On the Microscopic Foundations of Elasticity

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Abstract. The modeling of the elastic properties of disordered or nanoscale solids requires the foundations of the theory of elasticity to be revisited, as one explores scales at which this theory may no longer hold. The only cases for which microscopically based derivations of elasticity are documented are (nearly) uniformly strained lattices. A microscopic approach to elasticity is proposed. As a first step, microscopically exact expressions for the displacement, strain and stress fields are derived. Conditions under which linear elastic constitutive relations hold are studied theoretically and numerically. It turns out that standard continuum elasticity is not self-evident, and applies only above certain spatial scales, which depend on details of the considered system and boundary conditions. Possible relevance to granular materials is briefly discussed.

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1 Introduction

It is quite surprising that the existing microscopic justification of the time-honored theory of elasticity, which has been thoroughly researched in a variety of disciplines, is limited to lattice atomic configurations [1]. Classical continuum elasticity theory has been applied to a large variety of systems, including granular materials [2]. In recent years the same theory has been applied for the description of elastic properties of micro- and nano-scale systems (e.g., [3]). It is a-priori unclear whether this theory applies at such small scales.

The study presented below shows that the justification of elastic theory based on a microscopic picture is not entirely straightforward. As expected, one finds that linear continuum elasticity is valid on sufficiently large scales. Another result is that, like in granular matter, one observes force chains in strained elastic systems (also observed in [4]). These chains are not “visible” in the corresponding stress field. Classical mechanics is assumed throughout this paper. The case of isostatic systems, which has received considerable interest in the literature, is not specifically addressed here.

2 Coarse Graining and Constitutive Relations

2.1 Preliminaries

Consider a system of particles (indexed by \(i\)) whose masses, center of mass positions and velocities at time \(t\) are given by \(\{m_i; \mathbf{r}_i(t); \mathbf{v}_i(t)\}\). Following [5] define the coarse grained mass density at position \(\mathbf{r}\) and time \(t\) as

\[
\rho(\mathbf{r}, t) \equiv \sum_i m_i \phi(\mathbf{r} - \mathbf{r}_i(t)).
\]

Similarly, define the momentum density as

\[
p(\mathbf{r}, t) \equiv \sum_i m_i \mathbf{v}_i(t) \phi(\mathbf{r} - \mathbf{r}_i(t)),
\]

where \(\phi(\mathbf{R})\) is a normalized non-negative coarse graining function (with a single maximum at \(\mathbf{R} = 0\) of width \(w\), the coarse graining scale. Unlike in [5], here only spatial, and not temporal coarse graining, is invoked. Upon taking the time derivative of Eqs. (1,2) and performing straightforward algebraic manipulations [3], one obtains two of the equations of continuum mechanics. Eq. (1) yields the equation of continuity:

\[
\dot{\rho}(\mathbf{r}, t) = -\nabla \cdot \mathbf{p}(\mathbf{r}, t) = -\nabla \left[ \rho(\mathbf{r}, t) \mathbf{V}(\mathbf{r}, t) \right],
\]

where \(\dot{\rho} \equiv \frac{\partial \rho}{\partial t}\), and the coarse grained velocity field is defined by \(\mathbf{V}(\mathbf{r}, t) \equiv \mathbf{p}(\mathbf{r}, t)/\rho(\mathbf{r}, t)\). From Eq. (3) one obtains the momentum conservation equation:

\[
\dot{\rho}_\alpha(\mathbf{r}, t) = -\frac{\partial}{\partial r_j} \left[ \rho(\mathbf{r}, t) V_\alpha(\mathbf{r}, t)V_\beta(\mathbf{r}, t) - \sigma_{\alpha\beta}(\mathbf{r}, t) \right],
\]

where Greek indices denote Cartesian coordinates.

