Sound propagation in impure granular columns

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We present a detailed simulational study of the vertical propagation of *weak* and *strong impulses* in deep gravitationally compacted granular columns [see R. S. Sinkovits and S. Sen, Phys. Rev. Lett. **74**, 2686 (1995)]. The intergrain potential is assumed to be $V(\delta)\sim\delta^n$, $n\geqslant 2$, where δ is the overlap between the grains. Due to gravitational compaction, the magnitude of the overlap between the grains increases progressively with increasing depth. Therefore the sound velocity increases as an impulse travels vertically downward into a granular column. For *weak* impulses, our large scale simulational studies show that the sound velocity $c_{\rm weak} \propto z^{[1-1/(n-1)]/2}$, where z is the depth at which $c_{\rm weak}$ is measured. This result, which has been obtained from particle dynamical studies, is in perfect agreement with the predictions based upon elasticity theory. We then extend our analysis to show that (i) for columns with small void fractions, ϵ, $c_{\rm weak}\propto(1-\epsilon)z^{[1-1/(n-1)]/2}$ and (ii) for *large amplitude* impulses, the velocity of the perturbation $c_{\rm strong}$ behaves very differently compared to $c_{\rm weak}$ at shallow depths with $c_{\rm strong}\rightarrow c_{\rm weak}$ as $z\rightarrow\infty$. We also present a detailed numerical study of the velocity power spectra of the individual grains as a function of depth z. We close with a discussion of the effects of both light and heavy impurities on the vertical sound and shock propagation. [S1063-651X(96)04312-7]

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I. INTRODUCTION

The study of granular systems is a relatively new and developing research area that draws heavily from nonlinear dynamics, statistical physics, condensed matter physics, materials science, mechanics, and mechanical engineering [1–5]. While a significant body of literature [6] exists on the structural and the dynamical properties of granular systems using the ideas of continuum mechanics and fluid dynamics [7–10], much less appears to be known from the standpoint of microscopic grain dynamics [11–13].

The primary advantage of the latter approach lies in the possibility of understanding the dynamics of macroscopic granular beds and piles starting from Newtonian (or Newtonian-like) dynamics at the level of individual grains [11,12]. This microscopic approach allows one the flexibility to investigate the effects of modeling various granular beads with appropriate potentials to describe them and with simple and realistic constraints such as friction laws, etc. on the resultant dynamical equations. Further, given the fact that the intergrain interactions occur only when the grains are in contact, the ready availability of powerful workstations currently allows one to study the dynamics in compacted granular beds in meticulous detail with at least as many as 10 000 grains and often with many more [12,14,15]. Thus one can carry out subcontinuum and continuum level simulations for such granular systems with a modest amount of computational resources.

A characteristic feature of these systems, as briefly mentioned above, is that the grains, which are macroscopic (typically with radius $\sim$1mm, mass $\sim$0.1 g), interact with each other repulsively only upon contact and are noninteracting otherwise [11,12,14–16]. Being macroscopic, the grains are also strongly sensitive to gravity. Granular systems are hence excellent examples of many particle systems which are strongly affected by an external field [15,17]. Hence it is natural to expect that the grain piles will be loosely packed near the surface and progressively densely packed as one considers their packing at larger depths [14]. Detailed theoretical and experimental studies on the stress networks in uncompacted granular skeletons have recently been carried out by Liu *et al.* [18]. A consequence of this property concerning the packing of grain piles is that at sufficient depths, the following feature is found: an impulse, such as a sound wave, travels progressively faster at increasing depths [14,16].

Until now, the increase in sound speed as a function of depth has been analyzed in terms of the Hertzian contact theory, which is a long wavelength treatment [16]. Such an approach is, however, of limited value when one considers the fact that the small length scale structure of granular media often exhibits voids and mass mismatches which may locally affect the propagation of weak and strong impulses significantly at shallow depths [14,19]. The present study considers such propagation along the vertical direction in granular media, more specifically, in granular columns. The studies have been carried out using the molecular dynamics simulation technique [20]. The advantage of approaching the problem of sound and shock propagation in this manner lies in the fact that one can build the details of the microstructure in the granular media into the study. For sufficiently deep columns and weak impulses, typically, with depth $z\sim10^3$ grain diameters or more, one recovers the behavior predicted by Hertzian contact theory, i.e., continuum physics is recovered [14]. The behavior of large amplitude impulses or ''shocks'' is more complex. The present study also addresses the propagation of such shocks.

