Vibrational Modes in Granular Materials

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It is argued that a proper description of the vibrational properties of systems comprised of solid spheres interacting via forces exerted at their points of contact must take account of the *rotational* motion of the individual grains. The spectrum obtained by coupling these additional degrees of freedom to the familiar translational motion is studied in both ordered and disordered packings and, in the latter case, used to interpret data on compressional- and shear-wave speeds in systems with pressure-generated contacts.

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In describing the vibrational properties of solids, one usually assumes that the sizes of the vibrating particles are negligible compared to typical distances between particles. (In the simplest case, a solid is pictured as an array of point masses connected by springs.) By contrast, our concern is with granular composites in which the mass is distributed uniformly over grains whose size and nearest-neighbor distance are roughly comparable. Perhaps the simplest example of such a system is a dense packing of spherical glass beads under hydrostatic confining pressure.[1] Such model systems are a useful starting point in the description of ocean sediments and sedimentary rocks.

In recent experiments, the acoustic properties of granular composites have been studied under a variety of conditions and over a wide range of frequencies.[1,2] In this Letter we show (1) that to understand the normal-mode spectrum in terms of intergrain contact forces, the rotational and translational degrees of freedom of the grains must be treated on an equal footing; (2) that reasonably straightforward methods can be used to describe the spectrum in the case of dense disordered packings; (3) that in the static limit, our results reduce to those obtained by previous workers[3,4]; and (4) that our predictions are consistent with data on the pressure dependence of compressional- and shear-wave speeds in systems comprised of spherical glass beads.[1]

The static properties of granular composites are usually described[3,4] in terms of Mindlin's analysis of the two-grain problem.[5] The central notion in Ref. 5 is that the intergranular force arises because of *relative* motion of the contact points on adjacent grains. In the case of pressure-generated contacts, the component of this motion *normal* to the contact plane will set up a compressional restoring force, while the component *parallel* to this plane will be opposed by static friction. Formally, each contact point is characterized by longitudinal ($D_\parallel$) and transverse ($D_\perp$) force constants and the intergrain force matrix is written as $D(\vec{R}_{ij}) = D_\parallel \hat{R}_{ij}\hat{R}_{ij} + D_\perp(\underline{1} - \hat{R}_{ij}\hat{R}_{ij})$. [Here $\vec{R}_{ij} = \vec{R}_i - \vec{R}_j$ and the force, $\vec{F}_i$, on the ith grain due to a displacement $\delta\vec{u}_j$ of the jth grain from its equilibrium position, $\vec{R}_j$, is $\vec{F}_i = D(\vec{R}_{ij})\cdot\delta\vec{u}_j$.] For the moment, let us assume that the grains are arranged on a *periodic lattice.* Given this expression for $D(\vec{R}_{ij})$, one might naively suppose that the spectrum could be evaluated by diagonalizing the matrix $[\omega^2\underline{1} - D(\vec{k})]$, where $D(\vec{k}) = \sum_j D(\vec{R}_{ij})\exp(i\vec{k}\cdot\vec{R}_{ij})$. This would be equivalent to the nearest-neighbor Born model with $\alpha \rightarrow D_\parallel$ and $\beta \rightarrow D_\perp$ [α (β) is the central (noncentral) force constant]. It is known, however, that the underlying potential energy is *not rotationally invariant.*[6] In our view, a satisfactory description of the dynamics of granular systems should take account of the most important new degrees of freedom associated with the finite size of the particles. Since the grains are essentially rigid bodies subjected to external forces and torques exerted at each contact point, the principal new degrees of freedom are associated with rotations of the individual grains. Our aim, then, is to treat systems where, in addition to a mass M and an infinitesimal displacement $\delta\vec{u}$, we associate with each "particle" a moment of inertia I and an infinitesimal rotation $\delta\vec{\theta}$.

