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Force mobilization and generalized isostaticity in jammed packings of frictional grains

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We show that in slowly generated two-dimensional packings of frictional spheres, a significant fraction of the friction forces lie at the Coulomb threshold—for small pressure p and friction coefficient μ, about half of the contacts. Interpreting these contacts as constrained leads to a generalized concept of isostaticity, which relates the maximal fraction of fully mobilized contacts and contact number. For $p \to 0$, our frictional packings approximately satisfy this relation over the full range of μ. This is in agreement with a previous conjecture that gently built packings should be marginal solids at jamming. In addition, the contact numbers and packing densities scale with both p and μ.

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Models of *frictionless* polydisperse particles with finite-range repulsive forces exhibit a well-defined "jamming point" J in the limit that the confining pressure p goes to zero [1,2]. In the vicinity of J on the jammed side—i.e., for $p \gtrsim 0$—the average contact number, packing density, elastic constants, vibrational modes, and response functions all show scaling behavior as a function of pressure [2–4]. This scaling is intimately connected to the fact that when point J is approached by preparing packings at lower and lower pressures, such packings become *isostatic*: a simple constraint counting argument for hard spheres in d dimensions yields that for $p \to 0$, the average number of contacts per interacting particle, z, equals the fictionless isostatic value $z^0_{\rm iso}=2d$ [5,6].

The picture that is emerging for *frictional* packings is much more diffuse, since there are now two control parameters (p and μ), and more importantly, packing densities and contact numbers depend on the preparation method and history. This is because the Coulomb condition for the frictional force is an inequality: it specifies, for each static contact, that the tangential force f_t be less than or equal to the friction coefficient μ times the normal force f_n: $|f_t| \leq \mu f_n$. If in view of this inequality we treat these tangential forces as *independent* new degrees of freedom in the constraint counting, the isostatic value jumps from $z^0_{\rm iso}=2d$ to $z^\mu_{\rm iso}=d+1$, and in d dimensions frictional packings for $p \to 0$ can in principle occur for *any* z in the range $z^\mu_{\rm iso} \equiv d+1 \leq z \leq z^0_{\rm iso}$ [7].

In practice, however, for a given experimental [8] or numerical [9–11] protocol some reproducible value z is found. The sudden jump of the isostatic contact number with μ is not reflected in a jump of $z_J(\mu) \equiv z(\mu, p \to 0)$: numerically, $z_J(\mu)$ is found to vary smoothly from $z^0_{\rm iso}$ at small μ to some limiting value at large μ [9]. The large-μ limit may or may not coincide with $z^\mu_{\rm iso}$, and z is generally smaller and closer to the isostatic value the slower the packing is prepared [11].

As stressed by Silbert *et al.* [10] and Bouchaud [12], there is a natural way in which the discontinuity in the isostatic contact numbers is not reflected in $z_J(\mu)$, which hinges on the notion of maximizing the number of fully mobilized or "plastic" contacts—i.e., those at the Coulomb failure threshold for which $m=1$, where $m \equiv |f_t|/(\mu f_n)$ [10,12]. Since at fully mobilized contacts tangential and normal forces are related, this leads to additional constraints in the counting arguments: Introducing n_m as the number of fully mobilized contacts per particle in a packing with N_i interacting particles, the $zdN_i/2$ force degrees of freedom should be larger than the total number of constraints provided by the $N_i d(d+1)/2$ force and torque balance equations [7] and the $n_m N_i$ mobilization constraints. This gives

$$n_m \leq z - z^\mu_{\rm iso}. \tag{1}$$

From this point of view, packings with $n_m = z - z^\mu_{\rm iso}$ are in fact isostatic or marginal, while packings with $n_m < z - z^\mu_{\rm iso}$ are hyperstatic (see Fig. 1).

