Why Effective Medium Theory Fails in Granular Materials

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Experimentally it is known that the bulk modulus K and shear modulus μ of a granular assembly of elastic spheres increase with pressure p faster than the $p^{1/3}$ law predicted by effective medium theory (EMT) based on Hertz-Mindlin contact forces. To understand the origin of these discrepancies, we perform numerical simulations of granular aggregates under compression. We show that EMT can describe the moduli pressure dependence if one includes the increasing number of grain-grain contacts with p. Most important, the affine assumption (which underlies EMT), is found to be valid for $K(p)$ but breaks down seriously for $\mu(p)$.

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The study of nonlinear elasticity and sound propagation in unconsolidated granular matter is a topic of great current interest [1]. In the simplest experiments, a packing of spherical glass beads is confined under hydrostatic conditions and the compressional and shear sound speeds, v_p and v_s, are measured as functions of static confining pressure p [2,3]. In the long-wavelength limit, the sound speeds are related to the elastic constants of the aggregate: $v_p = \sqrt{(K + 4/3\mu)/\rho^*}$ and $v_s = \sqrt{\mu/\rho^*}$, where ρ^* is the system's density. In a recent Letter [4], acoustic measurements were made on bead packs under uniaxial stress and it was suggested that long wavelength compressional waves can be described in terms of an effective medium. Thus, it would be of great value to have a reliable effective medium theory (EMT) to describe sound propagation as a function of applied stress. However, our analysis, together with the work of others, raises serious questions about the validity of the generally accepted theoretical formulation. The EMT [5] predicts that K and μ both vary as $p^{1/3}$ (see below), and that the ratio K/μ is a constant (independent of pressure and coordination number) dependent only on the Poisson's ratio of the grains.

Experimentally (see Fig. 1), the bulk and shear moduli increase more rapidly than $p^{1/3}$ and the values of K/μ are considerably larger than the EMT prediction. These discrepancies between theory and experiment could be due to the breakdown of the Hertz-Mindlin force law at each grain contact as proposed in Ref. [6] for the case of metallic beads with an oxide layer, and in Ref. [7] for grains with sharp angularities. Alternatively, they could be associated with the breakdown of some of the assumptions underlying the EMT, for example, that the number of contacts per grain is pressure independent, which may not be the case as several authors have suggested [7,8].

In this Letter we report calculations of $K(p)$ and $\mu(p)$ based on granular dynamics (GD) simulations using the discrete element method developed by Cundall and Strack [9,10] for an assembly of spherical soft grains which interact via the Hertz-Mindlin force laws. We find good agreement with the existing experimental data, thus confirming the validity of the Hertz-Mindlin contact theory to spherical grain packings. Further, we can explain the two problems with the EMT described above. First, if the calculated increase of the average coordination number with p is taken into account, the modified EMT gives an accurate description of $K(p)$ found in the simulations; for $\mu(p)$ we obtain a curve whose shape is in good agreement with the simulation data but whose values are seriously offset therefrom. Second, the EMT is based on the *affine* approximation in which the motion of each grain follows the applied strain. Physically, this approximation follows from the *well-bonded* assumption that two grains originally in contact remain in contact after an external load is applied. We show that, while this assumption is approximately valid for the bulk modulus, it is seriously in error for the shear modulus; this is why the EMT prediction of K/μ differs significantly from the experimental value.

