Stress Field in Granular Systems: Loop Forces and Potential Formulation

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The transmission of stress through a marginally stable granular pile in two dimensions is exactly formulated in terms of a vector field of loop forces, and thence in terms of a single scalar potential. This leads to a local constitutive equation coupling the stress tensor to *fluctuations* in the local geometry. For a disordered pile of rough grains this means the stress tensor components are coupled in a frustrated manner. In piles of rough grains with long range staggered order, frustration is avoided and a simple linear theory follows. We show that piles of smooth grains can be mapped onto a pile of unfrustrated rough grains, indicating that the problems of rough and smooth grains may be fundamentally distinct.

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It has long been recognized in engineering practice that granular materials which lack cohesion cannot be regarded entirely as solids, nor (until "fluidized" or yielding) can they be regarded entirely as fluids [1]. In this Letter we explore the scenario that there exists a *marginal state* of granular matter in between solid and liquid. Most particularly, we are concerned with how that intermediate state transmits stress.

The marginal state is readily characterized in terms of the mean coordination number $\bar{z}$ for mechanical equilibrium. If external loads, such as gravity, are exerted on a pile of N grains [2] then the $N\bar{z}/2$ intergranular forces must be able to adjust so as to achieve $Nd(d+1)/2$ constraints balancing the force and torque on each grain in d dimensions. For perfectly rough grains, where every contact supports friction, this gives a critical coordination number $z_c = d+1$, while for ideally smooth asymmetric grains with no friction $z_c = d(d+1)$ [3–5]. For the special case of perfectly spherical smooth grains $z_c = 2d$, which matches the maximum mean coordination attainable by sequential packing [6], a fact exploited by Tkachenko and Witten [7].

For mean coordination numbers $\bar{z} < z_c$ the pile cannot be stable and under a general loading it must rearrange or consolidate. By contrast, for $\bar{z} > z_c$ the intergranular forces are underdetermined by the conditions of force and torque balance alone, and the deformation of individual grains, together with their local constitutive equations, becomes relevant: we then have a solid of constitution influenced by that of the individual grains.

The marginal case $\bar{z} = z_c$ is special in that the intergranular forces, and hence distribution of stress, are determined by conditions of balance of force and torque alone. This has been identified as a paradigm problem of theoretical granular mechanics [1,8,9]. What makes the problem intriguing is that the conventional macroscopic analogs of balancing force and torque,

$$\vec{\nabla} \cdot \hat{\sigma} = \vec{F}, \qquad \hat{\sigma} = \hat{\sigma}^T \tag{1}$$

(where $\hat{\sigma}$ and $\vec{F}$ are, respectively, the stress tensor and external load), are *not* a sufficient set of equations without $d(d-1)/2$ further *relations*. The central mystery we are seeking to unravel is the nature of the missing equations (one in two dimensions) when they also arise from local force and torque balance.

We resolve the issue by an analysis based on circulating loop forces. Our analysis is restricted to the case of boundary loading (i.e., $\vec{F} = 0$ in the bulk) and for simplicity to two dimensions of space. In two dimensions the grains enclose uniquely defined voids, as shown in Fig. 1, and around each void we have a corresponding loop of contacting grains. Around each loop we define a *loop force* $\vec{f}_l$ circulating in the anticlockwise direction, that is, $+\vec{f}_l$ contributes to each intergranular force around the loop with a (notionally) positive sign in the anticlockwise direction, and vice versa for the reaction forces. Each contact point is party to exactly two such loops, and the resulting total force across that contact is a difference between the two contributing loop forces.

The loop forces have two key features, the first being that they parametrize the intergranular forces in a manner that automatically satisfies the balance of force at each contact point and on each grain. In terms of them we can write the force moment for each grain as

$$\hat{S}_g = \sum_l \vec{r}_{lg}\vec{f}_l\,, \tag{2}$$

where $\vec{r}_{lg}$ is the vector connecting (anticlockwise) the two contact points shared by loop l and grain g. The vectors $\sum_g \vec{r}_{lg} = 0$ form an anticlockwise loop around the contact points of loop l and likewise $\sum_l \vec{r}_{lg} = 0$ form a clockwise loop around the contact points of grain g and play a central geometrical role in our discussion. The density of force moment gives the macroscopic stress.

