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Tail of the contact force distribution in static granular materials

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We numerically study the distribution $P(f)$ of contact forces in frictionless bead packs, by averaging over the ensemble of all possible force network configurations. We resort to umbrella sampling to resolve the asymptotic decay of $P(f)$ for large f , and determine $P(f)$ down to values of order 10^{-45} for ordered and disordered systems in two (2D) and three dimensions (3D). Our findings unambiguously show that, in the ensemble approach, the force distributions decay much faster than exponentially: $P(f) \sim \exp(-cf^\alpha)$, with $\alpha \approx 2.0$ for 2D systems, and $\alpha \approx 1.7$ for 3D systems.

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The contact forces inside a static packing of grains are organized into highly heterogeneous force networks, and can be characterized by the probability density of contact forces $P(f)$ [1]. Such force statistics were first studied in a series of experiments that measured forces through imprints on carbon paper at the boundaries of a granular assembly. Unexpectedly, the obtained $P(f)$ displayed an exponential rather than a Gaussian decay for large forces [2]. After these initial findings, other experimental techniques have revealed similarly exponentially decaying distributions of the boundary forces [3,4].

As it is difficult to experimentally access contact forces inside the packing, numerous direct numerical simulations of $P(f)$ have been undertaken [5,6]. While many of these studies claim to find an exponential tail as well, the evidence is less convincing than for the carbon paper experiments: apart from [5], nearly all numerical force probabilities bend down on a logarithmic plot, suggesting a faster than exponential decay [6]. In addition, new experimental techniques using photoelastic particles [7] or emulsions [8,9] have produced bulk measurements, and these also reveal a much faster than exponential decay for $P(f)$, consistent with a Gaussian tail.

Nevertheless, much theoretical effort has focused on explaining the exponential tail of $P(f)$, starting with the pioneering q model [10]. Here, scalar forces are balanced on a regular grid, but it was later realized that, in this model, the tail of $P(f)$ depends on details of the stochastic rules for the force transmission, and need not be exponential [11]. Other explanations for the exponential tail hinge on “entropy maximization” [12], or closely related, on an analogy with the Boltzmann distribution [13,14]. The essence of the latter argument is that a uniform sampling of forces that (i) are all positive (corresponding to the repulsive nature of contact forces), and (ii) add up to a constant value (set by the requirement that the overall pressure is constant) strongly resembles the microcanonical ensemble, in which configurations are flatly sampled under the constraint of fixed total energy.

In this paper, we will probe the tail of $P(f)$ in the force network ensemble [15–20]. This ensemble is obtained by flatly sampling all force configurations for which forces are repulsive and add up to satisfy overall stresses, i.e., (i) and

(ii) as listed above, under the additional constraints of force balance on all grains. We numerically resolve the probability for large forces using the technique of *umbrella sampling* [21], which yields accurate statistics for $P(f)$ for relative probabilities down to 10^{-45} and f up to $f=15$ (throughout, all forces are normalized such that $\langle f \rangle = 1$). This high accuracy is crucial for excluding any crossover effects and allows us to unambiguously identify the behavior for $f \gg 1$. We study the force ensemble for frictionless systems in two and three dimensions, with both ordered and disordered contact networks, and also explore the effect of system size and contact number.

For all systems, we have found that the ensemble yields force distributions that decay much faster than exponentially. The dimensionality of the system is crucial, while other factors hardly affect the asymptotics: $P(f)$ decays as $\exp(-cf^\alpha)$, with $\alpha = 2.0 \pm 0.1$ in two dimensions, while in three dimensions $\alpha = 1.7 \pm 0.1$ [22].

Our results thus underline the importance of the additional constraints that forces have to balance on each grain: these are ignored in the “Boltzmann”-type arguments, but completely alter the properties of $P(f)$.

The ensemble approach to force networks is inspired by the proposal of Edwards to assign an equal probability to all “blocked” states, i.e., states that are at mechanical equilibrium [23]. By limiting the Edwards ensemble to a single packing of fixed contact geometry [24], where the contact forces are the remaining degrees of freedom and all allowed force configurations are sampled with equal weight, one obtains the force network ensemble. Here we restrict ourselves to spherical particles with frictionless contacts, so that every contact force f_i corresponds to one scalar degree of freedom. Furthermore, we require all $f_i \geq 0$ due to the repulsive nature of the contacts. As the equations of mechanical equilibrium are linear in the contact forces, one can cast the solutions $\vec{f} = (f_1, f_2, \dots)$ in the form $\vec{f} = \vec{f}_0 + \sum_k c_k \vec{v}_k$. The solution space is spanned by the vectors \vec{v}_k and \vec{f}_0 , and can be sampled through the coefficients c_k —for details we refer to Refs. [15,16,19]. For a hexagonal packing (two dimensional), these vectors are easily constructed using so-called wheel moves [19], but for other packings we have obtained \vec{v}_k and

