Unilateral interactions in granular packings: A model for the anisotropy modulus

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Unilateral interparticle interactions have an effect on the elastic response of granular materials due to the opening and closing of contacts during quasi-static shear deformations. A simplified model is presented, for which constitutive relations can be derived. For biaxial deformations the elastic behavior in this model involves three independent elastic moduli: bulk, shear, and anisotropy modulus. The bulk and the shear modulus, when scaled by the contact density, are independent of the deformation. However, the magnitude of the anisotropy modulus is proportional to the ratio between shear and volumetric strain. Sufficiently far from the jamming transition, when corrections due to non-affine motion become weak, the theoretical predictions are qualitatively in agreement with simulation results.

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I. INTRODUCTION

Understanding the mechanical response of granular materials is still one of the remaining challenges in materials science and physics. The research is motivated by many industrial and geophysical applications. 1 2 A granular packing at rest does not behave like an ordinary elastic solid, because the relation between stress and strain is nonlinear, depends on the fabric and on the loading path, and gives rise to energy dissipation. 3 4 These properties have been investigated for packings of spheres, where they could be traced back to the nonlinearity of Hertzian contacts, disorder, and Coulomb friction law. In these studies the contacts between the spheres were supposed to remain closed under the strain.

However, there is another source of the nonlinear elastic response in granular media, which has not yet been studied in such detail yet. 5 Due to the absence of attractive contact forces in dry granular media, the contacts can open, and thus do not transmit any elastic restoring nor frictional force. Even in the case of linear (Hookean) elasticity on the particle level (e.g. for packings of parallel cylinders), the vanishing of the elastic response under tension renders the macroscopic elastic behavior nonlinear. It is this nonlinearity which we analyze in this paper.

It is known that the contact and force networks in sheared granular materials are anisotropic. 7 8 The present analytical approach links the fabric anisotropy to the shear deformation for fixed volumetric strain.

In the following, we investigate the incremental linear response of a pre-strained two dimensional packing of disks and relate the elements of the stiffness tensor to the mean packing properties and the probability distribution of contact orientations. Then, analytical expressions for the elastic moduli of isotropic and sheared contact networks are derived, and the results are compared with numerical simulations.

II. LINEAR ELASTIC RESPONSE

The elastic response of solids to deformations is classically expressed in terms of the relationship between the stress tensor \( \sigma \) and the strain tensor \( \epsilon \). Let us assume that the relation between the incremental stress tensor \( \delta \sigma \) and the incremental strain tensor \( \delta \epsilon \) can be expressed by analytical functions \( F_{ij} \) as

\[
\delta \sigma_{ij} = F_{ij} (\delta \epsilon_{kl}), \quad (1)
\]

where \( F_{ij} \) satisfy \( F_{ij} (\delta \epsilon_{kl}) = 0, \forall k, l \in \{1, ..., d\} = 0 \). Here, \( d \) is the dimension of the system. In the limit of small deformations, Eq. (1) can be approximated by Taylor expansion to first order in the strain increment

\[
\delta \sigma_{ij} = \sum_{k,l} C_{ijkl} \delta \epsilon_{kl}, \quad (2)
\]

where \( C \) is a tensor of rank 4, referred to as the stiffness or elasticity tensor. Equation (2) can be regarded as the generalization of Hooke’s law that describes the linear response of the medium to external perturbations. Although \( C \) has 16 elements in a two-dimensional system, symmetry considerations for the stress and strain tensors imply that there are usually less independent elements. For example, the symmetry of a completely isotropic material requires that \( C \) has only two independent elements, commonly represented by the Lamé coefficients or, alternatively, by Poisson’s ratio and Young’s modulus.

