Nonlinear Dynamics in Granular Columns

Robert S. Sinkovits
Code 6410, Naval Research Laboratory, Washington, D.C. 20375-5344

Surajit Sen
Physics Department, State University of New York, Buffalo, New York 14260
(Received 16 May 1994)

Atomistic simulations of the vertical propagation of perturbations in deep gravitationally compacted granular columns characterized by the intergrain potential $V(\delta) \propto \delta^n$, with $n \gtrsim 2$ and δ the grain overlap, are shown to recover the results of elasticity theory for weak perturbations. For strong perturbations, the sound velocity $c_{\text{strong}} \to c_{\text{weak}}$ as $z \to \infty$ with the deviations from c_{weak} best expressed via a certain recursion relation in z. We predict that voids in real granular columns lead to $c \propto 1 - \epsilon$, when the void fraction ϵ is small, and show that the velocity power spectrum of a grain resembles that of a harmonic oscillator chain as $z \to \infty$.

PACS numbers: 46.10.+z, 03.20.+i, 62.30.+d

Nonlinear elasticity and sound propagation in dry granular columns at small strains [1–5] has received significant attention in recent years. The characteristic feature of vertical sound propagation in granular columns as predicted by elasticity theory, referred to in the literature as Hertzian contact theory [3,4,6], is that the sound velocity c scales as $z^{1/6}$, z being the depth. This power law behavior is obtained from the assumption that the grains interact via the well accepted potential for contact between noncohesive spheres $V(\delta) \propto \delta^{5/2}$ for $r < r_c$, with r_c the cutoff radius, 0 otherwise, where δ denotes the normal displacement of one grain against another [7].

This prediction is consistent with experimental results for c at *large* depths or pressures. Discrepancies between Hertzian theory and experiments, however, persist at *shallow* depths [5,6], and one must invoke altered contact mechanisms to explain shallower depth sound propagation [5]. In general, however, the elasticity theoretic treatment of sound propagation, while simple and appealing, is possibly inadequate for describing the propagation in *real* granular columns at shallow depths, in the presence of voids, and when perturbations of large magnitude are important.

In this Letter, we use molecular dynamics simulations to first recover and generalize the elasticity theory based predictions mentioned above for very deep 1D granular columns of $\sim 10^4$ grains. We then extend our study and consider the problems of real granular systems by addressing the deviations from the scaling law for large amplitude perturbations at shallow depths followed by an extension of the study to 2D columns with voids and the role of voids in modifying the scaling law for c. We close with calculations of the velocity power spectra of the grains at large depths which reveal that the grain dynamics at various depths can be related to the simpler problem of the dynamics of particles in a harmonic oscillator chain subjected to a weak linear field. Thus, the present Letter discusses a simple way to study the propagation of strong perturbations in real granular media in a highly nonlinear regime.

We model the granular material (GM) as a collection of spheres interacting as follows (for studies on the properties of GM with other potentials, see [8,9]):

$$V(\delta_{ij}) = \begin{cases} a\delta_{ij}^n, & r_{ij} \leq r_c\,, \\ 0, & r_{ij} > r_c\,, \end{cases} \tag{1}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the separation between grains i and j, $\delta_{ij} \equiv r_c - r_{ij}$ is the grain overlap, and r_c is the cutoff distance for the potential. $V(\delta_{ij})$ leads to a repulsive force between grains in intimate contact [7]. For noncohesive spheres, it can be shown that $n = 5/2$ [5]. For grains with conical imperfections, on the other hand, $n = 3$ [5]. We study the system for arbitrary n to recover and extend upon the scaling law for c at large z. In addition, we subject the grains to the gravitational force $\mathbf{F} = -mg\hat{\mathbf{z}}$, $\hat{\mathbf{z}}$ being the unit vector in the vertically upward direction and m the mass of the grain. In all of the simulations units are employed in which m and $2r_c$ are set equal to 1 and g is set equal to 0.01. The system dynamics is obtained by time integration of the coupled Newtonian equations of motion for a N [$\sim O(10^4)$] grain system via the third-order Gear algorithm [10] using a time step in the range 1.0×10^{-3} to 5.0×10^{-4}.