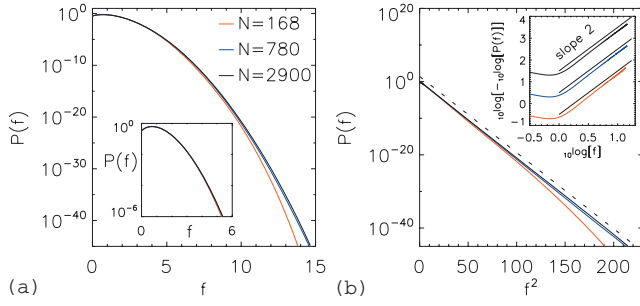


FIG. 1. (Color) Force probabilities in two-dimensional hexagonal packings of N particles with periodic boundary conditions. (a) $P(f)$ decays much faster than exponentially, and rapidly converges to its asymptotic form with N —larger N correspond to wider distributions. The inset illustrates that system size effects are hardly visible for $P(f)$ down to 10^{-6} . (b) $\log_{10} P(f)$ vs f^2 becomes a perfectly straight line for large systems, indicating that the tail of $P(f)$ is well described by a Gaussian decay $\sim \exp(-cf^2)$ (dashed line). The inset shows that, on a triple-logarithmic plot, the asymptotic decay attains a slope close to 2, confirming the Gaussian tail (see text). Curves are offset for clarity, and lines are guides to the eye.

\vec{f}_0 from a simulated annealing procedure [15]. Ensemble averages using a uniform measure in this force space then become

$$\langle q \rangle = \Omega^{-1} \int_{\mathcal{C}} d\vec{c} q, \quad \Omega \equiv \int_{\mathcal{C}} d\vec{c}, \quad (1)$$

where the integral runs over the coefficients c_k limited to the convex subspace \mathcal{C} for which all $f_i \geq 0$ [18].

To obtain accurate statistics for large forces, we perform umbrella sampling. The idea is to bias the numerical sampling toward solutions with large forces, using a Monte Carlo technique with a modified measure $d\vec{c} \rho(\vec{c})/\Omega$, and then correct for this bias when performing the averages, $\langle q \rangle = \langle q/\rho \rangle_{\text{umbrella}}$, since

$$\langle q \rangle = \Omega^{-1} \int_{\mathcal{C}} d\vec{c} \rho(\vec{c}) \left(\frac{q}{\rho(\vec{c})} \right). \quad (2)$$

Defining f_{\max} as the largest force for a given \vec{c} , we have used a measure $\rho(\vec{c}) \propto e^{W(f_{\max})}$, where W is chosen such that the

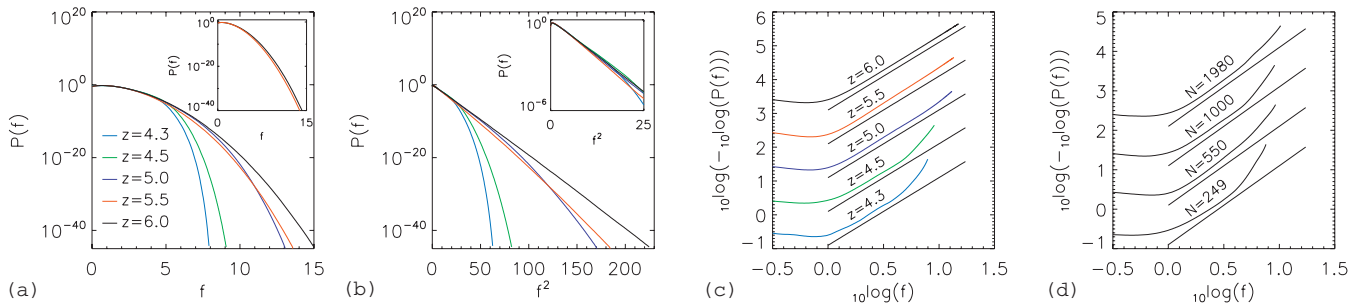


FIG. 2. (Color) Force distribution for two-dimensional systems. (a) For increasing values of the contact number z , $P(f)$ grows in width (disordered packings, $N=1000$). The inset compares $P(f)$ for a disordered packing with $z=6$ and $N=1000$ and the hexagonal packing for $N=2900$. (b) The same data as in (a), now plotted as $\log_{10} P(f)$ vs f^2 , tends to a straight curve for large z . The inset shows that on a smaller range, all curves look Gaussian. (c) Same data as in (a) and (b), now on a triple-logarithmic plot. The range in f over which $P(f)$ looks Gaussian grows with contact number z . (d) For fixed small $z=4.5$, $P(f)$ appears to approach a Gaussian tail for large N .

probability of f_{\max} in the modified ensemble is approximately flat in the range $1 < f_{\max} < 15$ (the precise form of W is irrelevant). We have verified that this procedure exactly reproduces $P(f)$ in the range accessible by the conventional unbiased sampling [19]. However, forces of the order of 15 are now sampled only 10^4 times less frequently than forces around 1, even though their relative probability is about 10^{-45} , leading to the spectacular improvement in numerical accuracy [25].