Nonlinear elasticity and sound propagation in dry granular columns at small strains [1,16,21–23] has received some attention in recent years. The characteristic feature of vertical sound propagation in granular columns as predicted by the Hertzian contact theory [22–24] is that the sound velocity c scales with depth z as $z^{1/6}$. This power law behavior is obtained from the assumption that the grains interact via the well-accepted potential for contact between noncohesive spheres (which constitute a granular system), $V(\delta)\propto\delta^{5/2}$, $r<r_c$, r_c is the cutoff radius and is 0 otherwise, where δ denotes the normal displacement of one grain against another [see Eq. (1) below] [25].

The above prediction concerning sound speed is consistent with the experimental results for the sound velocity at *large* depths or pressures. As alluded to above, discrepancies between the predictions of the Hertzian contact theory and the experiments, however, persist at *shallow* depths [16,24]. It is recognized that an understanding of the scattering processes associated with acoustic propagation at shallow depths holds the key to the development of the science and technology associated with the implementation of sonic probes to explore underground objects such as solid inclusions buried within a dry granular medium [19]. Hence it is of significant interest to acquire a broader understanding of sound and shock propagation at all depths.

The purpose of this article is to report a detailed study on the propagation of both small amplitude (sound) and large amplitude (shock) perturbations as they propagate through shallow as well as large depths. We shall also consider the effects of microstructure due to the presence of voids and of light and massive impurities on such propagation. The model granular systems are intentionally chosen to be very simple. Future studies will consider the effects of richer structural features of granular systems [26].

The details of the models studied, of the molecular dynamics simulations, and of the technical aspects of the simulations are presented in Sec. II. The results of our study are presented in Sec. III. We use molecular dynamics simulations to first recover the elasticity theory based predictions mentioned above for very deep and pristine one- and two-dimensional granular columns of $\sim 10^4$ grains (Sec. III A). We then extend the existing understanding to the case of the vertical propagation of large amplitude perturbations or ''shocks'' in the pristine granular columns. In Sec. III B we consider the effects of voids (as measured using ϵ as the void fraction) in the two-dimensional columns on the behavior of sound velocity c as a function of the depth z. Section III C focuses on the effects of heavy and light mass impurities in the granular columns. Section IV closes with a summary of the work and the direction of ongoing and future research.

II. THE MODEL AND THE SIMULATIONS

A. The model potential

We model the granular medium as a collection of disks interacting via the following well-accepted grain-grain potential [16] (for studies on the properties of granular materials with other potentials, see [11,12]):

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

where $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$ is the separation between grains i and j, $\delta_{ij}\equiv r_c-r_{ij}\equiv$ grain overlap, and r_c is the cutoff distance for the potential. $V(\delta_{ij})$ leads to a repulsive force between those grains which are in intimate contact [16,25]. In this study we shall consider grain-grain distances which are more than $r_c/2$, i.e., we shall not address the behavior of the granular system under extremely strong compaction.

For noncohesive spheres, it can be shown that $n=\frac{5}{2}$ [16] in Eq. (1). For grains with conical imperfections on the other hand, $n=3$ [16]. We shall study the two-dimensional system for arbitrary n to recover and extend upon the scaling law for c at large z obtained from Hertzian contact theory based analysis [16]. It is possible to extend our numerical calculations to three-dimensional systems. However, such studies are strongly computationally intensive. The behavior of sound and shock propagation may not be very different for pristine two- and three-dimensional granular columns. This somewhat rash claim is backed up by the excellent agreement between our numerical studies in two dimensions and the Hertzian contact theory based analysis which is, in general, valid for a three-dimensional system in the long wavelength regime [14]. 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 1.0 and g is set equal to 0.01. Choosing a small value of g allows us to probe the effects of gravity in compressing the grain column as it develops over an extended length scale. The system dynamics is obtained by time integration of the coupled Newtonian equations of motion for an N [$\sim O(10^4)$] grain system via the third-order Gear algorithm [20,27] using a time step in the range 1.0×10^{-3} to 5.0×10^{-4}. The large length scale involved in this study allows us to probe phenomena at continuum length scales [29]. Choosing a smaller time step does not significantly affect the accuracy of the calculations reported here. In comparative terms this is a rather large time step for a molecular dynamics based study [28]. The reasons why these time steps work very well are (i) the ground state of a close packed or nearly close packed grain column is well known and is built into the initial conditions that characterize the grain column and (ii) the amplitude of motion of individual grains is typically of the order of a fraction of the grain diameter. Given the fact that granular systems are inherently metastable [15,30], the dynamical behavior of a granular column is strongly sensitive to its proximity to the lowest energy structure during the passage of both weak and large amplitude impulses.