In this Rapid Communication, we will show that gently prepared packings support this scenario over a surprisingly wide range of friction coefficients. The distribution function $P(m)$ of such packings indeed naturally splits up in a peak at

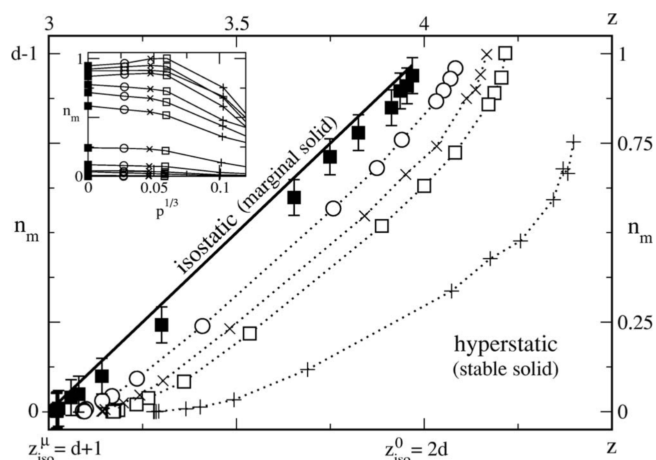

FIG. 1. Relation between the number of fully mobilized forces per particle, n_m, and contact number z. The solid line indicates the maximum of n_m, and such packings are marginal, while below this line one finds hyperstatic stable packings. The data points refer to numerically obtained values of n_m in two dimensions, for $p \sim 2 \times 10^{-4}$ (+), $p \sim 5 \times 10^{-5}$ (□), $p \sim 2 \times 10^{-5}$ (×), and $p \sim 5 \times 10^{-6}$ (○). n_m and z behave smoothly as function of $p^{1/3}$, and by extrapolation we obtain our $p=0$ estimate indicated by the solid squares (see inset and main text).

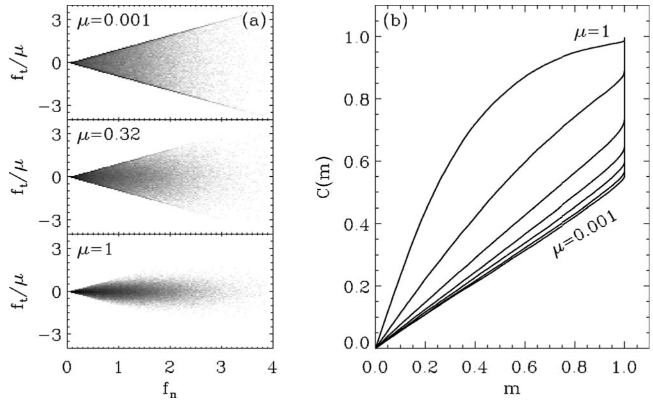

FIG. 2. Mobilization at $p=2\times10^{-5}$. (a) Scatter plots of f_t/μ versus f_{n} for three packings at $\mu=0.001$, 0.32, and 1. The probability density of normalized tangential (f_t/μ) and normal (f_n) forces exhibits a singularity on the Coulomb cone for small μ, which rapidly diminishes for larger μ (all forces are normalized so that $\langle f_n\rangle=1$). (b) The cumulative distribution of the mobilization $C(m)\equiv\int^m dm' P(m')$ exhibits a clear jump near $m=1$. Data shown here are for $\mu=10^0, 10^{-0.5}, 10^{-1}, \ldots, 10^{-3}$.

$m=1$ and a broad flat part for $m<1$ (Fig. 2), and these packings actually tend to be marginal at jamming—i.e., to lie close to this generalized isostaticity line in Fig. 1. The picture that emerges is that if we prepare the packings sufficiently slowly, they get stuck in a marginal state. Such a marginal scenario also occurs in, e.g., spin glasses [12], charge density waves [13], and phase organization [14].

The fact that our well-equilibrated packings approach a well-defined limit opens up the possibility to study the asymptotic scaling behavior as a function of pressure and friction coefficient μ. We have therefore also investigated the effect of applying pressure on repeatedly and gently created packings over a whole range of friction coefficients and find that contact numbers z and packing densities ϕ of the packings do exhibit scaling with p and μ. The scaling of ϕ and z with p is related to the form of the interparticle potential and is consistent with previous findings for the frictionless case. The scaling of z and ϕ with μ appears to be independent of the force law—we have at present no good physical understanding of this scaling.

