Force Network Ensemble: A New Approach to Static Granular Matter

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An ensemble approach for force distributions in static granular packings is developed. This framework is based on the separation of packing and force scales, together with an *a priori* flat measure in the force phase space under the constraints that the contact forces are repulsive and balance on every particle. We show how the formalism yields realistic results, both for disordered and regular triangular "snooker ball" configurations, and obtain a shear-induced unjamming transition of the type proposed recently for athermal media.

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The fascinating properties of static granular matter are closely related to the organization of the interparticle contact forces into highly heterogeneous force networks [1]. The probability density of contact forces, $P(f)$, has emerged as a key characterization of a wide range of thermal and athermal systems [2–8]. Most of these studies so far focused on the broad tail of this distribution. Recently, however, the nonuniversal shoulder of $P(f)$ for small forces has received increasing attention, since it appears to contain nontrivial information on the state of the system: $P(f)$ exhibits a peak at some small value of f for "jammed" systems which gives way to monotonic behavior above the glass transition [7–9]. This hints at a possible connection between jamming, glassy behavior, and force network statistics, and underscores the paramount importance of developing a theoretical framework for the statistics and spatial organization of the forces.

A first step towards a statistical description of force networks is the definition of a suitable ensemble over which to take averages. A popular approach is that of Edwards, who proposed to take an equal probability for all "blocked" states of a given energy and density [10,11]. Each point in this ensemble defines a contact geometry and a configuration of (balancing) contact forces. Even though the precise particle locations and contact forces are related, the crucial point is that for hard particles (most granular matter, hard-sphere colloids, particles with a steep Lennard-Jones interactions) a separation of scales occurs [7]: forces inside a pile of steel balls originate from minute deformations ($\simeq 10^{-3}$).

In this Letter we exploit this scale separation by focusing on the *ensemble of force configurations for a given fixed packing configuration*; see Fig. 1. As we will show, the forces can be considered underdetermined in this approach, since the number of unknown forces exceeds the number of balance equations: such packings are referred to as *hyperstatic*. Both packings of entirely rigid, frictional particles and packings of frictionless particles that deform $\simeq 10^{-3}$ are hyperstatic [12]. For transparency, however, we will restrict ourselves to two dimensional frictionless hyperstatic packings. In the spirit of Edwards, we sample all allowed force configurations for a given packing with equal probability. Interestingly, the idea to restrict the ensemble to fixed geometries has also been suggested by Bouchaud in the context of extremely weak tapping [13].

Our ensemble approach captures the essential features of force networks (Fig. 1) and leads to new insights on the nonuniversal "shoulder" of $P(f)$. In addition, by separating the contact geometry from the forces, we can start to disentangle the separate roles of contact and stress anisotropies in sheared systems. The conceptual advantage of not averaging over packing geometries is complemented by practical advantages: our protocol is numerically cheap and analytically accessible.

Formulation.—We study 2D packings of N frictionless disks of radii R_i with centers $\mathbf{r}_i$. We denote the interparticle force on particle i due to its contact with particle j by $\mathbf{f}_{ij}$. There are $zN/2$ contact forces in such

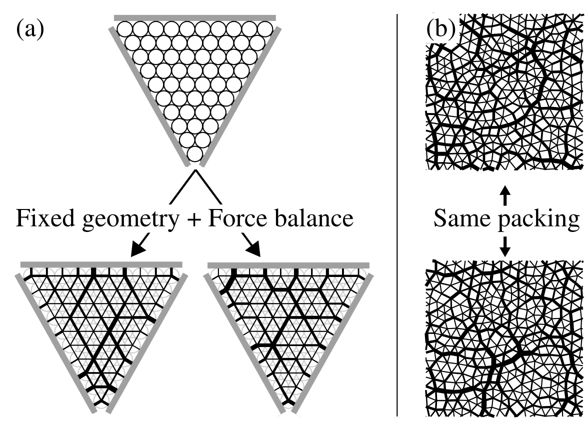

FIG. 1. Two different mechanically stable force configurations for (a) a "snooker-triangle packing" and for (b) an irregular contact network of 1024 particles (only part is shown); the thickness of the lines is proportional to the contact force. The "force network ensemble" samples all possible force configurations for a given contact network with an equal probability.