B. The preparation of pristine granular columns

We first focus on pristine granular columns [see Fig. 1(a)]. The detailed calculations for these systems are presented in Sec. III A. Given that the sound velocity c depends sensitively on δ, care is taken to ensure that the column is relaxed (to the extent possible in a numerical study) and is hence in its ''ground state.'' Thus the model system possesses zero effective granular temperature (i.e., total kinetic energy ~ 0). This step is critical for the study of the perturbation that we initiate into the system via a very low energy

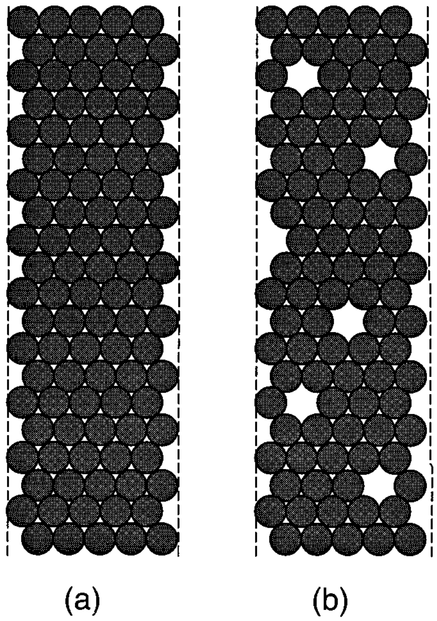

FIG. 1. (a) A pristine two-dimensional granular column. (b) A column with randomly distributed voids as discussed in Sec. II C.

impact at the top of the grain column to probe the nature of vertical sound propagation in granular columns.

The method of determining the ground state of the granular column can be described as follows. For a one-dimensional system consisting of a single gravitationally compacted column, the location of the bottom grain is first fixed. The positions of the remaining grains are then set such that the repulsive forces due to the overlap between 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 one-dimensional sum rule

$$g\sum_{j=i+1}^{N} m_j = an\,\delta_{i,i+1}^{n-1}. \tag{2}$$

For the two-dimensional 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 two-dimensional simulations, a large height to width aspect ratio $\geqslant 1000$ was chosen. In complete analogy with the one-dimensional systems, the overlap between the grains in adjacent rows is determined via the corresponding two-dimensional sum rule

$$g\sum_{j=i+1}^{N} m_j = an\,\delta_{i,i+1}^{n-1}\sqrt{1-1/(2-2\,\delta_{i,i+1}/r_c)^2} \tag{3}$$

for $\delta_{i,i+1}$. The two-dimensional 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

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

C. Preparation of the granular columns with voids and mass impurities

To prepare a weakly disordered system with a small density of voids we proceed as follows [see Fig. 1(b)]. Starting from the equilibrium configuration for the gravitationally compacted two-dimensional 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%). It is difficult to stabilize a column with a significantly higher void density even though we have chosen a relatively small value of g $(=0.01)$ for our studies. Such systems, typically, tend to reorganize themselves to lower their energies.

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 [see Fig. 1(b)].

The preparation of granular columns with mass defects was done in a very similar fashion except that there are no limits on the fraction or placement of the mass defects. While the inclusion of mass defects result in local inhomogeneities in the intergrain force network, all grain contacts are still present and there are no instabilities in the two-dimensional column.