We first focus on pristine systems. Given that c depends sensitively on δ, care is taken to insure that the column is relaxed (to the extent possible in a numerical study) and is hence in its "ground state" thus possessing zero effective granular temperature (i.e., total kinetic energy ~ 0). This step is critical for the study of the perturbation that we initiate in the system (via a very low energy impact) to probe the nature of vertical sound propagation in granular columns. The method of determining the ground state is as follows. For a 1D system consisting of a single gravitationally compacted column, the location of the bottom grain is first fixed and the positions of the remaining grains are set such that the repulsive forces due to the overlap between

 0031-9007/95/74(14)/2686(4)$06.00

the adjacent grains exactly equal the forces required to support the grain column. For a system of N grains in which the bottom grain is labeled 1, the overlap between grains i and $i+1$ is determined via the 1D sum rule $g\sum_{j=i+1}^{N} m_j = an\delta_{i,i+1}^{n-1}$. For the 2D case, the initial configuration is taken as the gravitationally compacted perfect triangular lattice. The coordinates of the bottom row of grains are fixed and periodic boundary conditions are imposed in the horizontal direction. In most of the 2D simulations, a large height to width aspect ratio ≥ 1000 was chosen. In complete analogy with the 1D systems, the overlap between the grains in adjacent rows is determined via the 2D sum rule $g\sum_{j=i+1}^{N} m_j = an\delta_{i,i+1}^{n-1}\sqrt{1 - 1/(2 - 2\delta_{i,i+1}/r_c)^2}$ for $\delta_{i,i+1}$. The 2D sum rule is obtained by allowing the separation between grains in adjacent rows to be reduced from r_c to $r_c - \delta$ so that the z components of the intergrain forces balance the weight of the supported column, while the distances between grains in the same row are kept constant. The separation between adjacent rows i and $i+1$ is then reduced from the uncompacted triangular lattice row separation by the amount

$$\Delta z = \frac{\sqrt{3}}{2} r_c \left[1 - \sqrt{1 - \frac{4}{3r_c}(2r_c\delta - \delta^2)} \right].$$

For the weakly disordered system, starting from the equilibrium configuration for the gravitationally compacted 2D triangular lattice, we remove the grains in a "semirandom fashion," i.e., a grain is removed from a randomly chosen site for every i rows. The configuration thus obtained, though significantly ordered in the sense that each grain still very nearly resides at a perfect triangular lattice site, possesses considerable disorder in the force network. The removal of grains using the above mentioned procedure allows one to tune the porosity and the degree of disorder in the system. The simulations were limited to cases with up to 12.5% of the grains removed (i.e., up to void concentrations of 12.5%). Upon removal of the grains from the lattice, the system is no longer in its ground state. Obtaining the new global ground state would require relaxing the system until all of the voids were filled and the compacted triangular lattice was recovered. Instead, we wanted to obtain a metastable state in which the energy is at a local minimum and the voids are trapped in the lattice. We have tried several approaches to find the metastable configuration. Although it is not the only viable approach, we found that integrating the Newtonian equations of motion with an additional time-dependent viscous damping term of the form $\mathbf{F}_v = -b(t)\mathbf{v}$ is an efficient way to relax the system into a metastable configuration in which the positions of the voids are preserved and the effective granular temperature does not rise significantly after the viscous damping is turned off.