packings (z being the average contact number), and for purely repulsive central forces we can write $\mathbf{f}_{ij} = f_{ij}\mathbf{r}_{ij}/|\mathbf{r}_{ij}|$, where all f_{ij} ($= f_{ji}$) are positive scalars. For a fixed contact geometry, we are thus left with $2N$ unknowns $\mathbf{r}_i$ and $zN/2$ unknowns f_{ij} [14]. These satisfy the conditions of mechanical equilibrium,

$$2N\text{eqs: } \sum_j f_{ij}\,\frac{\mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} = \mathbf{0}, \quad \text{where } \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \tag{1}$$

and once a force law F is given, the forces are explicit functions of the particle locations:

$$zN/2\text{eqs: } f_{ij} = F(\mathbf{r}_{ij}; R_i, R_j). \tag{2}$$

Packings of infinitely hard particles have $z = 4$ and are thus *isostatic*: For rigid particles Eqs. (2) reduce to $zN/2$ constraints on the $2N$ coordinates $\mathbf{r}_i$ which can only be satisfied if $z \leq 4$, while Eqs. (1) can only be solved if $z \geq 4$; combining these yields $z = 4$ [15,16].

However, for particles of finite hardness, packings are typically *hyperstatic* with $z > 4$. A key parameter which quantifies the separation of length scales is $\varepsilon = (\langle f\rangle/\langle r_{ij}\rangle)\langle dF_{ij}/dr_{ij}\rangle^{-1}$, where $\langle\ \rangle$ denotes an average over the packing. We will avoid the strict isostatic $\varepsilon = 0$ case, but focus instead on the regime where ε is small and variations of the force of order $\langle f\rangle$ result in minute variations of $\mathbf{r}_{ij}$, of relative size ε. Hence, for $\varepsilon \ll 1$, Eqs. (1) and (2) can be considered separated, and the essential physics is then given by the force balance constraints Eqs. (1) with fixed $\mathbf{r}_i$. In this interpretation, there are more degrees of freedom ($zN/2$) than constraints ($2N$), leading to an ensemble of force networks; see Fig. 1.

It is important to note that different points in our ensemble do not correspond to *precisely* the same packing of *exactly* the same particles. Our stochastic approach describes different force configurations arising in, e.g., experiments on "regular" packings of imperfect cannon balls [17] or packings under weak tapping [13]. Experimentally, it has become clear that the macroscopic properties of granular packings are sensitive to many (coarse grained) parameters such as local densities, anisotropies, and contact numbers, and that it is very difficult to establish the relevant characteristics of a packing. Our ensemble averages only over microscopic variations of the packing, which have a strong effect on the local forces but not on macroscopic properties, while keeping the important characteristics fixed. The restriction to a minute part of the Edwards ensemble may therefore help to disentangle the separate roles of contact and stress anisotropies.

The ensemble of force networks for a fixed contact geometry is constructed as follows. (i) Assume an *a priori* flat measure in the force phase space $\{f\}$. (ii) Impose the $2N$ *linear* constraints given by the mechanical equilibrium Eqs. (1). (iii) Consider repulsive forces only, i.e., $\forall f_{ij} \geq 0$. (iv) Set an overall force scale by applying a *fixed pressure*, similar to energy or particle number constraints in the usual thermodynamic ensembles.

We will first illustrate our formalism for a simple triangular snookerlike packing [Fig. 1(a)]. Then, for an irregular packing of 1024 particles [Fig. 1(b)], we compare our ensemble approach to MD simulations by varying the inverse "hardness" ε. The ensemble reproduces the $P(f)$ for sufficiently hard particles well. Finally, we find that applying a shear stress yields an "unjamming" transition in our framework.

Regular packings.—The triangular snookerlike packings shown in Fig. 1(a) have $3N$ unknown forces (boundary forces included) that are constrained by the $2N$ equations of mechanical equilibrium. Even though the packing geometry is completely regular, the ensemble approach yields irregular force networks and a broad $P(f)$.

Labeling each bond by a single index k, the mechanical equilibrium can be expressed as

$$A\vec{f} = \vec{0} \qquad \text{with } \vec{f} \equiv (f_1, f_2, \ldots, f_{3N}), \tag{3}$$

where A is a $3N$ times $2N$ sparse matrix. There is thus an N-dimensional subspace of allowed force configurations that obeys mechanical equilibrium. Equation (3) is homogeneous, but in physical realizations an overall force scale is determined by the externally applied stresses and/or the gravitational bulk forces. The simplest manner to do so here is to fix the external pressure by specifying the total boundary forces. For the snooker triangles it then follows that the sum of all forces is constant. We are thus considering the phase space defined by the force balance (3), the "pressure" constraint $\sum_k f_k = F_{\text{tot}}$, and the condition that all f's are positive:

$$\mathcal{A}\,\vec{f} = \vec{b} \quad \text{and} \quad \forall\ f_k \geq 0, \tag{4}$$

where the fixed matrix $\mathcal{A}$ is the matrix A extended by the pressure constraint and $\vec{b} = (0, 0, 0, \ldots, 0, F_{\text{tot}})$.