D. Calculation of the speed of sound

In all of our 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 grain or row of grains. For the *pristine* one- and two-dimensional systems, initiating the weak perturbation in this manner results in a spatially well-defined pulse that travels downward through the column (see Fig. 2). Although there

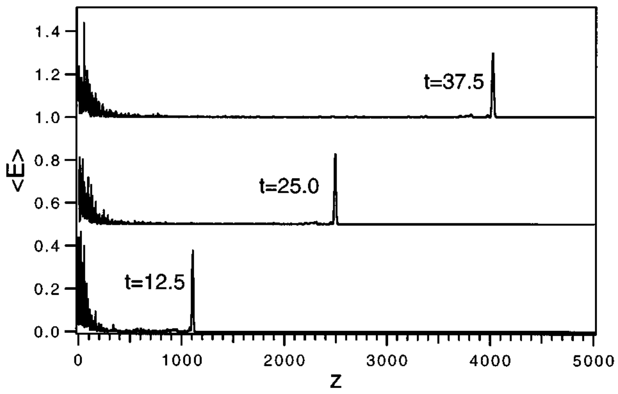

FIG. 2. Average kinetic energy as a function of depth for sound propagation in two-dimensional column with 3.3% void fraction, $v_{\mathrm{impact}}=0.1$, and $n=5/2$.

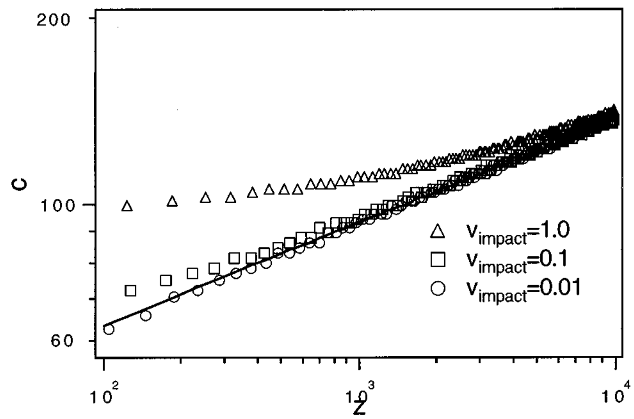

FIG. 3. Speed of vertical disturbances as a function of depth, c vs z, with the solid line showing the scaling law predicted by Hertzian contact theory. The calculations have been done for $n=5/2$ in one dimension. The slope is 1/6.

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 the local speed was determined from the time derivative of pulse location.

It may be noted that some years ago Nesterenko [31] and independently, Miller [32], theoretically studied the general problem of propagation of a compression pulse in granular and porous media. The work of Miller, which was an extension of Nesterenko's study, revealed that a propagating compression pulse is analogous to a solitonic excitation as it travels along a linear chain of spherical particles in the absence of gravity. Our analysis is similar to that of Miller's except for the fact that we consider gravitational compaction in our system. The slight broadening in the shape of the pulse in our problem is indicative of the fact that relatively weak gravity may not have the effect of making the pulse strongly dispersive.

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. As alluded to above, 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 $c \sim \sqrt{\mu/\rho}$ [25], 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.

III. RESULTS

A. Sound and shock propagation in pristine columns

In this subsection we present the results of our simulational study. We first discuss the results on the propagation of weak impulses, i.e., sound waves, in one- and two-dimensional pristine granular columns. Next we extend the analysis to the case of the propagation of strong impulses, i.e., shocks, in these pristine columns.

1. Sound propagation

We have performed the studies 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 which we call v_{impact}. Although experimental and theoretical studies suggest that the potentials that best describe systems composed of real sand 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 [16], calculations were carried out using a range of exponents from $n=\frac{5}{2}$ to $n=10$. The motivation for doing this is to study the power law dependence of sound speed as a function of depth z and n and also to check for possible deviations in the behavior of sound speed as a function of depth from the predictions of the Hertzian contact theory for impulses with large amplitudes for various n values.

The basic equation that describes the dependence of sound velocity c on depth z, measured from the surface of the column, can be arrived at as follows. If $f_{i,i+1}$ denotes the force between two adjacent grains i and $i+1$ that have an overlap of $\delta_{i,i+1}$, then the spring constant k between the two grains upon contact is

$$k_{i,i+1} = \frac{df_{i,i+1}}{d\delta_{i,i+1}}. \tag{5}$$

Given that $V(\delta_{i,i+1}) \sim \delta_{i,i+1}^n$ [see Eq. (1)], the force $f_{i,i+1} \sim \delta_{i,i+1}^{n-1}$. Hence $\delta_{i,i+1} \sim f_{i,i+1}^{1/(n-1)}$. Therefore one can write

$$k_{i,i+1} \sim \delta_{i,i+1}^{n-2} \sim \frac{f_{i,i+1}}{\delta_{i,i+1}} \sim f_{i,i+1}^{1-1/(n-1)}. \tag{6}$$