A well-studied geometry for which the force network ensemble yields nontrivial results is that when all particles are of equal size and form a hexagonal lattice [15,16,19]. The umbrella sampling allows us to access the statistics beyond $f=5$. Figure 1(a) shows that $P(f)$ decays much faster than exponentially, and that effects of the finite size of the system are weak. Figure 1(b) illustrates that, for increasingly large systems, $P(f)$ rapidly converges to an asymptotic form which is characterized by a purely Gaussian decay. This can also be seen in the inset of Fig. 1(b), where we exploit the fact that we have access to $P(f)$ over more than 40 decades: Assuming that, for large f , $P(f) \sim \exp(-cf^\alpha)$, one can infer the exponent α from the asymptotic slope of a triple-logarithmic plot in which $\log_{10}(-\log_{10} P)$ is plotted as function of $\log_{10} f$ [4]. The inset of Fig. 1(b) shows that $\alpha=2.0 \pm 0.1$, confirming that the tail of $P(f)$ is well described by a Gaussian decay [26].

To investigate the effect of packing disorder and coordination number z , we have created packings from molecular dynamics simulations of soft particles in periodic boundary conditions (see [15,17]). The coordination number z is controlled by the pressure in the simulations. Once a packing is obtained, all particle positions are kept fixed, and we subsequently explore the ensemble of force networks for these packings. At this point the interparticle potential is no longer used, so that grain rigidity is not a parameter in the ensemble.

For all 2D disordered packings, $P(f)$ decays much faster than exponentially, as shown in Fig. 2. Comparing the ordered hexagonal packings to a disordered system with equal coordination number, $z=6$, we find nearly indistinguishable $P(f)$ [inset Fig. 2(a)]. This suggests that the packing (dis)order and preparation history are not important for $P(f)$ in the ensemble. However, the contact number influences the

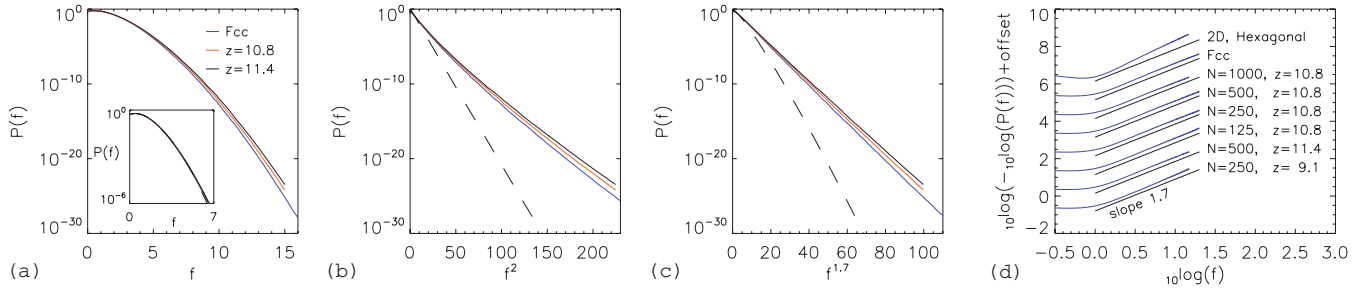


FIG. 3. (Color) Force distribution for three-dimensional systems. (a) $P(f)$ for two disordered and a regular fcc packing of $N=500$ particles—the fcc packing has the smallest width, while for the disordered packs the width grows with contact number. (b) The same, now plotted as function of f^2 . The dashed line corresponds to a hexagonal packing in 2D, which has a Gaussian tail—the tail of $P(f)$ for 3D systems is significantly less steep. (c) Same data, now plotted as function of $f^{1.7}$ —the tails for the $P(f)$ of 3D packings are now straight. (d) The change from 2 to 1.7 is also clearly visible in the triple-logarithmic plot. For a range of system sizes and contact numbers, we robustly find that $P(f) \sim \exp(-cf^\alpha)$ with an exponent $\alpha \approx 1.7$ for 3D systems—for comparison, we also show the Gaussian distribution for the 2D hexagonal packing. Note that, for small systems and small contact number ($N=250$, $z=9.1$), finite-size deviations, similar to those observed in two dimensions, can be seen.

asymptotic decay: a lower z leads to a faster decay [Figs. 2(a) and 2(b)], although in the restricted range $f < 5$, the force distribution appears very close to Gaussian for all z [inset Fig. 2(b)]. For the lowest z in particular, this tendency is cut off at large f , which can be clearly seen in the triple-logarithmic plot [Fig. 2(c)], where all curves tend toward a well-defined slope $\alpha=2.0$ for intermediate f , but cross over to a much faster decay for large f . We suggest that this is a finite-size effect, which is most severe when z approaches the isostatic point ($z=4$), where there are fewer and fewer degrees of freedom available [17,27]. Indeed, data for $z=4.5$ and increasing system sizes suggest that the “kink” in the triple-logarithmic plots becomes less severe for large systems [Fig. 2(d)]—our data are not conclusive as to whether this kink will disappear for $N \rightarrow \infty$.