To compute $P(f)$ for larger packings, we have applied a simulated annealing procedure [18]. Starting from an ensemble of random initial force configurations we sample the space of mechanically stable networks, using a penalty function whose degenerate ground states are solutions of Eq. (4). We have carefully checked that results do not depend on the initial configurations, and furthermore perfectly reproduce the distribution $P(f)$ for three and six balls, which can be worked out analytically [19].

The two force networks shown in Fig. 1 are typical solutions $\vec{f}$ obtained by this scheme. We limit the discussion to $P(f)$ for interparticle forces, and address the boundary forces which show different distributions elsewhere [19,20]. The interparticle $P(f)$ for packings of increasing number of balls are presented in Fig. 2. Note that all $P(f)$'s display a peak for small f, which is typical for jammed systems [7]. For large packings, this peak rapidly converges to its asymptotic limit. The tail of $P(f)$ broadens with system size, but the present data is not conclusive about its asymptotic characteristics.

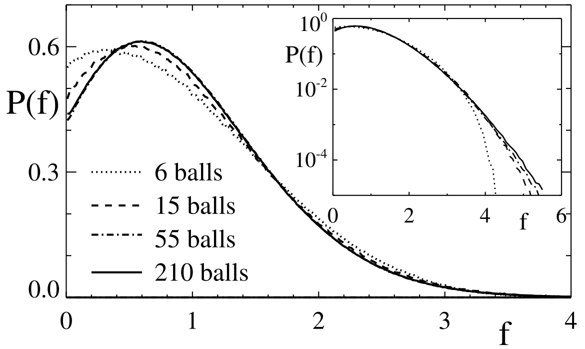

FIG. 2. Interparticle force $P(f)$ for various triangular "snooker" packings [Fig. 1(a)]. The inset shows the evolution of the tail for large systems.

Irregular packings.—We now apply our force ensemble approach to a more realistic system with a random packing geometry, and study a shear stress induced unjamming transition. To obtain a representative irregular contact geometry, we perform a standard molecular dynamics simulation of a 50:50 binary mixture of 1024 particles with size ratio 1.4 that have a purely repulsive 12-6 Lennard-Jones interaction (a shifted potential with the attractive tail cut off), the same system as the one studied by O'Hern *et al.* [7]. We then quench such a finite temperature simulation onto a $T = 0$ random packing with a steepest descent algorithm [18]. The static contact network that we obtain in this way then defines the matrix $\mathcal{A}$ in Eq. (3).

The $P(f)$ obtained for this fixed packing is displayed in Fig. 3: even for a single contact geometry, we clearly reproduce a realistic $P(f)$ which is very similar to both that of the triangular packings and to those obtained in experiments and simulations [2,5].

To investigate the role of the particle hardness, we have performed MD simulations of the same system with increasingly hard particles, obtained by varying the prefactor of the potential at constant pressure. For our original MD, which defined $\mathcal{A}$, the particles are fairly soft with $\varepsilon \sim 0.1$, and the corresponding $P(f)$ is somewhat different from the one in the force ensemble. When the

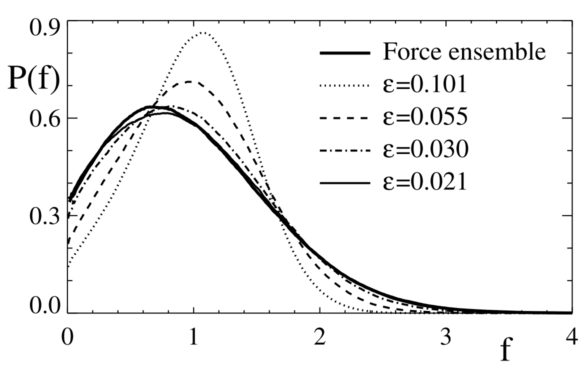

FIG. 3. Comparison of the $P(f)$ obtained by our sampling of a frozen geometry, and MD simulations of increasingly hard particles under constant pressure in the limit $T \to 0$.

hardness of the particles is increased, ε diminishes and the corresponding $P(f)$ indeed approaches the force ensemble $P(f)$. For the hardest particles ($\varepsilon \simeq 0.02$) these $P(f)$'s are virtually indistinguishable. We find that this holds for a variety of force laws [19]. This confirms the validity of our approach for hard particles.