The second key feature of the loop forces is that, being defined on the loops which are half as numerous as the grains, they are a comparatively coarse-grained quantity. The hidden nature of the constitutive equation can now be

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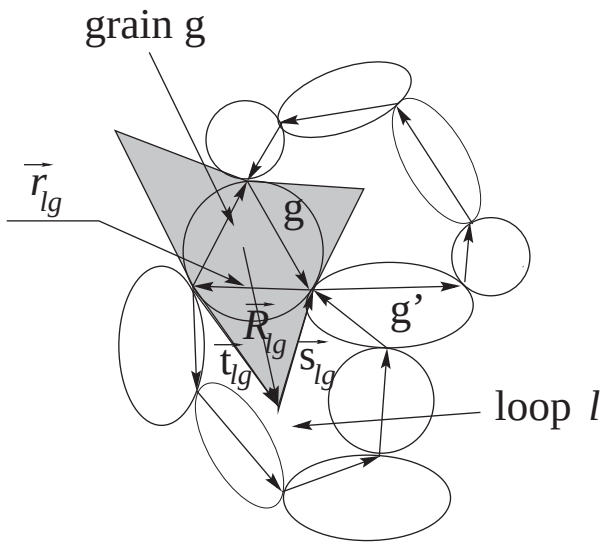

FIG. 1. The local geometry around a grain g. The vectors $\vec{r}_{lg}$ connect contact points clockwise around each grain g and anticlockwise around each void loop l, while the vectors $\vec{R}_{lg}$ connect from grain centers to loop centers. The stress field is coupled through tensors $\hat{C}_g = \sum_l \vec{R}_{lg}\vec{r}_{lg}$, whose antisymmetric part has a magnitude A_g which is the area shaded in the figure. The symmetric parts of these tensors evaluate to $\hat{P}_g = \frac{1}{2}\sum_l \vec{s}_{lg}\vec{s}_{lg} - \vec{t}_{lg}\vec{t}_{lg}$ and play a crucial role in the constitutive equation. As can be seen from the labeling of the vectors $\vec{s}_{lg}$ and $\vec{t}_{lg}$ in the figure, neighboring grains share equal and opposite contributions to their respective $\hat{P}_g$, $\vec{s}_{lg} = -\vec{t}_{lg'}$, so these tensors tend to zero upon local averaging.

readily appreciated, because the only remaining constraints that the loop forces have to obey is the balance of torque around each grain, that is,

$$\sum_l \vec{r}_{lg} \times \vec{f}_l = 0 \tag{3}$$

which gives *two* equations per loop.

The two torque equations per loop give us two macroscopic conditions, symmetry of the stress tensor $\hat{\sigma} = \hat{\sigma}^T$, *plus* a constitutive relation. To achieve this separation explicitly we interpolate the loop forces to a function of continuous position $\vec{f}(\vec{r})$, with each loop having a nominal center $\vec{R}_l$ so that $\vec{f}(\vec{R}_l) = \vec{f}_l$. For example, for a grain with $z = 3$ the loop centers form a triangle and $\vec{f}(\vec{r})$ is uniquely and exactly defined by linear interpolation from the vertex values. Then we can write

$$(\vec{\nabla}\vec{f})_g = 1/A_\triangle \sum_{l=1}^{3} \hat{R} \cdot (\vec{R}_{l+1} - \vec{R}_{l-1})\vec{f}_l\,, \tag{4}$$

where $\hat{R} = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ is the unit antisymmetric tensor corresponding to $\frac{\pi}{2}$ rotation in the plane, $A_\triangle$ is the triangle area, and $l \pm 1$ are the vertices cyclically before and after vertex l. A similar continuation of $\vec{f}$ is possible for grains with $z > 3$ although not as straightforward [10]. In terms of the continuous field $\vec{f}$, the force moment on grain g is

$$\hat{S}_g = \hat{C}_g \cdot (\vec{\nabla}\vec{f})_g \quad \text{where } \hat{C}_g = \sum_l \vec{r}_{lg}\vec{R}_l\,. \tag{5}$$