To illustrate the new features of the normal-mode spectrum, let us begin by looking at *ordered* systems and by setting all of the displacements $\delta\vec{u}_i = 0$. In Fig. 1 we show that there are important effects associated with the local geometry of the lattice. In open structures it is possible to set up counterrotating modes in which, to first order, there is no relative motion of the contact regions on adjacent grains and, therefore, no cost in elastic energy. By contrast, in systems with closed paths containing an odd number of grains, such zero frequency modes are eliminated by frustration. Although we are principally interested in close-packed systems, one surprising feature of the spectrum in open structures is worth discussing. It might be thought that the fully compensated mode shown in Fig. 1(a) can be formed only at the corner of the Brillouin zone. It turns out, however, that coupling to the translational degrees of freedom can, in fact, *enhance* the occurrence of compensation phenomena. This effect is especially dramatic in the case of one dimension (e.g., a single row on the left-hand side of Fig. 1). Displacements along the chain do not interact with the coupled rotations and transverse motion. We assume that the intergrain force is proportional (with force constant $D_\perp$) to the relative displacement of adjacent contact points. Taking δu_i along the y axis and counterclockwise $\delta\theta_i$ as positive, the equations describing the coupled transverse motion are

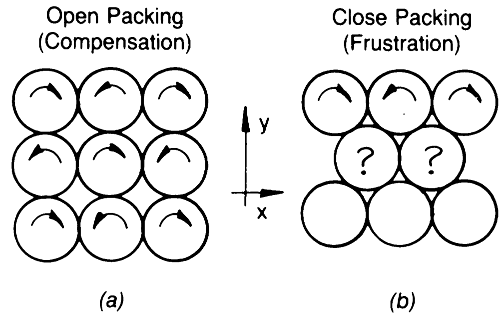

FIG. 1. Schematic illustration of pure rotational motion (i.e., $\delta\vec{u}=0$) in open and close ordered packings.

$$M\frac{d^2\delta u_i}{dt^2}=D_\perp\{(\delta u_{i-1}-\delta u_i)+(\delta u_{i+1}-\delta u_i)+R[(\delta\theta_{i-1}+\delta\theta_i)-(\delta\theta_{i+1}+\delta\theta_i)]\}, \tag{1a}$$

and

$$I\frac{d^2\delta\theta_i}{dt^2}=RD_\perp\{-R[(\delta\theta_{i-1}+\delta\theta_i)+(\delta_{i+1}+\delta\theta_i)]-(\delta u_{i-1}-\delta u_i)+(\delta u_{i+1}-\delta u_i)\}, \tag{1b}$$

where R is the grain radius. Invoking Bloch's theorem, the secular equation is

$$0=\omega^2\{\omega^2-\omega_0^2[\sin^2(ka/2)+\alpha\cos^2(ka/2)]\},$$

where $\omega_0^2=4D_\perp/M$ and $\alpha=MR^2/I$. Clearly, one solution is $\omega(k)=0$. (Physically, for each k, there is a balance between translation and rotation such that no relative motion of adjacent contact points is required.) Curiously, we note that for $\alpha=1$ (i.e., all the mass on the grain surface), the frequency of the upper branch turns out to be independent of k.

In two- and three-dimensional systems, the relative displacement of adjacent contact points must be treated as a vector and force constants associated with its components parallel ($D_\parallel$) and perpendicular ($D_\perp$) to the line joining the grain centers must be included in our description of the dynamics. The model potential energy is then

$$U=\tfrac{1}{4}\textstyle\sum_{ij}\{D_\perp[(\delta\vec{u}_i-\delta\vec{u}_j)-\tfrac{1}{2}(\delta\vec{\theta}_i+\delta\vec{\theta}_j)\times\vec{R}_{ij}]^2+(D_\parallel-D_\perp)[(\delta\vec{u}_i-\delta\vec{u}_j)\cdot\hat{R}_{ij}]^2\}. \tag{2}$$