In all of the simulations, the sound speed was determined by monitoring the position of the weak perturbation in the column as a function of time. The perturbation was initiated at time $t = 0$ by imparting an initial downward velocity to the top particle or row of particles. For the *pristine* 1D and 2D systems, initiating the weak perturbation in this manner results in a spatially well-defined pulse that travels downward through the column. Although there was some tendency for the pulse to broaden slightly over time, the shape of the pulse remains approximately invariant over the course of the simulation. The location of the pulse was defined by the position of the particle or row of particles with the highest velocity, and its local speed was determined from the time derivative of pulse location. To simplify the analysis of the results, the system parameters were chosen so that the density of the column as a function of depth does not change significantly due to compaction. This requires that $\delta_{1,2} \ll r_c/2$, or in terms of the system parameters $(mgN/an)^{1/(n-1)} \ll r_c/2$. Since sound speed scales as $c \sim \sqrt{\mu/\rho}$ [7], μ being the bulk modulus, and ρ being the density, variations in c as a function of depth in the column are due entirely to changes in the stiffness of the system.

We have performed the simulations for a family of potentials with a set of values for n in Eq. (1), and for a set of magnitudes of the initial perturbations, v_{impact}. Although experimental and theoretical works indicate that the potentials that best describe real systems are $V(\delta) \sim \delta^{5/2}$ for contact between perfect spherical grains and $V(\delta) \sim \delta^3$ for contact between grains with conical imperfections, calculations were carried out using a range of exponents from $n = 5/2$ to $n = 10$ in order to study the power law dependence of sound speed as a function of depth and deviations from the predictions of the theory. The results of these calculations are plotted in Fig. 1 for $n = 5/2$ and $n = 6$. For small v_{impact}, c_{weak} determined from the 1D simulations scaled with depth as $c_{\text{weak}} \sim z^{[1-1/(n-1)]/2}$. At higher v_{impact} and small z, we saw large deviations from the above law, with the deviation increasing with v_{impact}. In these studies, c_{strong} does not show a simple power law behavior (i.e., $z^{1/6}$ or like) until greater depths are reached where it asymptotically approaches that found in the low v_{impact} studies. c_{strong} increases more slowly with z than $z^{1/6}$ for small z (see Figs. 1 and 3). The relative difference between c for large v_{impact} and $v_{\text{impact}} \to 0$ can be defined as $\xi(z) \equiv (c_{\text{strong}} - c_{\text{weak}})/c_{\text{weak}}$. A functional form for $\xi(z)$ is expected to decrease monotonically as z increases and show the limiting behaviors $\lim_{z\to 0}\xi(z) \to \infty$ and $\lim_{z\to\infty}\xi(z) \to 0$.

Having attempted many different functional forms to fit $\xi(z)$ we conclude that $\xi(z)$ does not follow a simple power law behavior. The results of nonlinear curve fitting show that the functional form of $\xi(z)$ is well approximated by a function in z which is best expressed as $\sum_{k=-\infty}^{+\infty} b_k \exp(-d_k z)$ where the coefficients b_k and d_k follow the recursion relations $b_{k+1} = b_k\alpha$ and $d_{k+1} = d_k\beta$ with α and β constants that depend on the choice of system parameters. As an example, a best fit of $\xi(z)$ over the range $100 < z < 10\,000$ for $v_{\text{impact}} = 1.0$ and $n = 3$ to a triple exponential function gives