The geometric tensors $\hat{C}_g$ characterize the local geometry around grain g and their symmetric and antisymmetric parts have quite distinctive properties. It is readily shown that

$$\hat{C}_g = A_g\hat{R} + \hat{P}_g\,, \tag{6}$$

where A_g is the area associated with grain g shaded in Fig. 1. The areas A_g have the convenient property of tessellating the plane such that $\sum_g A_g$ is the area of the entire system. The symmetric part, $\hat{P}_g$, represents a *fluctuation* in the local chirality around grain g and can be expressed as

$$\hat{P}_g = \sum_l \frac{1}{2}\,(\vec{s}_{lg}\vec{s}_{lg} - \vec{t}_{lg}\vec{t}_{lg})\,, \tag{7}$$

where the vectors $\vec{s}_{lg}$ and $\vec{t}_{lg}$ are shown in Fig. 1. It is a crucial point that neighboring grains share equal and opposite contributions $\vec{s}\vec{s}$ and $-\vec{t}\vec{t}$ to their $\hat{P}$ tensors, $\vec{s}_{lg} = -\vec{t}_{lg'}$ in Fig. 1. From this it follows that the volume average $\langle\hat{P}\rangle$ vanishes up to boundary terms *independent* of any assumptions of isotropy. For periodic lattices $\langle\hat{P}\rangle$ vanishes over one unit cell.

To underpin the significance of C_g as the relevant geometrical order parameter, consider a region of area A whose boundary is defined by the contact points of the outermost grains. Averaging over $\hat{S}_g$ in the region, using Eq. (5), gives

$$\langle\hat{\sigma}\rangle = \frac{1}{A}\sum_g \hat{C}_g \cdot \vec{\nabla}\vec{f} = \langle\hat{C}_g \cdot \vec{\nabla}\vec{f}\rangle. \tag{8}$$

Carrying out the same summation using Eq. (2) we observe that the sum over loops inside the region cancels out and the only contribution comes from the boundary vectors, $\vec{r}_b$, between boundary contact points,

$$\langle\hat{\sigma}\rangle = \frac{1}{A}\sum_{\text{boundary}} \vec{r}_b\vec{f}_b\,, \tag{9}$$

where $\vec{f}_b$ is the external loading on the region. This contour sum can be converted, using Stokes theorem, into

$$\langle\hat{\sigma}\rangle = \frac{1}{A}\int ds\,\hat{R} \cdot \vec{\nabla}\vec{f} = \hat{R} \cdot \langle\vec{\nabla}\vec{f}\rangle. \tag{10}$$

Since $\langle\hat{P}_g\rangle = 0$ we identify $\langle\hat{C}_g\rangle = A\hat{R}$ and, on comparing to Eq. (8), we obtain

$$\langle\hat{C}_g \cdot \vec{\nabla}\vec{f}\rangle = \langle\hat{C}_g\rangle \cdot \langle\vec{\nabla}\vec{f}\rangle. \tag{11}$$

This result is particularly reassuring because it yields the effective response of a macroscopic granular region to a force field in terms of an effective macroscopic characteristic property $\langle\hat{C}_g\rangle$. It is equivalent to results in contexts such as disordered dielectrics and continuum elasticity that are derived by combining a field equation with either a constitutive relation or an energy functional [11].

We can now construct the constitutive equation in terms of a mean field continuum stress tensor based on Eq. (10) as

$$\hat{\sigma} = \hat{R} \cdot \vec{\nabla}\vec{f}\,. \tag{12}$$

This can be inverted to substitute $\vec{\nabla}\vec{f} = \hat{R}^T \cdot \hat{\sigma}$ into Eq. (5), and then for the torque on grain g to vanish requires the antisymmetric part of $\hat{C}_g \cdot \hat{R}^T \cdot \hat{\sigma} = -A_g\hat{\sigma} + \hat{P}_g \cdot \hat{R}^T \cdot \hat{\sigma}$ should vanish. This gives both the already anticipated requirement that $\hat{\sigma}$ is symmetric and a new relation which, in terms of the components P_{ij} of $\hat{P}$, is

$$P_{11}\sigma_{22} + P_{22}\sigma_{11} - 2P_{12}\sigma_{12} = 0\,. \tag{13}$$

Relation (13) is the continuum constitutive equation that provides the missing link between the stress and the local geometry. It has the striking feature that the coefficients $\hat{P}$ are spatially fluctuating quantities that locally add to zero, undermining any simple attempt to identify a nonvanishing mean field value $\langle\hat{P}\rangle$. In this sense the problem is analogous to spin glasses, in our case it being $\hat{\sigma}$ that is subject to spatial couplings of the random sign [12].