(The factor $\frac{1}{2}$ multiplying the $\delta\vec{\theta}$ term appears because the grain radius $R=\frac{1}{2}|\vec{R}_{ij}|$.) As we noted earlier, without the $\delta\vec{\theta}$ term, our model reduces to the Born model with noncentral forces. In the case of (either ordered or disordered) close-packed structures the interaction of translational and rotational motion will not lead to the compensation effects discussed above. Using Eq. (2), we show, in Figs. 2 and 3, respectively, the exact spectrum computed along the [100] direction in an fcc crystal, and approximate dispersion relations (calculated by two methods) for a disordered packing. In both figures the upper (lower) longitudinal (L) modes correspond to pure rotational (translational) motion, while, as in the one-dimensional case, the two effects are coupled in the transverse (T) modes. Figure 2 serves to illustrate the unphysical behavior associated with the neglect of rotational motion. Setting $\delta\vec{\theta}_i=0$, the spectrum consists of the lower dashed T band and the lower L band which are *identical* for the special case $D_\parallel=D_\perp$ shown here: At long wavelengths the compressional- and shear-wave speeds are then equal, a result that is known to be inconsistent with continuum elasticity theory.[6] The solid curves in Fig. 3 are derived with use of a model pair distribution function to construct a spherically averaged secular equation. In an earlier paper[7] it was shown that this method reproduces the essential features of the normal-mode spectrum

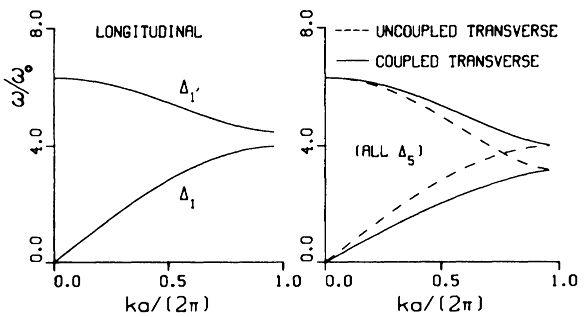

FIG. 2. Longitudinal and transverse modes in an fcc crystal. The upper (lower) uncoupled branch corresponds to motion with $\delta\vec{u}$ ($\delta\vec{\theta}$) set $=0$. Here $D_\perp = D_\parallel$, $I=\frac{2}{5}MR^2$, $2\sqrt{2}R=a$ (the cube edge), and $\omega_0^2 = 4D_\parallel/M$.

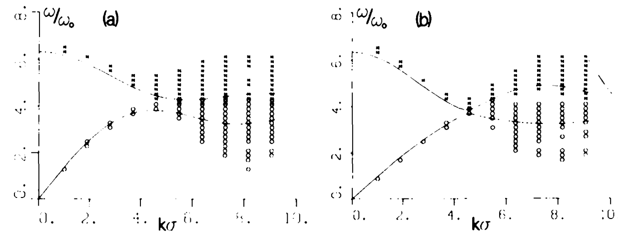

FIG. 3. (a) Longitudinal and (b) transverse dispersion relations in a disordered packing. The average coordination number and center-to-center grain separation are taken as $Z\approx 12$ and $\sigma \approx 2R$. The crosses and circles indicate the half-widths of the upper and lower peaks in the numerically computed spectral density functions.

in systems with purely longitudinal coupling between point particles. The vertical patterns in Fig. 3 are the results of machine simulations based on the application of the equation-of-motion method to a close-packed 500 site amorphous structure.[8] The general agreement between these two sets of calculations (for the disordered case) indicates that the averaged dynamical matrix again yields a reasonable picture of the average spectrum.

In the long-wavelength limit the dispersion relations shown in Figs. 2 and 3 can be related to expressions for static elastic coefficients obtained by previous workers. In the ordered case, the sound speeds along symmetry directions lead to relations between the elastic constants C_{ij} and the force constants $D_\parallel$ and $D_\perp$: $C_{11}=2C_{44}=(\sqrt{2}R)^{-1}[D_\parallel + D_\perp]$, and $C_{12}=(\sqrt{2}R)^{-1}[D_\parallel - D_\perp]$, obtained by Duffy and Mindlin.[3] In the disordered case, we find for the ratio of the sound speeds

$$\left[\frac{V_L}{V_T}\right]^2 = \frac{3[D_\parallel + 2D_\perp/3]}{[D_\parallel + 3D_\perp/2]} \leq 3 \tag{3}$$