In this section, it is recalled, how an approximate expression for the stiffness tensor of a dense assembly of grains can be obtained, which allows to calculate the elastic moduli from mean packing properties and the probability distribution of contact orientations. 9 10

The schematic figure 1(a) shows the undeformed shapes of two particles at positions A and B. Their overlap is a measure of the elastic deformation at their contact \( c \). The normal and tangential contact unit vectors are denoted by \( n^c \) and \( t^c \), and the branch vector \( l^c \) connects the centers of the particles. Each contact force is...
modeled by two linear springs in the normal and tangential directions with the spring constants $k_n$ and $k_t$, respectively. This harmonic force law approximates the interaction for two-dimensional disks for small deformations [12, 13]. Starting from an arbitrary weakly deformed state, the change in the force exerted by particle $B$ on particle $A$ due to an additional small deformation is

$$
\delta f^c = k_n (\delta t^c \cdot n^c) n^c + k_t (\delta t^c \cdot t^c) t^c,
$$

(3)

where $\delta t^c$ is the change of the branch vector due to the displacement of the particle centers. It is supposed that the contacts do not break due to the imposed deformation.

This is justified by the fact that during the measurement of the macroscopic elastic moduli, the material is subjected only to incremental strain changes so that the fabric remains nearly unchanged. The average stress increment can be approximated by

$$
\delta \sigma_{ij} \approx \frac{1}{V} \sum_{c=1}^{N_c} \delta f^c_{ij},
$$

(4)

where terms of order (overlap/particle radius) have been neglected. This is sufficiently accurate for small pre-strains. Here, the sum runs over all contacts $N_c$ within the volume $V$.

Using Eqs. (3) and (4) one obtains

$$
\delta \sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} \left( k_n \sum_k \delta l^c_{ik} n^c_k n^c_k + k_t \sum_k \delta l^c_{ik} t^c_k t^c_k \right) t^c_{ij}.
$$

(5)

A crucial simplification of this expression is obtained, if one assumes affine displacements of the particle centers, which states that the displacement gradient is constant or varies only slowly on the scale of the particle size. In this way, the non-affine parts of the relative displacements are neglected and the remaining part according to the macroscopic strain increment is given by

$$
\delta l^c_k = \sum_i \delta t_{ki} t^c_i.
$$

(6)

Inserting Eq. (6) into Eq. (5), one obtains

$$
\delta \sigma_{ij} = \sum_{k,l} \frac{1}{V} \sum_{c=1}^{N_c} |l^c|^2 \left( k_n n^c_j n^c_j n^c_i + k_t t^c_j t^c_j t^c_i \right) \delta \epsilon_{kl},
$$

(7)

For narrow size distributions and small pre-strain, one may replace $|l^c|$ by the average particle diameter $\ell$. Polydispersity leads, in first order, to an additional factor that only depends on the moments of the particle size distribution [16]. By comparing Eqs. (7) and (2) the stiffness tensor is identified as [17, 18]

$$
C_{ijkl} = \frac{\ell^2}{V} \sum_{c=1}^{N_c} \left( k_n n^c_j n^c_j n^c_i + k_t t^c_j t^c_j t^c_i \right).
$$

(8)

Denoting the normal and tangential unit vectors as $\vec{n} = (\cos \alpha, \sin \alpha)$ and $\vec{t} = (-\sin \alpha, \cos \alpha)$ [see Fig. 1(b)], the sum over the contacts located inside the volume $V$ can be replaced by an integral over the contact orientation distribution $P(\alpha)$ [11] so that

$$
C_{ijkl} = \frac{2}{\pi} \int_{-\pi}^{\pi} \left( k_n n_i n_j n_k n_l + k_t t_i t_j t_k n_l \right) P(\alpha) d\alpha,
$$

(9)

where $z = (2N_c/N)$ is the average coordination number, $\phi = N\pi \ell^2 / 4V$ is the volume fraction of the packing, and $P(\alpha) d\alpha$ denotes the probability to find a contact with an orientation between $\alpha$ and $\alpha + \Delta \alpha$. According to Eq. (9), the elements of the stiffness tensor are determined by the fabric properties: $z$, $\phi$, and $P(\alpha)$.