Define \(f_{ij}(t)\) to be the \(\alpha\)-th component of the force exerted on particle \(i\) by particle \(j\) \((j \neq i)\) at time \(t\) (assuming pairwise interactions), \(\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j\), and the fluctuating velocity
of particle $i$: $v_i'(r, t) \equiv v_i(t) - R(r, t)$. With these definitions, the stress tensor, $\sigma_{\alpha\beta}(r, t)$, is given by the following expression:

$$
\sigma_{\alpha\beta}(r, t) = -\frac{1}{2} \sum_{i, j \neq j} f_{ij\alpha}(r) r_{ij\beta}(t) \nabla r_{ij}(t) + \int_0^1 \sum_i m_i v'_i(r, t) u'_\alpha(r, t) \phi[r - r_i(t)]
$$

The first term in Eq. (8) is commonly referred to as the “contact stress” (or “collisional stress”), while the second term is a kinetic contribution (the “kinetic stress” or “streaming stress”), which vanishes for quasi-static deformations.

The energy conservation equation can be obtained in a similar way. Assume, for simplicity, that the forces are derived from a potential function: $f_{ij} = -\nabla \Phi(r_{ij})$, with obvious notation. Define the energy density as:

$$
e(r, t) \equiv \frac{1}{2} \sum_i m_i v_i^2(t) \phi[r - r_i(t)]
$$

Application of a time derivative to $e(r, t)$ and a rearrangement of terms yields the energy conservation equation:

$$
\dot{e}(r, t) = -\frac{\partial}{\partial r_{ij}} [V_{ij}(r, t)e(r, t) - V_{ij}(r, t) + c_{ij}(r, t)],
$$

where the heat flux, $c_{ij}$, is given by:

$$
c_{ij}(r, t) = \frac{1}{2} \sum_i \left[ m_i v_i^2(r, t) + \sum_{j \neq i} \Phi(r_{ij}(t)) \right] u'_{ij}(r, t) \phi[r - r_i(t)]
$$

$$
+ \frac{1}{4} \sum_{i \neq j, i \neq j} \left[ v'_i(r, t) + v'_j(r, t) \right] f_{ij\alpha}(r) r_{ij\beta}(t) 
\times \int_0^1 \sum_i m_i v'_i(r, t) u'_\alpha(r, t) \phi[r - r_i(t)] + s r_{ij}(t) \right].
$$

2.2 Displacement and Strain

Following elementary continuum mechanics, consider a material particle whose initial (Lagrangian, at time $t = 0$) coordinate is $R$. Its (Eulerian) coordinate at time $t$ is denoted by $r(R, t)$. The corresponding (Lagrangian) displacement field is given by $u^{la}(R, t) \equiv r(R, t) - R$. The material particle’s velocity is $V^{la}(R, t) = \partial u^{la}(R, t)/\partial t$. It therefore follows that $u^{la}(R, t) = \int_0^t V^{la}(R, t') dt'$. Using the definitions presented in Sec. 2.1, one obtains:

$$
u^{la}(R, t) \equiv \int_0^t \left[ \sum_i m_i v_i(t') \phi[r(R, t') - r_i(t')] / \sum_j m_j \phi[r(R, t') - r_j(t')] \right] dt'.
$$

The macroscopic displacement field $u$ is history dependent, i.e., the displacement at time $t$ depends on the trajectories of the particles from $t = 0$ to $t$. However, noting that $u_i = v_i$, where $u_i = r_i(t) - r_i(0)$ is the displacement of particle $i$, and invoking integration by parts in Eq. (9), one obtains (in the Eulerian representation):

$$
u(u, t) = u^{lin}(u, t)
$$

$$
+ \int_0^t \frac{1}{\rho(r, t')} \frac{\partial}{\partial t'} \left[ \sum_i m_i v'_i(r, t') u'_i(r, t') \phi[r - r_i(t') - r_i(t)] \right],
$$

where

$$
u^{lin}(u, t) \equiv \sum_i \frac{m_i u_i(t) \phi[r - r_i(t)]}{\sum_j m_j \phi[r - r_j(t)]}.
$$