In conclusion, for two-dimensional, frictionless systems, the ensemble approach yields force distributions $P(f)$ that decay at least as fast as a Gaussian.

We now turn to three-dimensional systems, which again have been generated using molecular dynamics. Similar to what happens in two dimensions, Fig. 3(a) shows that $P(f)$ decays faster than exponentially, and disordered and regular (fcc) packings have very similar force distributions. However, the decay is now *slower* than Gaussian and much more accurately described by $P(f) \sim \exp(-cf^\alpha)$ with an exponent $\alpha=1.7 \pm 0.1$ [see Figs. 3(b)–3(d)]. This exponent has been determined from the triple-logarithmic plots of Fig. 3(d) for a range of contact numbers and system sizes, and in all cases the slope is close to $\alpha=1.7$ over a decade.

For comparison we have, in Figs. 3(b)–3(d), also included the result for the hexagonal pack, which is seen to decrease significantly more rapidly than the $P(f)$'s of the three-dimensional systems. Surprisingly, we thus find that the dimensionality of the packing determines the nature of the tail of $P(f)$.

From experiments on (two-dimensional) sheared packs of photoelastic grains, it was found that the distribution broadened significantly, and developed an exponential-like regime in a range up to $f=4\langle f \rangle$ [7]. The ensemble indeed reproduces this qualitative feature for packs under shear. As can be seen

in Fig. 4, however, there does not seem to be a simple asymptotic decay. This is because the force anisotropy induced by the shear stress yields a variation in $\langle f \rangle$ depending on the orientation of the contact [17,19]. The total $P(f)$ becomes a superposition over all orientations, of mixed force statistics, and hence lacks a single characteristic feature.

We have shown for the force network ensemble that the tail of $P(f)$ decays faster than exponentially, in agreement with recent experiments [7,9], but inconsistent with others [2–4]. Some of our results required extremely accurate statistics, beyond the regime accessible by experiments or conventional simulations. In particular, it would be difficult to distinguish an exponent $\alpha=1.7$ from 2.0. Nevertheless the discrepancy between the exponential data sets [2–4] and the faster-than-exponential data sets [7,9] cannot be explained away by finite error bars, but is convincing and worthwhile of further investigations.

The experimental and numerical data for $P(f)$ have been obtained from a wide variety of systems and models, and parameters such as dimensionality, friction, hardness of grains [28], and bulk vs boundary measurements may ulti-

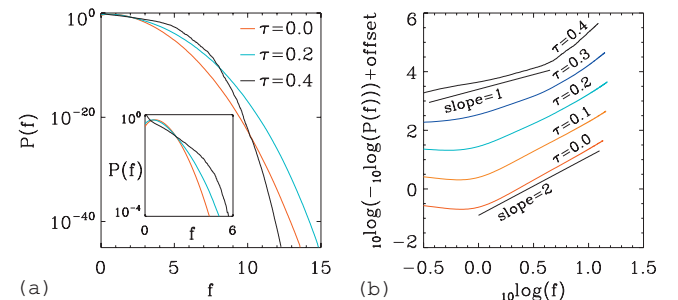


FIG. 4. (Color) Two-dimensional disordered system with $z=5.5$ experiencing a shear stress $\tau \equiv \sigma_{xy}/\sigma_{xx}$ [17]. (a) While, for large τ , the tail of $P(f)$ viewed over a limited range broadens and may appear exponential (inset), the asymptotic decay of $P(f)$ for $f > 10$ in fact increases with τ (main panel). (b) The same point is illustrated in the triple-logarithmic plots, which also show data for $\tau=0.1$ and 0.3.

mately all play a role in determining the asymptotics of $P(f)$. The ensemble can also be extended to include torque balance and to explore boundary measurements. Based on earlier work on boundary effects [29], however, we speculate that these extensions would not alter the tail of $P(f)$ significantly.

A crucial untested assumption in the ensemble is the flat measure, i.e., the sampling of all allowed configurations with equal weight. As argued in Ref. [4], different experimental

procedures and parameters can lead to a different $P(f)$, so that the effective sampling of force networks may not be universal.

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