Unjamming by shear.—It is also possible to study the effect of a shear stress on the force network ensemble by using the relation between the microscopic forces and the macroscopic stress field:

$$\sigma_{\alpha\beta} = \frac{1}{V}\sum_k (\mathbf{f}_k)_\alpha (\mathbf{r}_k)_\beta, \tag{5}$$

and extending the matrix of Eq. (4) with the three *linear* constraints of Eq. (5). The average value of the force is set to unity by requiring $\sigma_{xx} = \sigma_{yy} = 1/2$ [21], and we vary $\tau = \sigma_{xy}/\sigma_{xx}$.

We find that $P(f)$ evolves from a jammed distribution with a peak, to an "unjammed" monotonous distribution as a function of shear stress [Fig. 4(a)]. As a function of the angle ϕ, $\langle f \rangle$ varies in good approximation as $1 + 2\tau \sin(2\phi)$. This variation is consistent with Eq. (5) as well as with the alignment of the dominant contacts visible in Fig. 4(b)—note the similarity to experimentally obtained sheared networks [22]. Since $P(f)$ contains forces in all directions, the broadening of $P(f)$ with shear stress follows immediately from this angular modulation of $\langle f \rangle$. However, this is only part of the story: we find

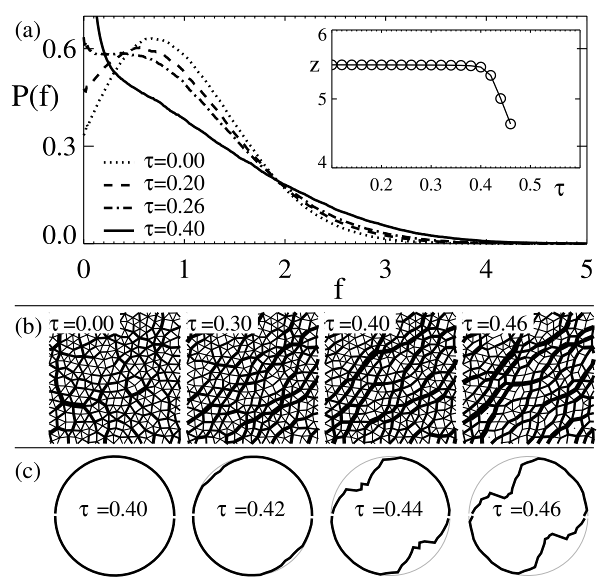

FIG. 4. Force networks under shear. (a) $P(f)$ for increasing shear showing an "unjamming" transition at $\tau \approx 0.26$. The inset shows the contact number as function of shear, where contacts are considered broken when $f < 10^{-4}$; for smaller values of the cutoff this curve remains essentially the same. (b) Examples of parts of the force networks under shear. (c) Ratio of number of contacts with $f > 10^{-4}$ and number of contacts as function of the contact angle show preferential breaking along the "weak" principal direction.

that the *shape* of $P(f)$ also varies with direction, from extremely jammed along the force lines, to almost purely exponential along the weak principle direction (not shown) [19].

When τ approaches 1/2, $\langle f \rangle$ becomes zero along the weak principle direction, which implies that all forces along the weak direction approach zero. This can be interpreted as the breaking of contacts [see Fig. 4(c)]. In addition, when $\tau \rightarrow 1/2$, the contact number drops to $z = 4$ [inset of Fig. 4(a)], and beyond this point, stable force networks are no longer possible. This simple mechanism thus provides $\tau = 1/2$ as a definite upper bound for the critical yield stress [1,17,23,24]. In terms of the "slip angle" this value corresponds to 30°. On the other hand, it has been speculated [7,8] that the qualitative change of $P(f)$ from peak to plateau could also be indicative of yielding; in our ensemble this occurs at $\tau = 0.26$ suggesting a slip angle of 15°.

Outlook.—We have proposed a novel ensemble approach to athermal hard particle systems. The full set of mechanical equilibrium constraints were incorporated, in contrast to more local approximations or force chain models [3,4,25–27]. A number of crucial questions can possibly be addressed within our framework. (1) Our approach is perfectly suited to include frictional forces, since these are difficult to express in a force law but simple to constrain by the Coulomb inequality. (2) The contact and force networks of sand piles exhibit different anisotropies under different construction histories [28,29]. We suggest that contact network anisotropies may be sufficient to obtain the pressure dip under properly created piles. (3) The problem defined by Eqs. (4) could be generalized to arbitrary $\mathcal{A}$ and $\vec{b}$, for which we can calculate $P(f)$ and may ask under what conditions $P(f)$ has an exponential tail, appear jammed, etc. Preliminary work indicates that for realistic $\mathcal{A}$ but taking $\vec{b}$ nonzero with mean square average proportional to T captures the effect of a finite temperature of $P(f)$ [19].

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