It is claimed that $u^{lin}$ represents the displacement field relevant to linear elasticity, i.e., the error is nonlinear in the strain. To this end, let $\epsilon^* = \max_j \epsilon_{ij}$. Linear elasticity is a theory which is linear in $\epsilon^*$. Following the above definitions,

$$
u'_{\alpha}(r, t) = \frac{\sum_j m_j [u_{\alpha}(t) - u_{\alpha}(t)] \phi[r - r_i(t)]}{\sum_k m_k \phi[r - r_k(t)]},
$$

hence $|v'_\alpha| < C_1 \epsilon^*$, where $C_1$ depends on the coarse graining scale, and $|v'_\alpha| < C_2 \epsilon^*/\tau$, where $\tau$ represents the typical time scale on which the particles change (in the quasistatic limit, $\tau \rightarrow \infty$, while $\epsilon^*$ remains finite). The integrand in Eq. (10) is thus $O(\epsilon^2)$. As a matter of fact, it is easy to show that the integral on the right hand side of Eq. (10) is bounded from above by $O(\epsilon^2)$. Note that $\partial u^{lin} / \partial \epsilon^* \neq V^{la}$, since $u_i$ is defined with respect to the linear displacement field and not the exact displacement field. A useful feature of the linear displacement, $u^{lin}$(r, t), is that, unlike the exact displacement field [Eq. (9)], it depends only on the macroscopic displacements at time $t$.

The linear strain field is $\epsilon_{\alpha\beta}(r, t) = \frac{1}{2} \left[ \frac{\partial u^{lin}_{\alpha}(r, t)}{\partial r_{\beta}} + \frac{\partial u^{lin}_{\beta}(r, t)}{\partial r_{\alpha}} \right]$. Notice that $\epsilon_{\alpha\beta} = O(\epsilon^2)$. Following the above arguments, this expression can be replaced by:

$$
\epsilon_{\alpha\beta}^{lin}(r, t) \equiv \frac{1}{2} \left[ \frac{\partial u^{lin}_{\alpha}(r, t)}{\partial r_{\beta}} + \frac{\partial u^{lin}_{\beta}(r, t)}{\partial r_{\alpha}} \right],
$$

the error being $O(\epsilon^2)$.

It is interesting to compare the above results with some previously defined heuristic calculations of the strain field. The mean field strain (e.g., $\bar{\epsilon}$) is based on the assumption that the relative particle displacements are described by the macroscopic strain, i.e., $u_{ij}(r, t) = \epsilon_{\alpha\beta} r_{ij\alpha\beta}$ where $u_{ij} \equiv u_i - u_j$ (an affine deformation). An improvement of this method, which enables a local evaluation of the strain field, is provided by the “best fit” hypothesis [7], whereby the rms difference between the actual relative displacements and the above mean field expression for them is minimized in a given volume, to produce
a ‘best’ strain field. The mean field approaches are in general inconsistent with local force equilibrium (except for homogeneous deformations of lattice configurations). Therefore, the mean field (or best fit) strain constitutes an uncontrolled approximation of the strain field. The difference between the exact strain field, the linear strain as given by Eq. (14), and the best fit approximation are demonstrated in Fig. 1. In this figure, the above three fields are presented for a one dimensional chain of 1000 point particles connected by linear springs of random rest lengths (mean rest length $a = 1$, relative standard deviation 0.29) and random spring constants (relative standard deviation 0.13), the global strain of the system being $\epsilon = 0.05$. To this end, a Gaussian coarse graining function $\phi(r) = \frac{1}{\sqrt{2\pi w^2}} e^{-(r/\mu)^2}$ with $w = 50a$ has been employed. In the calculation of the best fit strain, the fluctuations with respect to the mean field are weighted using the same coarse graining function as in the exact formulation. As seen in Fig. 1, the linear strain is very close to the exact strain, whereas the best fit provides quite a poor approximation (for the case of equal spring constants, the best fit method yields a uniform strain, while the correct strain is space dependent [8]). In general, heuristic approximations for the strain field may result in inaccurate constitutive relations.