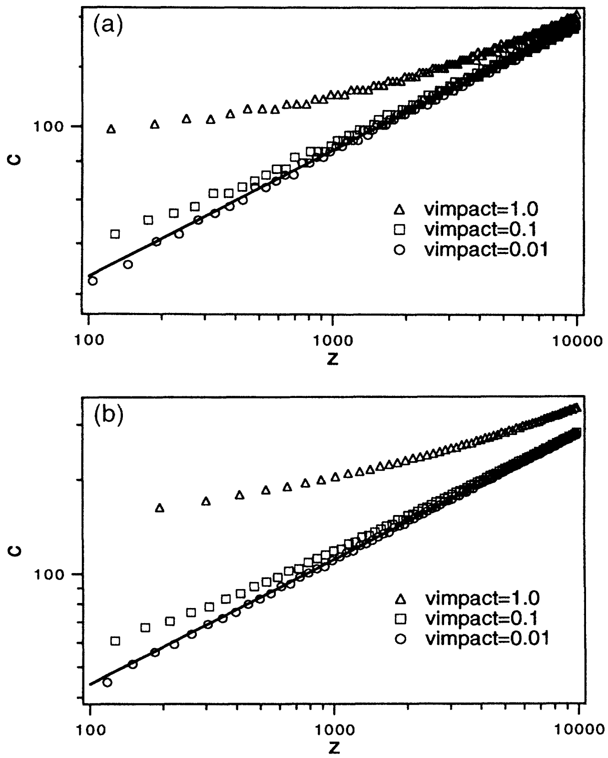

FIG. 1. Speed of vertical disturbances in 1D columns for (a) $n = 5/2$ and (b) $n = 6$. Solid lines show scaling behavior predicted from generalized Hertzian contact theory. Slopes of lines in (a) and (b) are 1/6 and 2/5, respectively.

the result $\xi(z) = 0.041\,07 + 0.2519\exp(-0.000\,3244z) + 0.4527\exp(-0.001\,911z) + 0.8019\exp(-0.010\,19z)$, which has four parameters. For this case $\alpha \simeq 1.8$ and $\beta \simeq 5.8$. α and β are both greater than unity, insuring that $\xi(z)$ converges for all $z > 0$ and diverges at $z = 0$. Although α and β depend on v_{impact} and n, in all cases studied both quantities are found to be greater than 1. It is reasonable to argue that at each value of z, as the strong perturbation propagates progressively downward, some energy goes to promote local excitations. It follows then that as $z \to \infty$ this energy loss becomes vanishingly small. Our calculations suggest that the origin of the above recursion relation lies in this iterative process. At this time we are unable to provide a simple explanation for the above functional form for $\xi(z)$ for this highly nonlinear process.

Typical velocity power spectra for grains at five different depths in the 1D column during the passage of a vertical disturbance are shown in Fig. 2. As one goes deeper and deeper into the column, one finds that the grains are more strongly confined to their equilibrium positions and that their velocity power spectra approach that of a mass in an infinite harmonic oscillator chain [11,12]. For a deep lying grain the total force on the grain is approximately $\mathbf{F} = a(\delta - dz)^{n-1} - a(\delta + dz)^{n-1} - mg$, where dz is the displacement of the grain from its equilibrium

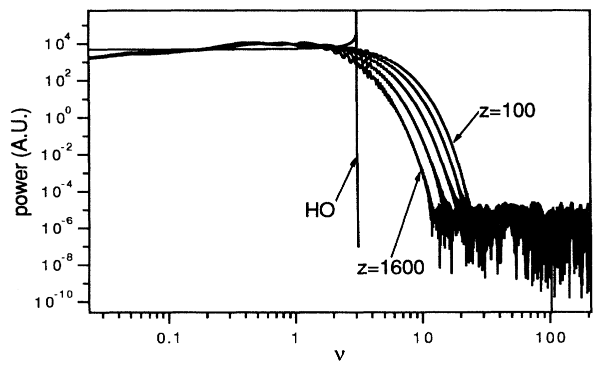

FIG. 2. Velocity power spectra for grains at five different depths, $z = 100$, 200, 400, 800, and 1600, in a 1D column due to passage of vertical disturbance. Shown for comparison is the velocity power spectrum for a particle in an infinite harmonic oscillator chain. The system parameters are $n = 5/2$ and $v_{\text{impact}} = 0.05$.

position. The leading term in a power series expansion of the force about $dz = 0$ is $-2a(n - 1)\delta^{n-1}dz$, hence for a strongly confined grain in the limit of small amplitude oscillations the behavior approaches that of a harmonic oscillator.