Model and simulation method. We numerically build two-dimensional (2d) packings of $N_{\mathrm{p}}=1000$ polydisperse spheres that interact through 3D Hertz-Mindlin forces or through one-sided linear springs plus friction [15] in a square box with periodic boundary conditions. The data reported below are all for the 3D Hertz-Mindlin forces. Following [16] our units are such that the mass density, the average particle diameter, and the Young's modulus of the grains are 1. The Poisson ratio of the grains is taken to be zero, and there is no gravity. As in [16] the packings are constructed by cooling an initial low-density state where the particles have a small velocity, while slowly inflating the particle radii by multiplying them with a common scale factor r_s. This factor is determined by solving the damped equation $r_s''=-4\omega_0 r_s' - \omega_0^2[p(t,r_s)/p-1]r_s$, where $\omega_0\sim6\times10^{-2}$, $p(t,r_s)$ is the instant value of the pressure, and p is the target pressure. This ensures a very gentle equilibration of the packings. In our analysis of forces and contact numbers, we always take out rattlers by considering contact forces less than 10^{-3} times the average force broken and removing particles, with less than two contacts. For each packing, we determine the total number of contacts, N_{c}, and the total number of interacting particles, N_{i} (the total number of particles minus the rattlers)—$z\equiv2N_c/N_{\mathrm{i}}$. For each value of p and $\mu\in[10^{-3},10^3]$, 30 realizations have been constructed with a polydispersity of 20%. We occasionally checked that taking 60 realizations and a different polydispersity or different damping parameters leads to similar results. In comparison with other simulations where the particles settled under gravity [10] or were quenched rapidly [11], our algorithm prepares the packings more gently, in the sense that it results in low packing densities and coordination numbers.

The density n_{m} of fully mobilized contacts. The joint probability distribution of the normal and frictional contact forces clearly shows that for small μ, a substantial amount of forces lie on the Coulomb cone—i.e., have $m=1$—while for larger μ the fraction of fully mobilized contacts diminishes [Fig. 2(a)]. *A priori* it would appear to be difficult to determine numerically whether a contact is fully mobilized with $m=1$ or elastic (nonmobilized) with $m<1$, but as Fig. 2(b) shows, the cumulative distribution $C(m)\equiv\int^m dm' P(m')$ exhibits a clear jump at $m=1$. The value of n_{m} equals $\lim_{m\to1} z/2[1-C(m)]$, and we find that for a small friction about half of the contacts (one contact per particle) are at the Coulomb treshold. Especially for small μ, $C(m)$ is linear in m, which means that the distribution of nonmobilized forces is flat—in other words, nonmobilized contacts are not biased towards higher contact numbers.

Our estimates for n_m and z for $p\to0$ and a range of μ lie very close to the generalized isostaticity line (Fig. 1). Note that we have extrapolated contact numbers and n_{m} to estimate the zero-pressure limit (see the inset of Figs. 1 and 3). The close proximity of n_{m} and z to the marginal line presents, to our knowledge, the strongest support to date for the marginal solid scenario described above: when frictional packings are sufficiently gently prepared, they form a marginally stable jammed solid which in a generalized sense is an isostatic solid. We expect that the deviations from the generalized isostaticity will be larger the faster the granular particles are compressed or quenched; earlier simulations already give indications for this [10,11].

Scaling behavior of z and ϕ. Since our packings for small p approach the generalized isostaticity line, one may wonder how the contact number and packing density ϕ change when moving away or along this line. Since the number of rattlers is strongly dependent on the pressure p and on the friction coefficient μ, we have found it illuminating to study both the density with the rattlers excluded and included, $\phi_{-\mathrm{R}}$ and $\phi_{+\mathrm{R}}$, respectively. Note that for small pressure and small friction about 4% of the particles are rattlers, which rises to 12% for large values of the friction. The results of our analysis are shown in Figs. 3(a)–3(c). As a function of μ, the overall variation of z in Fig. 3(a) is very similar to results obtained by contact dynamics [9], and again the density variations in Figs. 3(b) and 3(c) mimic that of z. As a function of p, our data are consistent with the scaling relation $z(\mu,p)-z(\mu,0)$