Consider, for sake of simplicity, only systems with pairwise interactions. In order to develop linear elasticity one can assume, without loss of generality, harmonic interactions:

$$\Phi(r_{ij}(t)) = \frac{1}{2} K_{ij} (|r_{ij}| - l_{ij})^2,$$  \hspace{1cm} (15)

where $l_{ij}$ is the equilibrium separation of particles $i$ and $j$. The force on particle $i$ exerted by particle $j$ is given, to linear order in the relative particle displacements, $u_{ij}$, by:

$$f_{ij} \simeq -K_{ij} (r_{ij}^0 \cdot u_{ij}) \dot{r}_{ij}^0,$$  \hspace{1cm} (16)

where the superscript 0 denotes the reference configuration, in which all particle pairs are at their equilibrium separation ($|r_{ij}^0| = l_{ij}$), i.e., an unstressed configuration (prestressed states are not considered here).

It is apparent that even in this case, the microscopic expressions for the contact stress [the first term in Eq. (5)] and the strain [Eq. (14)] are not manifestly proportional. Therefore macroscopic elasticity is not a-priori obvious. To see how it still comes about, substitute Eq. (16) in Eq. (5). The contact stress, to linear order in $\{u_{ij}\}$, is:

$$\sigma_{\alpha\beta}^{lin}(r, t) = \frac{1}{2} \left[ \sum_{ij} K_{ij} \epsilon_{ij\gamma} F_{ij\gamma} \dot{F}_{ij\gamma}^{0} \right] \times \int_{0}^{1} ds \phi(|r - r_{i} + s \dot{r}_{ij}|) \left[ u_{ij\gamma} - u_{ij\gamma}^{0} \right].$$  \hspace{1cm} (17)

Consider a volume $\Omega$, whose linear dimension, $W$, is much larger than the coarse graining scale, $w$, and let $r$ be an interior point of $\Omega$ which is ‘far’ from its boundary. Let upper case Latin indices denote the particles in the exterior of $\Omega$ which interact with particles inside $\Omega$. Since the considered system is linear, there exists a Green’s function $G$ such that $u_{ia} = G_{ia\beta} u_{j\beta}$ for $i \in \Omega$. Let $L_{ija\beta} \equiv G_{ia\beta} - G_{ja\beta}$. It follows that $L_{ija\beta} = L_{ija\beta}^{0} + K_{ij} \epsilon_{ij\gamma} F_{ij\gamma}^{0}$. Under a rigid translation (all $\{u_{j}\}$ equal): $u_{ij\alpha} = 0$, hence: $u_{ij\alpha} = L_{ija\beta} [u_{j\beta} - u_{j\beta}(r)]$.

It follows that:

$$u_{ij\alpha} = L_{ija\beta} [u_{j\beta}(r_{j}) - u_{j\beta}(r)] + L_{ija\beta} [u_{j\beta} - u_{j\beta}(r_{j})],$$  \hspace{1cm} (18)

where $u_{j\beta} - u_{j\beta}(r_{j})$ is a fluctuating displacement. The sum over $J$ in the second term can be shown to be subdominant when $W$ sufficiently exceeds $w$. The first term equals, to leading order in a gradient expansion:

$$u_{j\beta}(r_{j}) - u_{j\beta}(r) \simeq \frac{\partial u_{j\beta}(r)}{\partial r_{\gamma}} (r_{j\gamma} - r_{\gamma}).$$  \hspace{1cm} (19)

Substituting Eq. (19) in Eq. (17):

$$\sigma_{\alpha\beta}(r) \simeq \frac{1}{2} \left[ \sum_{ij} K_{ij} L_{ija\beta} \left( r_{ij\mu}^{0} - r_{ij\mu} \right) F_{ij\mu}^{0} F_{ij\mu}^{0} \epsilon_{\mu\nu}(r) \right] \times \int_{0}^{1} ds \phi(|r - r_{ij}^0 + s \dot{r}_{ij}^0|) \epsilon_{\mu\nu}(r),$$  \hspace{1cm} (20)

where rotational symmetry has been invoked. Thus linear elasticity is valid when $||\epsilon|| < 1$ (the strain components are small).