It is convenient to choose the principal axes of the strain tensor increment $\delta \epsilon$ as coordinate system so that

$$
\delta \epsilon = \frac{1}{2} \begin{pmatrix} \delta \epsilon_n + \delta \gamma & 0 \\ 0 & \delta \epsilon_n - \delta \gamma \end{pmatrix}
$$

(10)

with $\delta \epsilon_n (= \text{Tr} \delta \epsilon = \delta V/V)$ and $\delta \gamma$, the change in the volumetric strain and in the shear deformation, respectively. Then Eq. (2) can be written as

$$
\begin{pmatrix}
\delta \sigma_{11} \\
\delta \sigma_{22} \\
\delta \sigma_{12}
\end{pmatrix} = \begin{pmatrix}
C_{1111} & C_{1122} & 0 \\
C_{2211} & C_{2222} & 0 \\
C_{1121} & C_{2212} & C_{2222}
\end{pmatrix} \begin{pmatrix}
\delta \epsilon_n + \delta \gamma \\
\delta \epsilon_n - \delta \gamma \\
0
\end{pmatrix}/2.
$$

(11)

The balance of torques requires that the average stress tensor remains symmetric, i.e. $\delta \sigma_{12} = \delta \sigma_{21}$. Hence, the following constraints must hold in equilibrium

$$
C_{1211} = C_{1222}, \quad C_{2212} = C_{2222}.
$$

(12)

Using (12) this implies that only those incremental deformations do not induce torques inside the packing (and hence lead to particle rotations), whose principal axes are compatible with the contact orientation distribution in the sense that

$$
\sin 2\alpha = \int_{-\pi}^{\pi} \sin 2\alpha P(\alpha) d\alpha = 0.
$$

(13)

Evaluating (12) for fabrics that fulfill the constraint [13] gives the following expressions for the elements of the
stiffness tensor:
\[
\begin{align*}
C_{1111} &= \frac{z\phi}{\pi} \left( k_n (1 + \cos 2\alpha) - \frac{k_n - k_i}{2} (\sin 2\alpha)^2 \right) \quad (14) \\
C_{2222} &= \frac{z\phi}{\pi} \left( k_n (1 - \cos 2\alpha) - \frac{k_n - k_i}{2} (\sin 2\alpha)^2 \right) \quad (15) \\
C_{1122} &= \frac{z\phi}{\pi} \frac{k_n - k_i}{2} (\sin 2\alpha)^2 \quad (16) \\
C_{2112} &= C_{2211} = -C_{1221} = -C_{2122} = \frac{z\phi}{\pi} (k_n - k_i) (\sin 4\alpha) \quad (17)
\end{align*}
\]

III. BIAXIAL DEFORMATIONS

In the following we consider biaxial deformations, which means that the principal axes of the strain tensor do not change, while the sample is deformed. If the deformation starts from an isotropic configuration, the fabric \((P(\alpha))\) will remain symmetric with respect to \(\alpha = 0\). Hence (13) is fulfilled and (17) vanishes, as one averages odd functions with an even distribution. This simplifies matters considerably, as it implies that the principal axes of stress and strain coincide so that
\[
\delta \sigma = \begin{pmatrix} \delta \sigma_{11} & 0 \\ 0 & \delta \sigma_{22} \end{pmatrix} = - \begin{pmatrix} \delta P + \delta \tau & 0 \\ 0 & \delta P - \delta \tau \end{pmatrix},
\]
where \(\delta P\) and \(\delta \tau\) are the incremental pressure and shear stress.