But the sound velocity c_{weak} is

$$c_{\mathrm{weak}} \sim \sqrt{\mu} \sim \sqrt{k_{i,i+1}} \sim f_{i,i+1}^{[1-1/(n-1)]/2}, \tag{7}$$

where μ is the bulk modulus of the granular medium. Clearly, at large depths $k_{i,i+1}, f_{i,i+1}$ become independent of i. Thus

$$c_{\mathrm{weak}} \sim f^{[1-1/(n-1)]/2}. \tag{8}$$

The results of our simulations for the one-dimensional columns are plotted in Figs. 3 and 4 for two specific cases,

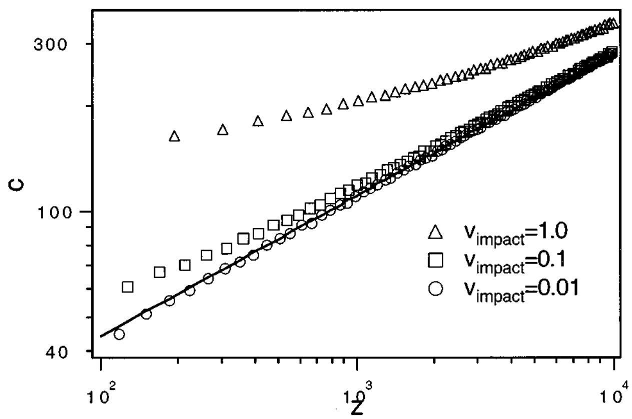

FIG. 4. Plot of c vs z for $n=6$ in one dimension. The slope of the solid line predicted by Hertzian contact theory is 2/5.

$n=\frac{5}{2}$, and $n=6$, respectively. For small v_{impact}, i.e., ~ 0.01, c_{weak} determined from the one-dimensional simulations scaled with depth z as

$$c_{\text{weak}} \sim z^{[1-1/(n-1)]/2}. \tag{9}$$

At large depths, the grains are very strongly compressed. Since the pressure P at depth z is $\rho g z$, where ρ is the density of the material and z is the depth, it naturally follows that Eqs. (8) and (9) are completely equivalent. The arguments given here are independent of dimensionality.

We present our results from simulations of sound propagation in two-dimensional granular columns in Figs. 5 and 6. The results are essentially indistinguishable with respect to the one-dimensional cases reported in Figs. 3 and 4.

2. Shock propagation

One would envisage from the arguments given above that the scaling law for c_{weak} presented above will not be valid at shallow enough depths or alternately, for large enough impulses (i.e., large v_{impact}). This is indeed what we find in our studies. The data for $v_{\text{impact}} \geqslant 0.1$ in Figs. 3–6 show a clear departure from the scaling law in Eq. (9) above for small z. The deviations become more pronounced as v_{impact} is in-

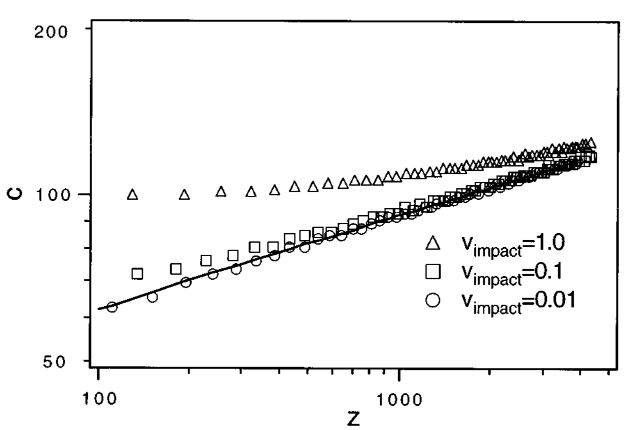

FIG. 5. Plot of c vs z for $n=5/2$ in two dimensions. Observe that there is very little difference between Figs. 5 and 3.