Fig. 1. The Eulerian strain $\epsilon(x)$ vs. position $x$ in the central region of a linear chain of particles connected by linear springs of random spring constants and rest lengths, calculated by three methods (see text).

### 2.3 Stress-Strain Relation

It is not a-priori clear that the stress field can be expressed as a linear functional of the strain field, even for small deformations. Each of these two macroscopic fields, cf. Eqs. (4[4]), is a different average of microscopic entities. Once averaging is invoked to produce macroscopic fields, on cannot deduce the microscopic entities from these fields. This is one of the fundamental flaws of the mean field approaches, which rely on such a deduction. Below, an exact method for obtaining linear elasticity, which demonstrates the above problem and highlights the scale limitations of this theory, is outlined.
and $|W_{\alpha \beta} u| \ll 1$. Note that the elastic moduli depend, in principle, on the position as well as the resolution (through the coarse graining function $\phi$). Our numerical results (see below) indicate that the contribution of the second term on the right hand side of Eq. (18) to the stress is smaller than a naive bound based on surface to volume ratios implies.

### 2.4 Elastic Energy

In the quasistatic limit, the energy density reduces, cf. Eq. (9), to:

$$e(\mathbf{r}, t) = \frac{1}{2} \sum_{i,j: i \neq j} \Phi (\mathbf{r}_{ij}(t)) \phi[\mathbf{r} - \mathbf{r}_i(t)].$$  \hspace{1cm} (21)

To lowest nonvanishing order in the strain, the potential energy corresponding to Eq. (15) is given by $\frac{1}{2} K_{ij} (\mathbf{r}^{0}_{ij} \cdot \mathbf{u}_{ij})^2$. Hence, at this order:

$$e(\mathbf{r}, t) = \frac{1}{4} \sum_{i,j: i \neq j} K_{ij} (\mathbf{r}^{0}_{ij} \cdot \mathbf{u}_{ij})^2 \phi[\mathbf{r} - \mathbf{r}_i(t)].$$  \hspace{1cm} (22)

If linear elasticity is to hold, one must have: $e = \frac{1}{2} \sigma \cdot \epsilon$. A set of straightforward transformations on Eq. (22) yields:

$$e(\mathbf{r}, t) = \frac{1}{2} \sigma \cdot \epsilon - \frac{\partial}{\partial \mathbf{r}_\beta} \left[ \frac{1}{4} \sum_{i,j: i \neq j} (\mathbf{f}_{ij} \cdot \mathbf{u}^0_{ij}) r_{ij\beta} \right] \times \int_0^1 d\lambda \phi[\mathbf{r} - \mathbf{r}_i(t) + s \mathbf{r}_{ij}(t)].$$  \hspace{1cm} (23)

It can be shown that the second term on the right hand side of Eq. (23) represents the adiabatic limit of the divergence of the heat flux [Eq. (8)], i.e., the work of the fluctuating forces at the surface of a control volume. As this term is a divergence of a flux, its average over a sufficiently large volume tends to zero, i.e., the average of $\frac{1}{2} \sigma \cdot \epsilon$ over a sufficiently large volume (not its ‘local value’) is the elastic energy density. As in the previous section, one obtains that classical elasticity is valid only for sufficiently large scales, in particular scales for which “surface contributions”, as explained above, vanish.