Numerical Simulations.—At the microscopic level the grains interact with one another via nonlinear Hertz-Mindlin normal forces and transverse forces. Our

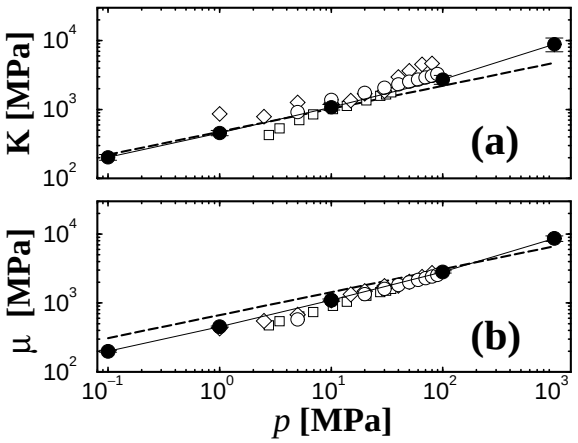

FIG. 1. Pressure dependence of the elastic moduli from GD (•), experiments [Domenico (□) [2], Yin (◇) [3], and ours (○)], and EMT equations (2a) and (2b) (dashed line): (a) bulk modulus and (b) shear modulus.

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approach is valid for grains in contact at a point which is not singular, and may not be applicable to packings of grains with sharp angularities, as may be present in many granular materials with a distribution of contact asperities. The normal force is $f_n = \frac{2}{3} C_n R^{1/2} w^{3/2}$ (the $3/2$ power law gives rise to the $p^{1/3}$ dependence of the moduli), and the transverse force is given as [11] $\Delta f_t = C_t (Rw)^{1/2} \Delta s$. Here the grain radii are R_1 and R_2, $R = 2R_1R_2/(R_1 + R_2)$, the normal overlap is $w = (1/2)\,[(R_1 + R_2) - |\vec{x}_1 - \vec{x}_2|] > 0$, where $\vec{x}_1$, $\vec{x}_2$ are the positions of the grain centers and $2s$ is the relative shear displacement between the two grain centers. The normal force acts only in compression, $f_n = 0$ when $w < 0$. $C_n = 4\mu_g/(1 - \nu_g)$ and $C_t = 8\mu_g/(2 - \nu_g)$, where μ_g is the shear modulus, and ν_g is the Poisson's ratio of the material from which the grains are made. In our simulations we set $\mu_g = 29$ GPa and $\nu_g = 0.2$. We assume a distribution of grain radii in which $R_1 = 0.105$ mm for half the grains and $R_2 = 0.095$ mm for the other half. Our results are, in fact, insensitive to the choice of the distribution, as long as the distribution is not very broad. We also include a viscous damping term to allow the system to relax toward static equilibrium.

Our calculations begin with a numerical protocol designed to mimic the experimental procedure used to prepare dense packed granular materials. In the experiments the initial bead pack is subjected to mechanical tapping and ultrasonic vibration in order to increase the solid phase volume fraction ϕ_s. The simulations begin with a gas of 10 000 spherical particles located at random positions in a periodically repeated cubic unit cell approximately 4 mm on a side. At the outset, the transverse force between the grains is turned off ($C_t = 0$). The system is then compressed slowly until a specified value of ϕ_s is attained (see dashed lines in Fig. 2). The compression is then stopped and the grains are allowed to relax. If the compression is stopped before reaching the critical volume fraction, $\phi_s \sim 0.64$, corresponding to random close packing (RCP) [1], the system will relax to zero pressure and zero coordination number, since the system cannot equilibrate below RCP. The compression is then continued to a point above the critical packing fraction and a target pressure is maintained with a "servo" mechanism [9] which constantly adjusts the applied strain until the system reaches equilibrium. Because there are no transverse forces, the grains slide without resistance during the relaxation process and the system reaches the high volume fractions found experimentally.

The simulated granular aggregate relaxes to equilibrium states in which the average coordination number $\langle Z(p)\rangle$, increases with pressure as seen in Fig. 2. For low pressures compared with μ_g, $\langle Z\rangle \approx 6$, while in two dimensions the same preparation protocol gives $\langle Z\rangle \approx 4$. Such low coordination numbers can be understood in terms of a constraint argument for frictionless rigid balls [12,13], which gives $\langle Z\rangle = 2\mathrm{D}$, where D is the dimension.