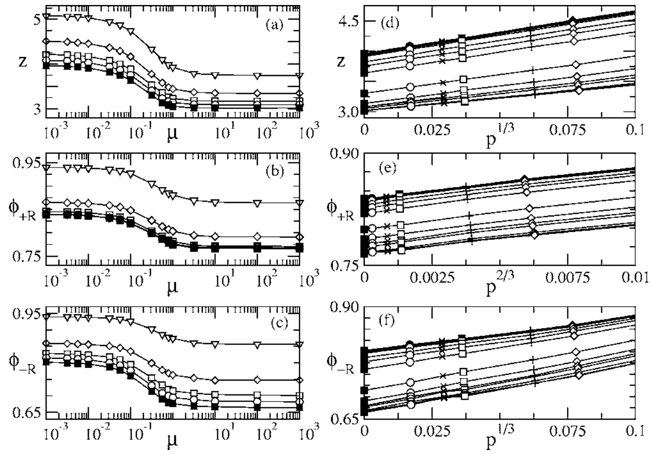

FIG. 3. Variation of contact numbers z and packing density ϕ as function of pressure p and friction coefficient μ. Error bars are smaller than the symbol size. (a)–(c) The variation of the contact number z, the packing density including rattlers ϕ_{+R}, and the packing density excluding rattlers ϕ_{-R} as a function of μ. Symbols indicate data at pressures $p \sim 4\times10^{-3}$ (▽), 5×10^{-4} (◇), 2×10^{-4} (+), 5×10^{-5} (□), 2×10^{-5} (×), and 5×10^{-6} (○). Based on the extrapolation illustrated in panels (d)–(f), we also show the estimated values at $p=0$ (■). Even though ϕ_{+R} and ϕ_{-R} differ substantially, their variation with μ appears very similar. (d)–(f) z scales as $p^{1/3}$ and ϕ_{+R} as $p^{2/3}$, which allows us to extrapolate to zero pressure. Surprisingly, the packing density ϕ_{-R} does not scale convincingly with $p^{2/3}$, but rather as $p^{1/3}$. Symbols are as in panels (a)–(c).

$\sim p^{1/3}$ [Fig. 3(d)]. This allows us to extrapolate with confidence to zero pressures, giving $z(\mu \ll 1,0)=3.98\pm0.02$ and $z(\mu \gg 1,0)=3.00\pm0.02$, which are close to the frictionless and frictional isostatic bounds, $z^0_{\rm iso}=4$ and $z^\infty_{\rm iso}=3$, respectively. For the whole range of μ we find that the change in density including rattlers scales as $\phi_{+R}(\mu,p)-\phi_{+R}(\mu,0) \sim p^{2/3}$ [Fig. 3(e)]. This is consistent with the scaling of the density in frictionless packings upon compressing a given packing [2] and with the variation $K\sim(d\phi_{+R}/dp)^{-1}\sim p^{1/3}$ of the compression modulus K with pressure [2,17]. Interestingly, the density excluding rattlers, ϕ_{-R}, appears to vary instead as $p^{1/3}$ [Fig. 3(f)].

For our Hertz-Mindling forces, the $p^{1/3}$ scaling for z is consistent with the scaling $z-z^0_{\rm iso}\sim\sqrt{\delta}$ observed also for frictionless particles [2,17], where δ is the typical dimensionless overlap of the particles. We have checked that our results do only trivially depend on the details of the force law: for one-sided harmonic springs the z and ϕ scale as function of $p^{1/2}$ (not shown). The fact that z scales with p similarly as for frictionless systems was seen in some studies [11] but not in others [10]. Both the presence of this scaling and the fact that our packings reach the generalized isostaticity line for $p \to 0$ may be related to our very slow rate of equilibration.

From the zero-pressure extrapolations discussed above, we can study the variation of the contact number and densities at jamming. The results of this analysis are summarized in Fig. 4, with details given in the figure caption. In particular we find $z(\mu,0)$ to decrease for small μ as $\mu^{0.7\pm0.1}$. That indeed z decreases rapidly with μ is also clear from the 3D data of [10], which appear to fit a power-law behavior Δz