### 3 Numerical Results

The above results are demonstrated on a two dimensional (2D) system of particles with harmonic interactions [Eq. (16)]. As a first test case, consider a square-shaped triangular lattice configuration, with uniform nearest-neighbor spring constants $K$ and rest lengths equal to the lattice constant $d$, subjected to the following boundary conditions. The displacements of the particles at the boundary (whose positions are denoted by $\mathbf{r}^{0}_{ij}$) are chosen to yield a homogeneous deformation, i.e., the boundary is subject to an “applied strain”, $\epsilon_{\alpha\beta}$:

$$u_{1\alpha} = \epsilon_{\alpha\beta}(r_{1\beta} - r_{0\beta}),$$  \hspace{1cm} (24)

where $r_{0\beta}$ is an arbitrary point, chosen to reside at a corner of the system. The (linear) static equilibrium equations are solved (by matrix inversion) for a given applied $\epsilon_{\alpha\beta}$, yielding (for each choice of $\epsilon_{\alpha\beta}$) a set of displacements $\{u^i_{1\alpha}\}$. The latter are used for calculating the linear strain field [using Eq. (14) and linear stress, Eq. (17)]. The coarse-graining function used is,

$$\phi(R) = \phi(r) = \frac{A}{1 + e^{-w\frac{R - \lambda}{\beta}}},$$  \hspace{1cm} (25)

(\text{the Fermi distribution}), chosen as a smoothed Heaviside function. The length on which the function decays to zero, $\lambda$, can be chosen independently of the coarse graining scale, $w$. In all the calculations presented below, $\lambda = \frac{2}{3}$. The constant $A$ is fixed by the normalization: $\int_0^\infty R\phi(R) dR = 1$.

In this case of an ordered lattice, the strain components converge to the applied strain components even for $w = d$. This should be expected, since, as mentioned, for a lattice configuration (with uniform spring constants) under homogeneous deformation, the particle displacements correspond to an affine transformation, rendering the mean field approximation exact. The corresponding stress components are scale-independent as well, and consistent with the continuum isotropic elastic moduli for a triangular lattice (Lamé constants $\lambda = \mu = \frac{\sqrt{3}}{2} K$).

For disordered systems, even for a “homogeneous applied strain” as described above, the stress and strain fields are inhomogeneous, in general. Linear elasticity should still be valid (at least as an approximation, as described in Sec. 3), i.e. the local stress should depend on the local strain by an appropriate local linear relation on a sufficiently large coarse graining scale. In order to examine the influence of disorder on the validity of linear elasticity, disordered systems were generated, based on the triangular lattice configuration: a random number, uniformly distributed in the range $[-\delta d, \delta d]$, is added to the $x$ and $y$ coordinates of the particles. Particles whose distance is less than $c_{\max} = 1.1 d$ are connected by springs, with rest lengths equal to the particle separation in the initial configuration (ensuring an unstressed configuration), and spring constants uniformly distributed in the range $[K - \delta K, K + \delta K]$. Note that this choice of $c_{\max}$ can decrease the coordination number, for some of the particles, to a value smaller than 6, for sufficiently large $\delta d$ (this kind of topological disorder can give rise to qualitatively different effects than positional disorder). To evaluate the extent to which disordered systems are described by the equations of linear elasticity, the following procedure is used. Three independent global strains $\epsilon^0_{\alpha\beta}$: $i = 1, 2, 3$ are applied, and the stress and strain fields are calculated at a given point. According to linear elasticity, these fields should be linearly related, though the elastic moduli may be position dependent. In a 2D system with central forces (as used here), there are, in general, 6 independent elastic moduli. Each deformation provides three linear equations for these moduli (however, it can be shown that two independent deformations are insufficient for determining them, and three deformations are required). The elastic moduli are determined using 6 of the 9 linear equations. The stress components which are not used in this procedure are then calculated using these elastic moduli, and their values are compared to those computed directly using Eq. (17). The root mean square of the differences between the stress components calculated by employing the measured moduli and their directly measured exact values (normalized by the norm of the exact values), $\Delta$, is used as a measure of the extent to which
the system is described by linear elasticity at a given position and for a given value of the coarse graining scale.