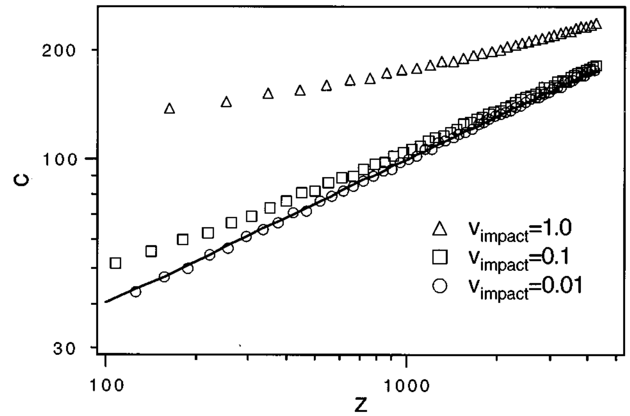

FIG. 6. Plot of c vs z for $n=6$ in two dimensions. Observe that there is very little difference between Figs. 6 and 4.

creased in magnitude. In these studies, c_{strong} does not show a simple power law behavior (i.e., $z^{1/6}$ or similar) 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 $z^{[1-1/(n-1)]/2}$ for small z (see Figs. 3–6). The relative difference between c for large v_{impact} and $v_{\text{impact}} \rightarrow 0$ can be defined as

$$\xi(z) \equiv (c_{\text{strong}} - c_{\text{weak}})/c_{\text{weak}}. \tag{10}$$

A functional form for $\xi(z)$ is expected to decrease monotonically as z increases and show the limiting behaviors $\lim_{z\rightarrow 0}\xi(z)\rightarrow\infty$ and $\lim_{z\rightarrow\infty}\xi(z)\rightarrow 0$.

One way to understand the departure from the scaling law that describes the propagation of a weak impulse is to recognize that the grains, which barely touch one another in the shallow reaches of the column, are suddenly strongly compressed against one another when a large impact is introduced into the system. As a result, the propagation of the perturbation is intrinsically strongly anharmonic in nature.

Having attempted many different functional forms to fit $\xi(z)$ we conclude that $\xi(z)$ does not follow a simple power law behavior. This conclusion suggests that there may be a single or a set of length scales that enter into the description of $\xi(z)$, i.e., in the manner in which $c_{\text{strong}}(z)$ converges to $c_{\text{weak}}(z)$. 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

$$\sum_{k=-\infty}^{+\infty} b_k \exp(-d_k z), \tag{11}$$

where the coefficients b_k and d_k follow the recursion relations

$$b_{k+1} = b_k \alpha \tag{12}$$

and

$$d_{k+1} = d_k \beta, \tag{13}$$

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

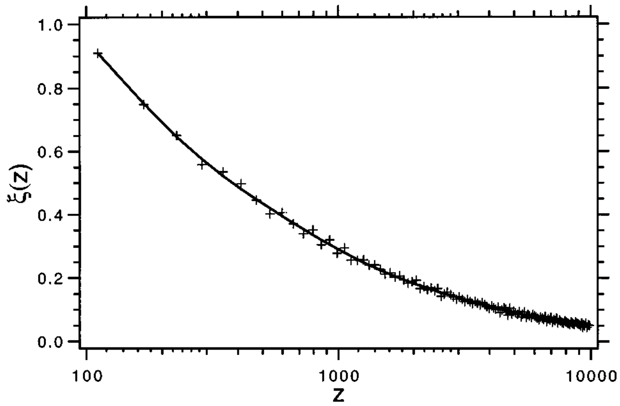

FIG. 7. Relative velocity difference $\xi(z)$, as defined in Eq. (10), for $v_{\rm impact}=1.0$ and $n=3$. The markers are results of numerical simulations and the solid line is the best fit of the data to a triple exponential function.

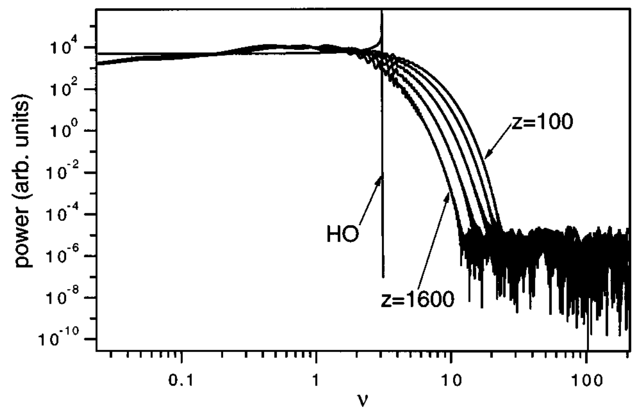

FIG. 8. Velocity power spectra for grains at five different depths, $z=100$, 200, 400, 800, and 1600, in a one-dimensional column due to the passage of a vertical disturbance. Shown for comparison is the velocity power spectrum for a particle in an infinite harmonic oscillator chain. The system parameters are $n=5/2$ and $v_{\rm impact}=0.05$.