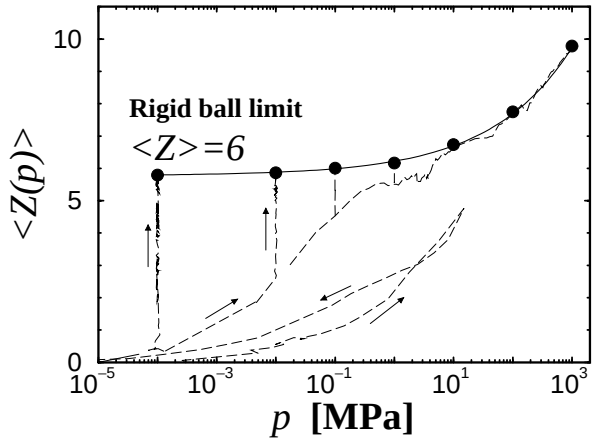

FIG. 2. Average coordination number $\langle Z\rangle$ from GD at a given pressure p (•). The dashed lines show the various out-of-equilibrium trajectories taken by the system to reach equilibrium as described in the text. The solid line is a fit according to Eq. (1).

These values should be valid in the limit of low pressure when the beads are minimally connected near RCP [13] (or in the rigid ball limit $\mu_g \to \infty$). For large values of p more grains are brought into contact, and the coordination number increases. Empirically, we find

$$\langle Z(p)\rangle = 6 + \left(\frac{p}{0.06\ \mathrm{MPa}}\right)^{1/3}. \qquad (1)$$

Comparison with Experiment.—Consider now the calculation of the elastic moduli of the system as a function of pressure. Beginning with the equilibrium state described above, we first restore the transverse component of the contact force interaction (finite C_t). We then apply an infinitesimal distortion, $\Delta\epsilon_{ij}$, and measure the linear response [14]. The shear modulus is calculated in two ways, from a pure shear test, $\mu = (1/2)\Delta\sigma_{12}/\Delta\epsilon_{12}$, and also from a biaxial test, $\mu = (\Delta\sigma_{22} - \Delta\sigma_{11})/2(\Delta\epsilon_{22} - \Delta\epsilon_{11})$. The bulk modulus is obtain from a uniaxial compression or tension test, $K + 4/3\mu = \Delta\sigma_{11}/\Delta\epsilon_{11}$. Here the stress σ_{ij} is determined from the measured forces on the grains [9], and the strain ϵ_{ij} is determined from the imposed dimensions of the unit cell.

In Fig. 1 our calculated values of the elastic moduli as a function of pressure are compared with EMT and with experimental data. Because there is a considerable degree of scatter in the experimental results we performed our own experiments with standard sound propagation techniques. A set of high quality glass beads of diameter 45 μm was deposited in a flexible container of 3 cm height and 2.5 cm radius. Transducers and a pair of linear variable differential transformers (for measurement of displacement) were placed at the top and bottom of the flexible membrane, and the entire system was put into a pressure vessel filled with oil. Before starting the measurements, a series of tapping and ultrasonic vibrations were applied to the container in order to let the grains settle into the best possible packing. We then

applied confining pressures ranging from 5 to 100 MPa. The pressure was cycled up and down several times until the system exhibited minimal hysteresis. At this point, shear and compressional waves were propagated by applying pulses with center frequencies of 500 KHz. The sound speeds and corresponding moduli were obtained by measuring the arrival time for the two sound waves.