One defines the bulk modulus \(E\), the shear modulus \(G\) and the anisotropy modulus \(A\) by
\[
\begin{pmatrix} \delta P \\ \delta \tau \end{pmatrix} = - \begin{pmatrix} E & A \\ A & G \end{pmatrix} \begin{pmatrix} \delta \varepsilon_v \\ \delta \gamma \end{pmatrix}.
\]

According to (14) and (15) - (16)

\[
\begin{align*}
E &= \frac{C_{1111} + C_{1122} + C_{2211} + C_{2222}}{4} = \frac{z\phi}{2\pi} k_n, \\
G &= \frac{C_{1111} - C_{1122} - C_{2211} + C_{2222}}{4} = E \left( (\cos 2\alpha)^2 + \frac{k_i}{k_n} (\sin 2\alpha)^2 \right) \\
A &= \frac{C_{1111} - C_{2222}}{4} = E \cos 2\alpha.
\end{align*}
\]

For an isotropic fabric, \(P(\alpha) = \frac{1}{2\pi}\), the result of Kruyt and Rothenburg [18] is reproduced:
\[
E = \frac{z\phi}{2\pi} k_n, \quad G = \frac{z\phi}{4\pi} (k_n + k_i), \quad A = 0.
\]

In the next section a simple model is proposed for the kind of anisotropy; a granular packing develops under the influence of shear.

IV. ANISOTROPY INDUCED BY UNILATERALITY

In order to elucidate the effect of unilaterality on the stress-strain relationship, we must consider the closing respectively opening of contacts, as a finite volumetric strain \(\epsilon_v\) and shear deformation \(\gamma\) build up, starting from an isotropic, stress-free, jammed packing (unstrained reference state with zero overlap). Assuming again that the particle displacements may be approximately regarded as affine, the distance between the centers of neighboring particles changes due to the strain \(\epsilon\) by
\[
\Delta \xi_n(\alpha, \epsilon) = -\ell \sum_{i,j} \epsilon_{ij} n_i n_j = - \ell \left( \frac{\epsilon_v}{2} + \frac{\gamma}{2} \cos 2\alpha \right).
\]

The change depends on \(\epsilon\) as well as on the direction of the branch vector, \(\alpha\). If the two particles touched each other, i.e. \(\xi_n = 0\) in the unstrained state, a positive \(\Delta \xi_n\) means that the deformation leads to an overlap, while a negative value indicates that the particles are no longer in contact in the strained state. When there is a gap between the particle surfaces in the unstrained configuration, an overlap can also form, if \(\Delta \xi_n\) is larger than the gap. Therefore we extend the notion of an overlap to include small negative values, \(\xi_n < 0\), which tell the size of the gap.

We introduce the probability density \(Q(\xi_n, \alpha, \epsilon)\) that a particle pair has a branch vector at an angle \(\alpha\) with respect to the principal axis of the strain tensor \(\epsilon\), belonging to the eigenvalue \(\epsilon_v + \gamma\), and that the overlap respectively the negative gap has a value \(\xi_n\). This probability density depends on the strain \(\epsilon\). For \(\epsilon = 0\) it is assumed to be isotropic, i.e. independent of \(\alpha\), and it fulfills \(Q_0(\xi_n) = 0\) for \(\xi_n > 0\), as there are no overlaps in the unstrained configuration, and \(Q_0(\xi_n) \neq 0\) for \(\xi_n \leq 0\), as the unstrained configuration is jammed. We assume that the probability distribution simply shifts by \(\Delta \xi_n\), Eq. (22), under the influence of strain:
\[
Q(\xi_n, \alpha, \epsilon) = Q_0(\xi_n - \Delta \xi_n(\alpha, \epsilon))
\]

The probability that a pair of neighbor particles is actually in contact is
\[
\mathcal{N} = \int_{-\pi}^{\pi} d\alpha \int_0^{\infty} d\xi_n \; Q(\xi_n, \alpha, \epsilon)
\]

The probability density, that a contact has a certain angle \(\alpha\) with respect to the principal axis of the strain, which belongs to the eigenvalue \(\epsilon_v + \gamma\), is
\[
P(\alpha, \epsilon) = \frac{1}{\mathcal{N}} \int_0^{\infty} d\xi_n \; Q(\xi_n, \alpha, \epsilon).
\]