which is equivalent to the results for the effective Lamé moduli derived by Digby.[4] We emphasize that, because of problems related to rotational invariance, the above results cannot be derived from the conventional continuum limit of the Born model. We have, however, formulated a more general theory in which one allows for two vector fields $\delta\vec{u}(\vec{r})$ and $\delta\vec{\theta}(\vec{r})$.[9] The underlying potential-energy density

$$U(\vec{r}) = \tfrac{1}{2}\{\textstyle\sum_{ij}(\lambda\epsilon_{ii}\epsilon_{jj} + 2\mu\epsilon_{ij}\epsilon_{ij}) + \nu|\delta\vec{\theta} - \tfrac{1}{2}\nabla\times\delta\vec{u}|^2\} \tag{4}$$

is positive definite and invariant under rigid rotations. Here ϵ_{ij} is the usual symmetric strain tensor, and λ, μ, and ν are generalized Lamé coefficients. The relevant long-wavelength equations are

$$\rho_I\omega^2\delta\vec{\theta} = \nu(\delta\vec{\theta} - \tfrac{1}{2}\nabla\times\delta\vec{u}), \tag{5a}$$

$$\rho_M\omega^2\delta\vec{u} = -(\lambda+2\mu)\nabla(\nabla\cdot\delta\vec{u}) + \mu\nabla\times(\nabla\times\delta\vec{u}) - \tfrac{1}{2}\nu\nabla\times(\delta\vec{\theta} - \tfrac{1}{2}\nabla\times\delta\vec{u}), \tag{5b}$$

where ρ_M and ρ_I are the mass and moment of inertia densities. [For the specific microscopic model defined by Eq. (2), the relations between $\{\lambda,\mu,\nu\}$ and $\{D_\parallel, D_\perp\}$ are given in Ref. 9.] Note that as $\omega \to 0$, Eq. (5a) leads to the condition $\delta\vec{\theta} - \frac{1}{2}\nabla \times \delta\vec{u} = 0$. [In the low-frequency transverse mode rotation and translation couple so as to guarantee, not that $\delta\vec{\theta}=0$, but that the *local torque* vanishes!]

For systems comprised of unconsolidated spherical grains under hydrostatic pressure, Mindlin[5] has calculated the dependence of the parameters $D_\parallel$ and $D_\perp$ on (1) the diameter, d, of the contact area (which increases with pressure) and (2) the elastic properties of the grain material (roughly independent of pressure). Since both $D_\parallel$ and $D_\perp$ turn out to be proportional to d, their ratio is independent of d and, therefore, of the confining pressure. It follows from Eq. (3) that $(V_L/V_T)^2$ should be independent of pressure and should have a value between 2.44 and 2.0 [under the assumption that $(D_\perp/D_\parallel)$ has a value between 0.33 and 1.0]. Experiments by Domenico[1] on disordered packings of spherical glass grains indicate that $(V_L/V_T)^2$

remains essentially constant (≈ 2.43) as the (hydrostatic) confining pressure is increased from 2.7 to 34.0 MPa. While the value 2.43 is somewhat high, the fact that the measured ratio does not vary with pressure is consistent with our Eq. (3) and Mindlin's argument that $D_{\parallel}$ and $D_{\perp}$ are both proportional to a single contact area.[10] Mindlin's work also indicates that, in the weak-contact regime, the ratio $(D_{\perp}/D_{\parallel})$ should be rather insensitive to the elastic properties of the material from which the individual grains are made. Further measurements on systems in which the composite geometries are similar, but the elastic properties of the grains vary greatly, would be useful in testing this prediction.

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[10]While our Eq. (3) is equivalent to Eq. (33) and Eq. (34) of Ref. 4, there is a significant point regarding the interpretation of $D_{\parallel}$ and $D_{\perp}$ on which we differ with Digby. Although he claims to be using Mindlin's results, Digby assumes that $D_{\parallel}$ and $D_{\perp}$ depend on *different* effective contact diameters ($d_{\parallel} = a$ and $d_{\perp} = b$) only one of which, $d_{\parallel}$, varies with pressure. Accordingly, his calculations indicate that $(V_L/V_T)^2$ should increase with pressure to the value 3.0 as the ratio $d_{\parallel}/d_{\perp}$ increases. This prediction is not consistent with the data presented in Ref. 1.