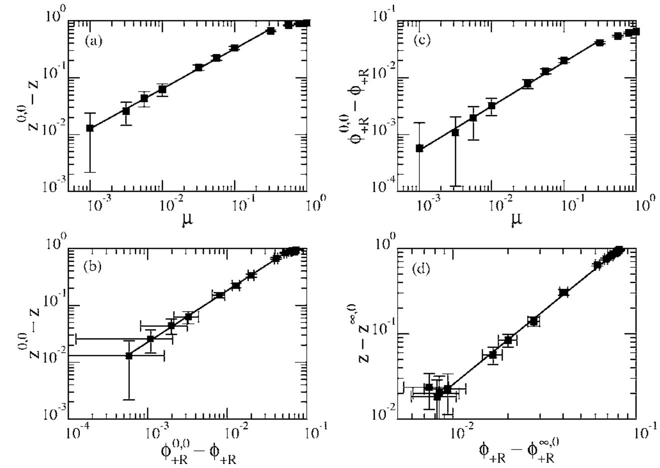

FIG. 4. Scaling of the zero pressure, extrapolated, contact numbers, and packing densities with the friction coefficient μ. The extrapolated values at zero (infinite) friction are labeled as 0,0 (0,∞). (a)–(c) When $\mu\to0$ and $p\to0$, z approaches $z^{0,0}\approx3.975$ [20], while ϕ_{+R} approaches $\phi^{0,0}_{+R}\approx0.8395$ [5]. For finite but small μ, z and ϕ_{+R} appear to scale as (a) $(z^{0,0}-z)\sim\mu^{0.70[10]}$ and (b) $(\phi^{0,0}_{+R}-\phi_{+R})\sim\mu^{0.77[10]}$. (c) The contact number and packing deviate similarly from this scaling when μ approaches 1, and so $(z^{0,0}-z)\sim(\phi^{0,0}_{+R}-\phi_{+R})^{0.91[10]}$. (d) In the limit of infinite friction and zero pressure, z approaches $z^{\infty,0}=3.00$ [2], while ϕ_{+R} approaches $\phi^{\infty,0}_{+R}=0.758$ [10]. The deviations from these limiting values also appear to be related by a scaling relation of the form $(z-z^{\infty,0})\sim(\phi_{+R}-\phi^{\infty,0}_{+R})^{1.7[2]}$.

$\sim\mu^{0.5}$ reasonably well. Whether the density changes for small μ with a nontrivial exponent different from 1 is less clear from our data. We cannot draw any firm conclusion from our data regarding the functional μ dependence for large friction but the variation of contact number with density appears to be consistent with an exponent of 1.7. Similar scalings are obtained for linear instead of Hertzian contact laws.

Summary and outlook. Our results substantiate the scenario that when a packing is gently prepared, it gets jammed in a (near) marginal state, where enough contacts get stuck at the Coulomb failure threshold to make the packing a marginal solid. Note that this is different from what engineers refer to as "incipient failure everywhere"—the idea that one can deal with the Coulomb inequality by turning it into an equality for *all* contacts [18]. Our results here show that this overestimates the number of fully mobilized contacts. Our results suggest a lower boundary for the contact number, and possibly for the packing densities too, that can be obtained for finite μ, whereas naive counting would suggest that d-dimensional packings with any contact number between $d+1$ and $2d$ could arise.

An immediate implication of our results is that the response properties of such gently prepared packings will have a strong tendency to show a nonlinear response, depending very sensitively on the behavior of the plastic contacts: if these remain fixed at the Coulomb threshold, the fact that these packings are near isostaticity will give many low-frequency modes and will make these packings very soft. If these contacts yield, however, irreversibility effects will dominate.

The contact numbers and densities that characterize gently prepared packings show various nontrivial scaling relations as a function of μ and p. The scaling of $z \sim p^{1/3}$ and $\phi_{+R} \sim p^{2/3}$ with p is similar to that found for frictionless Hertzian packings—but these scalings seem to work equally well over the whole range of μ. The scaling of ϕ_{-R} is more puzzling. It is very well possible that the asymptotic behavior for very small p crosses over to the familiar $p^{2/3}$ behavior, but we cannot access this regime at present. In addition, for 3D packings the fraction of rattlers may be smaller than for 2D, so that there we expect less of this effect. Nevertheless, the question whether one should include or exclude rattlers is subtle—see also [19].

The scaling of z and ϕ_{+R} with μ is new and presently not understood, but may give indirect evidence for strong correlations between the tangential forces. Suppose we think of the tangential forces f_t as small randomly pointing perturbations of the net forces on the particles for $\mu \ll 1$. In a domain of linear scale L, these tangential forces add up to a total force of order $\mu f_n L^{d/2}$. This is comparable to the normal force scale f_n on a scale $L_\mu \simeq \mu^{-2/d}$. It might therefore be natural to suppose that on this scale the tangential forces allow one to reduce z by replacing a single contact. Since $\Delta z L_\mu^d = O(1)$, this would suggest $\Delta z \sim \mu^2$, in strong contrast to the data.

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