The stress and strain components at the center of a disordered system of size $40d \times 40d$, with $\delta d = 0.1d$, $\delta K = 0.1K$ and applied strain $\epsilon^1 = \begin{pmatrix} 0.005 & 0.0075 \\ 0.0075 & 0.01 \end{pmatrix}$, are shown in Figs. 2, 3, respectively, for different coarse graining scales. These fields are obviously inhomogeneous, hence the observed scale dependence (note that for coarse graining scales approaching the system size, the values of the strain components do approach their imposed global values, as expected).

![Fig. 2. The strain components vs. the coarse graining scale, $w$, in a disordered configuration (see text), for an applied strain $\epsilon^1$ (see text).](image1)

![Fig. 3. The stress components vs. the coarse graining scale, $w$, in a disordered configuration (see text), for an applied strain $\epsilon^1$ (see text).](image2)

Fig. 4 shows the deviations from elasticity, measured by $\Delta$ as defined above, for the same disordered system. The deviation is quite large for small coarse graining scales, but it decreases to less than 1% for $w > 12d$, indicating that linear elasticity holds reasonably well beyond this scale. Note that at this scale, the stress and strain are still scale dependent, or inhomogeneous, which implies that linear elasticity does hold locally inside the system, with elastic moduli which depend on position (and scale). The deviations from elasticity for a similar system with higher disorder (with $\delta d = 0.15d$, $\delta K = 0.15K$) is shown in Fig. 5. One may interpret the observed fluctuations as an indication that the scale required to obtain linear elasticity exceeds the size of the system, as even at scales close to this size there is no clear saturation to a linear elastic relation.

![Fig. 4. The deviation from elasticity in a disordered configuration (see text), measured by $\Delta$ (see text), vs. the coarse graining scale, $w$.](image3)

![Fig. 5. The deviation from elasticity in a configuration with higher disorder compared to Fig. 4 (see text), measured by $\Delta$ (see text), vs. the coarse graining scale, $w$.](image4)
4 Concluding Remarks

It is important to note that the results presented in Sec. 3 have been obtained with boundary conditions chosen to obtain a homogeneous strain field. Indeed, in the case of a lattice, a uniform strain is obtained. Thus the inhomogeneity in the disordered case is not a result of the applied boundary conditions but of the disorder itself. When inhomogeneous boundary conditions are applied one expects an inhomogeneous strain field even in a homogeneous system. In this case one should observe deviations from linear elasticity on small scales or close to the boundary. The deviations from standard linear elasticity should be particularly prominent in small systems. This is indeed the case [8] for an ordered (lattice configuration) slab of particles resting on a rigid support (“bottom”) with a point force applied to the center particle at the “top” (motivated by experiments on granular systems [10,11]). A comparison of the stress field obtained at the bottom of slabs of different heights (number of layers of particles) with corresponding continuum elastic solutions [8] shows significant deviations, for a small number of layers. These deviations decrease as the size of the system increases, rendering continuum elasticity a good approximation for a sufficient number of layers [O(10)] in 2D, [O(60)] in 3D.

For disordered systems, this effect is even more pronounced, as elasticity sets in on larger coarse graining scales (which should be compared to the size of the system). An additional factor which is expected to influence the crossover to linear elasticity is a possible inhomogeneous stress in the reference state, as observed in [4] (in the examples presented here, the reference state is unstressed). In [4], a similar crossover has been observed for the vibrational modes of disordered systems, in which the strain is typically inhomogeneous. While not mentioned in [4], their results appear to suggest that the crossover is obtained for larger system sizes as the frequency (wavelength) is increased, i.e., as the strain gradients are larger, consistently with the above arguments.

The above considerations, as well as the theoretical calculations described in Sec. 3, suggest that the general constitutive description of the systems considered here, even for small deformations, should involve a non-local relation between the stress and the strain field, a leading approximation thereof being provided by gradient elasticity. Larger deformations should obviously require nonlinear elasticity.