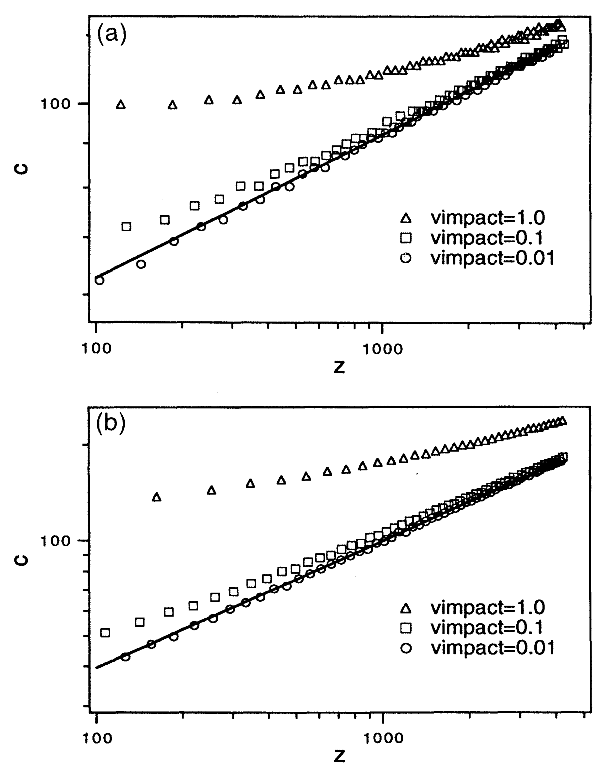

FIG. 3. Speed of vertical disturbances in 2D columns for (a) $n = 5/2$ and (b) $n = 6$. Solid lines show scaling behavior predicted from generalized Hertzian contact theory. Slopes of lines in (a) and (b) are 1/6 and 2/5, respectively.

To understand the behavior of c_{strong} let us return to the Hertzian contact theory in which $c_{\text{weak}} \sim \sqrt{k}$, $k = df/d\delta$, $f \sim \delta^{n-1}$ for $V(\delta) \sim \delta^n$, $n \geq 2$. In this theory, one assumes that although k is a function of z or P it is essentially constant during the passage of a perturbation. This assumption fails for large perturbations and hence c_{strong} does not scale with z as c_{weak} does. To study $c_{\text{strong}}(z)$ one must therefore solve for $\delta(t)$ in $d^2\delta/dt^2 = -an\delta^{n-1}$ subjected to appropriate initial conditions on δ. For fixed total energy, knowledge of $\delta(t)$ and hence of $V(t)$ will yield information about $v_i(t)$ of the individual grains, which in turn will yield the behavior of c_{strong} as a function of z.

The results of calculations on 2D systems are consistent with those from the 1D simulations. The same scaling of sound speed on depth and deviations from the generalized Hertzian theory for strong perturbations are observed in the 2D calculations. The results of the 2D simulations on the systems without voids are shown in Fig. 3. We find that in the limit of weak perturbation $c_{\text{weak}} \propto P^{[1-1/(n-1)]/2}$ in pristine 2D systems (see Fig. 3), while $c \propto (1-\epsilon)P^{[1-1/(1-n)]/2}$ for weakly disordered 2D systems with void fractions of up to 12.5% (see Fig. 4). The main difference between the perfect and perturbed systems is that in the 2D systems, with voids, inhomogeneities in the force network lead to a significant transfer of energy from the coherent elastic disturbance into the random motion of the particles. Figure 5 shows the average grain kinetic energy as a function of z for a system with 3.3% void fraction. With the exception of the strong dissipation of the pulse in the topmost, loosely packed layers of the system, the details of the sound propagation in the 2D systems with and without voids are unchanged. On the basis of our calculations for 2D columns, we find it reasonable to expect similar behavior for close-packed (hcp) 3D systems. The issue of sound propagation in both close-packed and randomly packed 3D columns will be addressed in the future to definitively answer this point.