From Fig. 1 we see that our experimental and numerical results are in reasonably good agreement. Also shown are measured data from Domenico [2] and Yin [3] for spherical glass beads. Clearly, the experimental data are somewhat scattered. This scatter reflects the difficulty of the measurements, especially at the lowest pressures where there is significant signal loss. Nevertheless, our calculated results pass through the collection of available data. Also shown in Fig. 1 are the EMT predictions [5]

$$K = \frac{C_n}{12\pi}(\phi_s Z)^{2/3}\left(\frac{6\pi p}{C_n}\right)^{1/3}, \tag{2a}$$

$$\mu = \frac{C_n + (3/2)C_t}{20\pi}(\phi_s Z)^{2/3}\left(\frac{6\pi p}{C_n}\right)^{1/3}. \tag{2b}$$

The EMT curves are obtained using the same parameters as in the simulations; we also set $Z = 6$ and $\phi_s = 0.64$, independent of pressure. At low pressures we see that K is well described by EMT. At larger pressures, however, the experimental and numerical values of K grow faster than $p^{1/3}$. The situation with the shear modulus is even less satisfactory. EMT overestimates $\mu(p)$ at low pressures but, again, underestimates the increase in $\mu(p)$ with pressure.

To investigate the failure of EMT in predicting the correct pressure dependence of the moduli, we plot $\mu/p^{1/3}$ in Fig. 3. For such a plot, EMT predicts a horizontal straight line but we see that the numerical and experimental results are clearly increasing with p. We can explain this behavior by modifying Eq. (2b) to take into account the pressure dependence of the coordination number $\langle Z(p)\rangle$ from Fig. 2 [Eq. (1)] and also $\phi_s(p)$ (which is a much smaller effect).

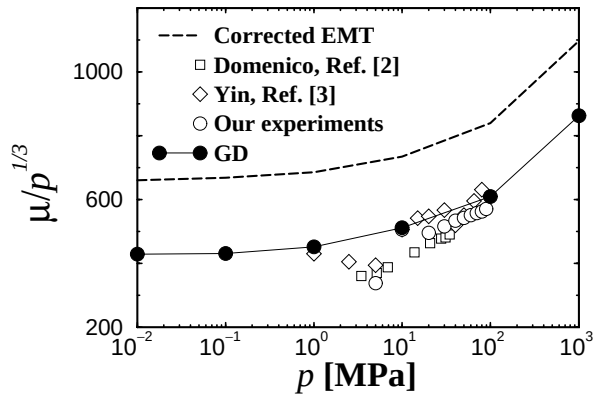

FIG. 3. Shear modulus from GD (•), experiments (open symbols as in Fig. 1), and corrected EMT (dashed line), taking into account the pressure dependence of $\langle Z(p)\rangle$ from Fig. 2 [Eq. (1)], as well as $\phi_s(p)$.

The modified EMT is also plotted in Fig. 3, and we see that it predicts the same trend with pressure as the simulations but has a significantly larger magnitude. The experimental data also seem to be following this trend but more data over a larger pressure range are clearly needed. Not shown in Fig. 3 is a similar analysis of $K(p)$, but the result is that the modified EMT is in essentially exact agreement with our numerical simulations. It is for this reason that we focus on $\mu(p)$.

To understand why μ is overpredicted by EMT we must examine the role of transverse forces and rotations in the relaxation of the grains. (These effects do not play any role in the calculation of the bulk modulus.) Suppose we redefine the transverse force by introducing a multiplicative coefficient α, viz., $\Delta f_t = \alpha C_t (Rw)^{1/2}\Delta s$; with $\alpha = 1$ we recover our previous results. To quantify the role of the transverse force on the elastic moduli, we calculate $K(\alpha)$ and $\mu(\alpha)$ at a given pressure $p =$ 100 KPa (Fig. 4a). Surprisingly, μ becomes negligibly small as $\alpha \to 0$. As expected, K is independent of the strength of the transverse force. To compare with the theory we also plot the prediction of the EMT [Eqs. (2a) and (2b)] in which C_t is rescaled by αC_t. We see that the EMT fails in taking into account the vanishing of $\mu(\alpha)$ as