While in granular matter, the interactions among the grains are not harmonic, we believe that the above discussion may still be relevant for quasi-static deformation of granular materials. First, the interactions are often described by elastic contact models for which the force-displacement law, even when nonlinear, may be linearized around a reference state (though to conform with the nature of cohesionless grains, the springs should be “one-sided”, i.e., allow for compressive forces only). A deformation under which the contact network does not change should then still be described by linear elasticity on sufficiently large scales. As the interactions among the grains are only compressive, some contacts may break under a given applied boundary conditions, yielding a modified contact network. For small deformations, the changes in this network may be sufficiently small for the elastic moduli not to be affected. When this is not the case, incremental elasticity, whereby the elastic moduli are modified by the deformation, may still be appropriate for describing the deformation. Furthermore, when the boundary conditions result in tensile stress components in a given region, contacts may break there preferentially in specific directions [13,13]. A similar type of stress-induced anisotropy has been suggested in the context of plastic models for soil mechanics [13]. Another source of deviations from elasticity is granular friction. Note, however, that static friction is not dissipative, and it may actually prevent the breaking of contacts, extending the elastic range of frictional systems with respect to the (idealized) frictionless case. Once the limit of static friction is exceeded, friction is kinetic and dissipation does occur. In this case one expects plastic failure, which is clearly beyond the limits of validity of elastic theory.

As a final remark, force chains, which have been observed in both experiments [14] and simulations [15] of granular materials, are also observed in elastic systems [4,12]. However, as shown in [4], force chains appear even in inhomogeneously strained lattices which are macroscopically isotropic, due to the inherent small-scale anisotropy of discrete systems. The corresponding stress field, even at small scales, does not exhibit similar structures in an isotropic system, i.e., force chains do not necessarily imply an inhomogeneous stress field.

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References

1. C. Kittel, Introduction to Solid State Physics (Second Edition) (Wiley, 1956); R. P. Feynman, R. B. Leighton, and M. Sands, The Feynman Lectures on Physics, Vol. II (Addison-Wesley, 1964); M. Born and K. Huang, Dynamical Theory of Crystal Lattices (Clarendon Press, 1954).
2. R. M. Nedderman, Statics and Kinematics of Granular Materials (Cambridge University Press, 1992); S. B. Savage, in Proc. NATO ASI on Physics of Dry Granular Media, Cargèse, France, 1997, edited by H. J. Herrmann, J. P. Hovi, and S. Luding, pp. 25–95, Kluwer, 1998.
3. J. Schiøtz et al., Phys. Rev. B 60, 11971 (1999); A. G. Khachatryan, S. Semenovskaya, and T. Tsakalakos, Phys. Rev. B 52, 15909 (1995); R. Lifshitz and M. L. Roukes, Phys. Rev. B 60, 5600 (2000).
4. J. P. Wittmer et al., cond-mat/0104509.
5. B. J. Glasser and I. Goldhirsch, Physics of Fluids 13, 407 (2001).
6. R. J. Bathurst and L. Rothenburg, J. Appl. Mech. 55, 17 (1988).
7. C.-L. Liao, T.-P. Chang, D.-H. Young, and C. S. Chang. Int. J. Solids and Structures 34, 4087 (1997).
8. C. Goldenberg and I. Goldhirsch, unpublished.
9. C. Goldenberg and I. Goldhirsch, cond-mat/0108297.
10. G. Reydellet and E. Clément, Phys. Rev. Lett. 86, 3308 (2001); D. Serero et al., Eur. Phys. J. E 6, 169 (2001).
11. J. Geng et al., Phys. Rev. Lett. 87, 035506 (2000).
12. S. Luding, Phys. Rev. E 55, 4720 (1997).
13. M. Oda, Mech. Mat. 16, 35 (1993).
14. A. Drescher and G. de Jesselin de Jong, J. Mech. Phys. Solids 20, 337 (1972).
15. P. A. Cundall and O. D. L. Strack, Geotechnique 29, 47 (1979); F. Radjai, S. Roux, and J. J. Moreau, Chaos 9, 544 (1999).