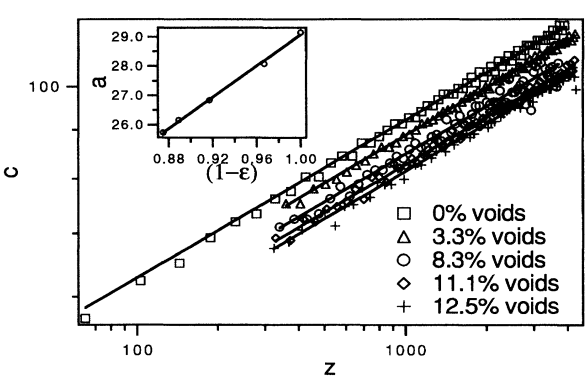

FIG. 4. Speed of vertical disturbances in 2D columns with voids for $n = 5/2$ in the limit of weak impact. Solid lines are the best fits of the data to the functional form $c = az^b$. Inset shows the prefactor a plotted against $1-\epsilon$ illustrating linear dependence of c on void fraction.

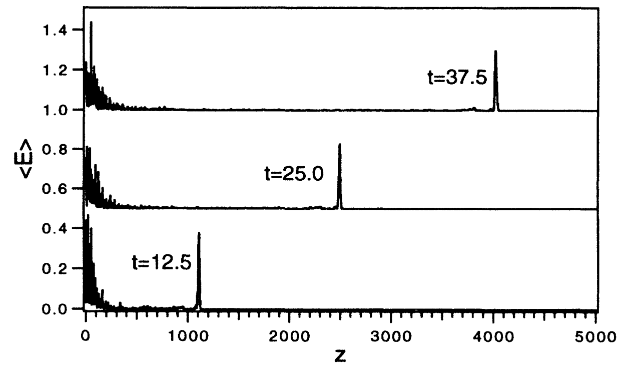

FIG. 5. Average kinetic energy as a function of depth for sound propagation in 2D column with 3.3% void fraction, $v_{\text{impact}} = 0.1$ and $n = 2.5$.

In conclusion, we have performed molecular dynamics simulations to recover the elasticity theory based result $c_{\text{weak}} \sim P^{1/6}$ at large depths from microscopic considerations. Our approach allows us to probe new issues with regard to the propagation of perturbations in real granular columns. These issues are (i) propagation of weak perturbations in shallow depths, (ii) propagation of strong perturbations at all depths, and (iii) propagation of weak perturbations in granular columns with voids. In addition, we argue that the velocity power spectra of grains at large depths can be understood by studying the velocity power spectrum of particles in a harmonic oscillator chain.

We thank Professor J. T. Jenkins, Dr. Elaine Oran, and Mark Wedloe for valuable conversations. R. S. S. was supported by an ONR postdoctoral fellowship and by DARPA. S. S. acknowledges support of the Physics Department at SUNY, Buffalo.

[1] H. M. Jaeger and S. R. Nagel, Science **255**, 1523 (1992).
[2] C-h. Liu and S. R. Nagel, Phys. Rev. Lett. **68**, 2301 (1992); Phys. Rev. B **48**, 15 646 (1993).
[3] P. J. Digby, J. Appl. Mech. (ASME) **48**, 803 (1981).
[4] K. Walton, J. Mech. Phys. Solids **35**, 213 (1987).
[5] J. D. Goddard, Proc. R. Soc. London A **430**, 105 (1990).
[6] J. Duffy and R. D. Mindlin, J. Appl. Mech. (ASME) **24**, 585 (1957).
[7] A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity* (Dover, New York, 1944), 4th ed.; K. L. Johnson, *Contact Mechanics* (Cambridge Univ. Press, Cambridge, 1985).
[8] P. A. Thompson and G. S. Grest, Phys. Rev. Lett. **67**, 1751 (1991).
[9] S. Sen, N. Mousseau, and G. Overney, Phys. Rev. E **49**, 4712 (1994).
[10] C. W. Gear, *Numerical Initial Value Problems in Ordinary Differential Equations* (Prentice-Hall, Englewood Cliffs, 1971).
[11] M. H. Lee, J. Florencio, Jr., and J. Hong, J. Phys. A **22**, L331 (1989).
[12] S. Sen and R. Sinkovits (to be published).