$100<z<10\,000$ for $v_{\rm impact}=1.0$ and $n=3$ to a triple exponential function gives the result

$$\begin{aligned}\xi(z)\approx\,&0.04\,107+0.2519\,\exp(-0.000\,3244z)\\&+0.4527\,\exp(-0.001\,911z)\\&+0.8019\,\exp(-0.010\,19z),\end{aligned}\tag{14}$$

which has four parameters (see Fig. 7). For this case $\alpha\simeq1.8$ and $\beta\simeq5.8$. α and β are both greater than unity, ensuring that $\xi(z)$ converges for all $z>0$ and diverges at $z=0$. Although α and β depend on $v_{\rm impact}$ 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 is used up in promoting local excitations. It follows then that as $z\rightarrow\infty$ 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 derivation or a simple explanation for the above functional form for $\xi(z)$ for this highly nonlinear process. Our analysis suggests that each of the exponential terms in Eq. (14) roughly relates to each decade in z traversed by the strong perturbation. The precise magnitudes of the prefactors and the coefficients of z are perhaps sensitive to details such as n and $v_{\rm impact}$.

3. Velocity power spectra of grains in the column

In order to understand the dynamics of individual grains as the perturbation propagates downward through the column it is instructive to calculate the velocity power spectra of the grains at various depths. Typical velocity power spectra obtained by calculating $|v(\omega,z)|^2$ for grains at five different depths in the one-dimensional column during the passage of a vertical disturbance are shown in Fig. 8.

As one goes deeper and deeper into the column, one finds that the grains are more strongly confined to their equilibrium positions. Therefore one would expect that as depth $z\rightarrow\infty$, one would recover the known results for the velocity power spectrum of any mass in an infinite harmonic oscillator chain.

The calculations suggest that this is indeed the case [33,34]. 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 position. The leading term in a power series expansion of the force about $dz=0$ is $-2a(n-1)\delta^{n-2}dz$, hence for a strongly confined grain in the limit of small amplitude oscillations the behavior approaches that of a harmonic oscillator. Subsequently the velocity power spectrum of the grains at progressively larger depths approaches that of any mass in an infinite harmonic oscillator chain (see Fig. 8), which is given by [33]

$$\langle|v(\omega)|^2\rangle\equiv\sqrt{\frac{2}{\pi}}\int_0^\infty\frac{\langle v(t)v(0)\rangle}{\langle v(0)^2\rangle}\cos(\omega t)dt.\tag{15}$$

In the above equation, $\langle v(t)v(0)\rangle/\langle v(0)^2\rangle=(2k_BT/m)J_0(\omega_0t)$, where k_B is the Boltzmann constant, T is the temperature, $\omega_0=\sqrt{k/m}$, $\langle\rangle$ denotes canonical ensemble averages, and J_0 is a zeroth-order Bessel function. Recall here that $m=1$ in our study. The resultant power spectrum is

$$\langle|v(\omega)|^2\rangle=\frac{1}{\sqrt{4\omega_0^2-\omega^2}},\quad 0<\omega<2\omega_0\tag{16}$$

and is zero otherwise [35]. Our numerical calculations reveal that at finite depths within the grain column the velocity power spectrum does not have a cutoff at $2\omega_0$. This cutoff is asymptotically approached as depth $z\rightarrow\infty$.

B. Sound propagation in columns with voids

It is well known that granular materials are, in general, loosely packed and often contain a large void fraction [36,37]. This section presents our numerical investigations on how sound propagation may be affected by the presence of a small fraction of voids.

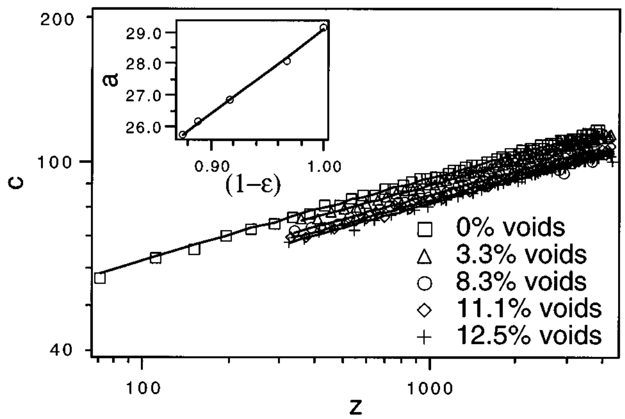

FIG. 9. Speed of the vertical disturbance in two-dimensional columns with voids for $n=5/2$ in the limit of weak impact. Solid lines are the best fits to data of form $c=az^b$. Inset shows the prefactor a plotted against $1-\epsilon$. The linear behavior of a for small ϵ suggests that $c \propto (1-\epsilon)z^{1/6}$.