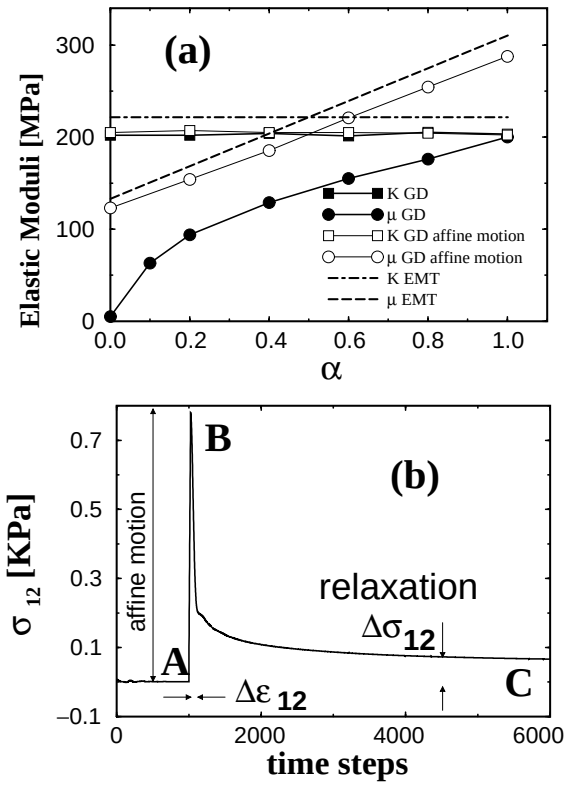

FIG. 4. (a) $K(\alpha)$ (squares), and $\mu(\alpha)$ (circles) versus α for a fixed $p(=$ 100 KPa) calculated from GD using only the affine motion (open symbols), and using the full relaxation [nonaffine motion (solid symbols)]. We also plot the corresponding EMT prediction, [Eqs. (2a) and (2b)], as dashed lines. (b) Relaxation of the shear stress ($B \to C$) after an affine motion ($A \to B$) in the calculation of the shear modulus.

$\alpha \to 0$. However, it accurately predicts the value of the bulk modulus, which is independent of α.

There are two main approximations in the EMT: (1) All of the spheres are statistically the same, and an isotropic distribution of contacts around a given sphere is assumed. (2) A sphere at position X_j is moved a distance δu_i in a time interval δt according to the macroscopic strain rate $\dot{\epsilon}_{ij}$: $\delta u_i = \dot{\epsilon}_{ij} X_j \delta t$ (affine approximation). The spheres are always at equilibrium due to the assumption of isotropic distribution of contacts, and further relaxation is not required.

In the GD calculation of the shear modulus an affine perturbation is first applied to the system. The shear stress increases instantaneously (from A to B in Fig. 4b), and the grains are out of equilibrium since the system is disordered. The grains then relax towards equilibrium (from B to C), and we measure the resulting change in stress from which the modulus is calculated. To better understand the approximations involved in the EMT, suppose we repeat the GD calculations, taking into account only the affine motion of the grains and ignoring the subsequent relaxation. The resulting values of the moduli are plotted in Fig. 4a as open symbols and we see that the moduli calculated in this way are very close to the EMT predictions. Thus, the difference between the GD and EMT results in shear lies in the relaxation of the grains, this difference being largest when there is no transverse force. As noted earlier, relaxation and rearrangement of the grains violate the well-bonded assumption which underlies EMT. By contrast, grain relaxation after an applied *isotropic* affine perturbation is not particularly significant, and the EMT predictions for the bulk modulus are quite accurate.

The surprisingly small value of μ found as $\alpha \to 0$ can be understood as a melting of the system that occurs when the system is close to the RCP fraction. This fluidlike behavior (when $C_t = 0$) is closely related to the melting transition seen in compressed emulsions [15] and foams [16]. At the RCP fraction the system behaves like a fluid with no resistance to shear. By contrast, molecular dynamics simulations of glasses, in which the atoms interact by purely longitudinal forces, predict nonvanishing shear speeds [17]. The crucial difference between these two systems is the local coordination of the particles. In the granular system, the coordination number near RCP (where the balls are nearly rigid) is $\langle Z \rangle = 6$; the system is quite tenuous. In glasses, however, the number of neighbors is closer to 10 and the motion of each grain is highly constrained, even for strictly longitudinal forces.