Applying the assumption [23], the integral is in first order of \(\epsilon\) given by
\[
\int_0^{\infty} d\xi_n \; Q(\xi_n, \alpha, \epsilon) \approx Q_0(0) \Delta \xi_n(\alpha, \epsilon) = -Q_0(0) \ell \left( \frac{\epsilon_v}{2} + \frac{\gamma}{2} \cos 2\alpha \right).
\]
Integrating this over $\alpha$ gives the corresponding first order approximation of $N$:

$$N \approx -Q_0(0) \epsilon_v \pi. \quad (27)$$

Hence the properly normalized first order approximation of the probability density of contact directions is

$$P(\alpha, \epsilon) \approx \frac{1}{2\pi} \left( 1 + \frac{\gamma}{\epsilon_v} \cos 2\alpha \right). \quad (28)$$

This approximation can at most be applied for $|1/\epsilon_v| \leq 1$, as otherwise the probability density would not be positive semi definite. $\alpha = 0$ is the direction of the principal axis belonging to the eigenvalue $\epsilon_v + \gamma$. For $\epsilon_v < 0$ (compressive strain) and $\gamma \geq 0$ (by definition) this is the direction in which the precompressed system expands during biaxial deformation. Therefore contacts preferentially open in this direction so that $P(0, \epsilon) \approx \frac{1}{2\pi} \left( 1 + \frac{1}{\epsilon_v} \right) < \frac{1}{2\pi}$.

Equation (28) is the main new result of this paper. In this approximation, $\langle (\cos 2\alpha)^2 \rangle = \langle (\sin 2\alpha)^2 \rangle = \frac{1}{2}$ and $\langle \cos 2\alpha \rangle = \frac{\pi}{2\pi}$ so that the elastic moduli of a granular packing are approximately

$$E = \frac{z\phi}{2\pi} k_n, \quad G = \frac{z\phi}{4\pi} (k_n + k_t), \quad A = \frac{z\phi}{4\pi} k_n \gamma. \quad (29)$$

Note that due to the presence of the nonzero element $A$ in Eq. (19), two independent experimental tests are required to determine the elastic moduli of an anisotropic material, for example:

(I) incremental $\delta \epsilon_v$ while $\delta \gamma = 0$:

$$E = -\frac{\delta P}{\delta \epsilon_v} \bigg|_{\delta \gamma = 0}, \quad A = -\frac{\delta P}{\delta \epsilon_v} \bigg|_{\delta \gamma = 0}. \quad (30)$$

(II) incremental $\delta \gamma$ while $\delta \epsilon_v = 0$:

$$G = -\frac{\delta P}{\delta \gamma} \bigg|_{\delta \epsilon_v = 0}, \quad A = -\frac{\delta P}{\delta \gamma} \bigg|_{\delta \epsilon_v = 0}. \quad (31)$$

This is in contrast to the isotropic case, where a single experiment with simultaneous incremental $\delta \epsilon_v$ and $\delta \gamma$ is sufficient to measure both bulk and shear moduli. In granular media, in contrast to an isotropic elastic material, a pure shear leads to a pressure increase, $\delta P = -A\delta \gamma > 0$ as $A < 0$.

V. SIMULATION RESULTS

We tested the theoretical predictions of Sec. IV by numerical simulations. The unstrained initial packing consists of 3000 rigid disks with particle radii uniformly distributed between $a_{\text{min}}=0.95$ and $a_{\text{max}}=1.05$ to avoid crystalline order. It was generated by a method based on Contact Dynamics simulations, which leads to homogeneous, isotropic, jammed configurations [19]. Such a packing is taken as unstrained initial configuration in a Molecular Dynamics simulation of soft particles using the LAMMPS code [20, 21]. The interactions between particles are modeled with normal and tangential Hookean springs (with $k_1/k_2=0.5$). We checked that the results do not depend on the friction coefficient, when it is chosen larger than 0.5. The data shown here are for $\mu=1$.