Constitutive equations for stress components in the form of (13) have been suggested for modeling empirically stress transmission in sandpiles [8,13]. These presume that a nonvanishing macroscopic version of $\hat{P}$ exists, e.g., the hypotheses of "fixed principal axes" (corresponding to $\hat{P}$ being traceless) and "oriented stress linearity" [13]. Our observation that the simple grain average of $\hat{P}$ vanishes suggests that this assumption is far from straightforward. We are therefore particularly motivated to consider any case where a nonzero effective $\hat{P}$ can be identified.

Drawing inspiration from spin problems, we focus on granular systems with antiferromagneticlike order. The key idea is that, for systems where every loop has an even number of edges, we can uniquely label all grains $+$ and $-$ (or vice versa) such that each grain is surrounded only by opposite sign neighbors, a pattern that is commonly termed unfrustrated. In such systems we can distinguish locally averaged values $\hat{P}_+$ and $\hat{P}_-$, restricted to the respective $+$ and $-$ grains, and Eq. (13) holds with either replacing $\hat{P}$. Thus the problem is solved because we now have a local nonvanishing order parameter, say, $\hat{P}_+$, whose volume average does not vanish macroscopically and we have a nontrivial additional equation for the stress field. The simplest class of systems where we can see this work is a periodic lattice with the connectivity of a honeycomb and a generally anisotropic unit cell comprising two grains, which we duly label $+$ and $-$ (see Fig. 2). Then the condition that both $\hat{S}_+ - \hat{S}_-$ and $\hat{\sigma} \propto (\hat{S}_+ + \hat{S}_-)$ be symmetric leads to the constitutive equation (13) with $\hat{P}$ replaced by $\hat{P}_+(\neq 0)$ whose value holds for the *entire* periodic structure.

The idea of a staggered order parameter can be further exploited to formulate a mapping from perfectly smooth to perfectly rough systems. We note that the behavior of a pile of perfectly smooth grains is identical to the same pile of rough grains provided that at each contact point we insert a vanishingly small perfectly rough ball bearing. It is readily checked that starting from $\bar{z} = 6$ for the smooth grains leads to $\bar{z} = 3$ for the resulting set of rough grains (three-fourths of which are the new bearings, each having $z = 2$), so we duly arrive at a marginally connected set of rough grains. Furthermore, in the rough system we automatically have a staggered order since each original grain $(+)$ is surrounded only by bearings $(-)$ and vice versa. Explicit evaluation shows that for each bearing $\lim_{\epsilon\to 0}\hat{P}_- \propto \epsilon$ where ϵ is the bearing radius and so, in this case, the appropriate order parameter is $\hat{p} = \lim_{\epsilon\to 0}\hat{P}_+/\epsilon$. This order parameter, and hence the corresponding $\hat{P}_{\rm eff}$, will generally have a nonzero average for any orientationally ordered assembly of smooth grains, and in particular for a periodic array where such a calculation has been computed explicitly [5].