In conclusion, our GD simulations are in good agreement with the available experimental data on the pressure dependence of the elastic moduli of granular packings. They also serve to clarify the deficiencies of EMT. Grain relaxation after an infinitesimal affine strain transformation is an essential component of the shear (but not the bulk) modulus. This relaxation is not taken into account in the EMT. The failure of EMT is attributed to the fact that grains which are initially in contact at a given pressure can be separated under a shear perturbation, but they are likely to remain in contact under a compressional or tensional additional load. In the limit $\alpha \to 0$ a packing of nearly rigid particles responds to an external isotropic load (compression or tension) with an elastic deformation and a finite K [14]. By contrast, such a system cannot support a shear load ($\mu \to 0$) without severe particle rearrangements: The network supporting shear stress appears to be more tenuous than the network supporting compressional loads. This may indicate a "fragile" state of the system [18], where interparticle forces are organized along "force chains" (stress paths carrying most of the forces in the system) oriented along the principal stress axes. Such fragile networks support, elastically, only perturbations compatible with the structure of force chains and deform plastically otherwise. Clearly, there is a need for an improved EMT; recent work on stress fluctuations in minimally connected networks [12,13] may provide an alternative formulation and allow one to properly describe the linear response of granular materials.

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[1] *Powders and Grains 97*, edited by R. P. Behringer and J. T. Jenkins (Balkema, Rotterdam, 1997); *Physics of Dry Granular Matter*, edited by H. J. Herrmann, J.-P. Hovi, and S. Luding (Kluwer, Dordrecht, 1998).
[2] S. N. Domenico, Geophysics **42**, 1339 (1977).
[3] H. Yin, Ph.D. thesis, Stanford University.
[4] X. Jia *et al.*, Phys. Rev. Lett. **82**, 1863 (1999).
[5] K. Walton, J. Mech. Phys. Solids **35**, 213 (1987); P. J. Digby, ASME J. Appl. Mech. **48**, 803 (1981).
[6] P.-G. de Gennes, Europhys. Lett. **35**, 145 (1996).
[7] J. D. Goddard, Proc. R. Soc. London A, **430**, 105 (1990).
[8] P. A. Cundall, J. T. Jenkins, and I. Ishibashi, in *Powder and Grains 1989*, edited by J. Biarez and R. Gourvès (Balkema, Rotterdam, 1989); S. Roux, D. Stauffer, and H. J. Herrmann, J. Phys. **48**, 341 (1987).
[9] P. A. Cundall and O. D. L. Strack, Géotechnique **29**, 47 (1979).
[10] C. Thornton and D. J. Barnes, Acta Mech. **64**, 45 (1986).
[11] K. L. Johnson, *Contact Mechanics* (Cambridge University Press, Cambridge, England, 1985).
[12] S. F. Edwards and D. V. Grinev, Phys. Rev. Lett. **82**, 5397 (1999).
[13] S. Alexander, Phys. Rep. **296**, 65 (1998); A. V. Tkachenko and T. A. Witten, Phys. Rev. E **60**, 687 (1999).
[14] Since K and μ vanish as $p \to 0$, $\Delta\epsilon_{ij}$ (whether compression, tension, or shear) must also decrease in order to remain in the linear response regime at low p.
[15] M.-D. Lacasse *et al.*, Phys. Rev. Lett. **76**, 3448 (1996).
[16] D. J. Durian, Phys. Rev. Lett. **75**, 4780 (1995).
[17] G. S. Grest *et al.*, Phys. Rev. Lett. **49**, 1271 (1982).
[18] M. E. Cates *et al.*, Phys. Rev. Lett. **81**, 1841 (1998).