the microstate statistics in macroscopic granular systems treated as a collection of nearly independent small subsystems. We will also dial in frictional contacts to generate continuous geometrical families of MS packings that occur even at fixed γ , and then compare the statistics of these continuous sets of packings to that for discrete MS packings.

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