In a quasi-static compression process, the volume of the unstrained packing is gradually decreased by applying incremental volumetric strain steps and allowing the system to relax between those steps. The process is stopped when the total volumetric strain $\epsilon_v = \Delta V/V$ reaches a given value ($\epsilon_v = -0.04$ respectively $\epsilon_v = -0.09$). This precompressed packing is then sheared in a biaxial geometry, while keeping the volume of the system constant. The shear deformation is imposed via incremental steps, and the system is allowed to relax between the steps.

Two different methods are used to determine the elastic moduli:

1. Using Eq. (8) the elastic constants can be computed from the fabric. This formula assumes affine deformations and that the contact network remains unchanged for incremental strains.

2. An incremental strain test is simulated by molecular dynamics and the elastic moduli are determined from Eqs. (30) and (31). This method allows for a change of the contact network and non-affine motions of the particles.

Fig. 2 shows that the bulk and shear moduli divided by $z\phi$ are approximately constant for strong enough compression, $-\epsilon_v > 0.04$, in agreement with Eq. (29).
However, as one approaches the unstrained configuration (at the jamming transition), the elastic moduli obtained from evaluating incremental strain tests soften, whereas the ones calculated from the fabric remain unchanged. This shows that close to the jamming transition the assumption that the incremental particle movements are affine fails, in agreement with the findings of \[22, 23\]. Therefore we concentrate on the regime \(-\epsilon_v \geq 0.04\) in the following. Remarkably, the ratio of the two moduli, \(G/E\), differs from this behavior for small shear, \(\gamma/\epsilon_v\), and show can be fitted by a linear dependence on \(\gamma/\epsilon_v\). Further simulations are needed to clarify the origin of \(\epsilon_v\) as well as the ones from the incremental shear tests for \(\gamma/\epsilon_v\). The model predicts, however, that the system presumably forms a shear band and begins to flow. Then the contact density must become independent of \(\gamma\). The transition from elastic to plastic response can be seen in Fig.3. The shear stress first increases linearly with \(\gamma\) and saturates for large deformation, indicating the plastic regime. This shows, that one can speak about elastic response only for \(\gamma/\epsilon_v < 1\).

Fig.4 also shows that the contact density (= \(\frac{2}{\pi} z \phi\)) increases the more compressed the packing is, while it decreases, if a precompressed sample is sheared at fixed volume, see Fig.4 provided \(\gamma\) remains small enough. For large shear deformation, the system presumably forms a shear band and begins to flow. The results for \(A/E\) determined from the fabric, as well as the ones from the incremental shear tests for \(\epsilon_v = -0.04\) agree with each other within the error bars and show can be fitted by a linear dependence on \(\gamma/\epsilon_v\). Only the shear test simulation data for \(\epsilon_v = -0.09\) deviate from this behavior for small shear, \(\gamma/\epsilon_v < 0.7\), although the evaluation of the fabric perfectly agrees. Further simulations are needed to clarify the origin of this peculiar behavior. The simulation data essentially confirm the linear dependence of the anisotropy modulus on the ratio \(\gamma/\epsilon_v\). However, the theory overestimates the slope by a factor of about 7.

**VI. CONCLUSION**

We have shown that the opening and closing of contacts can explain the anisotropy modulus which is characteristic for the elastic response of dense granular packings under biaxial shear. The theory predicts a linear dependence of the anisotropy modulus on the ratio \(\gamma/\epsilon_v\), which is the only zeroth order combination of the scalar invariants \(\gamma = \sqrt{\text{Tr} \epsilon^2 - 2 \det \epsilon} \) and \(\epsilon_v = \text{Tr} \epsilon\). This is confirmed by simulations, but the theory overestimates the anisotropy modulus by a factor of 7. The bulk and shear moduli are predicted correctly by the theory, as long as one is not too close to the jamming transition, where the assumption of affine deformation of the packing fails.
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