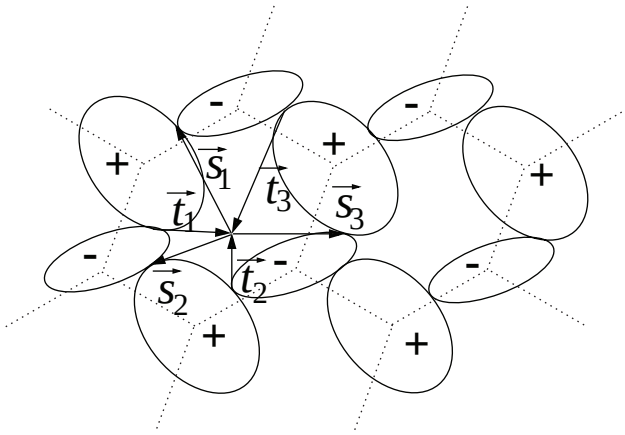

FIG. 2. Part of an anisotropic periodic lattice, where there are two distinct grains, labeled $+$ and $-$, per unit cell. Stress transmission is controlled by the tensor $\hat{P}_+ = -\hat{P}_- = \frac{1}{2}\sum_k \vec{s}_k\vec{s}_k - \vec{t}_k\vec{t}_k$. The lattice vectors are $\vec{t}_1 + \vec{s}_1$, $\vec{t}_2 + \vec{s}_2$, and $\vec{t}_3 + \vec{s}_2$ and, because these are not independent, the value of $\hat{P}_+$ turns out to be independent of the choice of loop center.

Returning to rough grains, general piles may clearly have loops with odd numbers of edges and therefore there is no way to tag the grains by $+$ or $-$ in the above pattern. Such piles are frustrated in the sense that they must contain neighbors of like sign, which undermines the above definition of a global nonvanishing order parameter $\hat{P}$. This implies that there is an inherent difference between frustrated and unfrustrated systems which has macroscopic implications for the stress field in the sense that only for the latter can we find a missing equation for the stress field. Since perfectly smooth systems can always be mapped to unfrustrated rough systems, it follows that there may be an inherent difference between the smooth and rough grain piles.

Finally, to underpin the exact nature of our analysis, we introduce an alternative formulation of the problem in terms of a potential field. The circulating loop forces

amount to two degrees of freedom per loop and hence can be represented in terms of one scalar per grain, a grain potential ψ_g. A natural way to achieve this is via

$$\vec{f}_l = \frac{-1}{A_l} \sum_g \vec{r}_{lg} \psi_g \,, \tag{14}$$

where A_l is the loop area analogous to the grain area A_g described above. The A_l's tessellate the systems uniquely and $\sum_l A_l$ is the entire system area. The potentials are determined by substituting (14) into Eq. (3), leading to

$$\sum_{l,g'} \frac{1}{A_l} \vec{r}_{lg} \times \vec{r}_{lg'} \psi_{g'} = 0 \,. \tag{15}$$

We emphasize that the above potential formulation is exact. We now continue the ψ field throughout the system just as we did previously for the force field and show that this leads to identification of ψ with the conventional Airy stress function [14]. We expand around the loop centers and obtain

$$\vec{f}_l = \frac{1}{A_l} \hat{C}_l \cdot \vec{\nabla} \psi \,. \tag{16}$$

The geometrical tensor $\hat{C}_l = \sum_g \vec{r}_{lg} (\vec{R}_l - \vec{R}_g)$ is the loop analog of $\hat{C}_g$ and its antisymmetric part is likewise associated with the area A_l. The symmetric part of $\hat{C}_l$ is sensitive to the choice of grain center positions $\vec{R}_g$: as there are two grains per loop these constitute four degrees of freedom per one $\hat{C}_l$ tensor and therefore these tensors can be chosen to be purely antisymmetric, $\hat{C}_l = A_l \hat{R}$. We can now express our continuum stress field [Eq. (12)] as

$$\hat{\sigma} = \hat{R} \cdot \vec{\nabla} \hat{R} \cdot \vec{\nabla} \psi = \vec{\nabla} \times \vec{\nabla} \times \psi \tag{17}$$

which reassuringly recovers Airy's representation of a symmetric divergence-free stress field [14].

To conclude, we have formulated a theory of stress transmission in granular matter at the marginal state between solid and fluid in terms of loop forces, which in turn can be defined in terms of a scalar potential. These results apply strictly to two-dimensional systems and their validity to three dimensions remains an open question.

The theory provides the elusive missing equation without resorting to phenomenological assumptions and exposes the sensitivity of granular matter to local geometrical fluctuations. These have zero average, preventing us from developing a simple mean field theory in the general case. Where these fluctuations have an antiferromagneticlike order we obtain a global consitutive relation leading to a macroscopic theory. In particular, we have shown that piles of smooth grains map into such an unfrustrated case. Nonfrustration for smooth grains is supported by exact lattice calculations [5] and by the simulations of Tkachenko and Witten [7]. These results point to an inherent difference between rough (frustrated) and smooth (ordered) systems, suggesting that there may be a subtle transition of behavior somewhere in between.

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