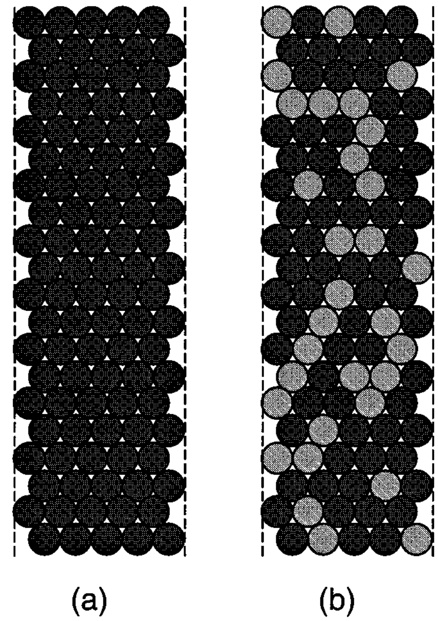

FIG. 10. Picture of a column with randomly distributed masses of two different magnitudes as indicated by the shade in (b). Observe that the positions of the grains remain very nearly the same as that in the pristine system in (a).

This study is technically somewhat challenging. It is nontrivial to stabilize voids in a column. Typically, the voids introduced into a system by randomly removing grains from a regular array of grains tend to disappear upon relaxing the system to its lowest energy state. As described in Sec. II C, the locations of the voids were carefully chosen so as to avoid the removal of adjacent grains. The voids were frozen into the lattice by first integrating the equations of motion with an additional viscous term until the metastable state was obtained before initiating the pulse. Due to the inherent fragility of the column with voids we report our studies of sound propagation (i.e., $v_{\mathrm{impact}} \ll 1$) here for columns with void fractions of up to about 12.5%.

The presence of voids in the two-dimensional column has a profound effect on the sound propagation. First, a large fraction of the energy in the vertically propagating disturbance is converted into random motion of the grains in the bulk of the column, particularly near the surface of the column as shown in Fig. 2. Second, the sound velocity now has the scaling behavior given by (see Fig. 9)

$$c \propto (1-\epsilon)z^{[1-1/(n-1)]/2}, \tag{17}$$

where ϵ is the void fraction. These two results are due to the fact that the presence of voids in the column leads to strong inhomogeneities in the force network.

Although we have not carried out calculations of a three-dimensional system due to computational limitations, our studies suggest that one should expect behavior similar to the one cited in Eq. (17) in close packed (hcp) three-dimensional systems.

It is worth mentioning that the amount of the amplitude of sound velocity (and hence the kinetic energy) that is lost to the voids ends up being transported approximately horizontally at the depth in which a void is present. In this sense the physical mechanism underlying the behavior given in Eq. (17) is very similar to what one finds in fracture physics [38]. Hence the presence of this energy is simply not picked up by the vertically propagating perturbation as it travels downward past the voids. As a result the amplitude of the sound velocity is decreased linearly by the void fraction. The effects of larger void fractions on sound propagation remain a challenging problem.

C. Sound propagation in columns with mass defects

A number of simulations were carried out to study the propagation of weak vertical disturbances in two-dimensional columns with randomly distributed mass defects (see Fig. 10). The systems were prepared by replacing a fraction of the grains in the pristine column with grains of an identical size but different mass. Generalizing Eq. (7) to account for the dependence of the sound speed on the mass, i.e., using $c_{\mathrm{weak}} \sim \sqrt{\mu/\rho}$, of the grains leads to the scaling relation

$$c_{\mathrm{weak}} \sim (mz)^{[1-1/(n-1)]/2}/\sqrt{m}. \tag{18}$$

Figure 11 shows the quantity $\overline{m}^{1/3}c$ plotted as a function of depth for both pristine columns and columns with a bimodal mass distribution for the case $V(\delta) \propto \delta^{5/2}$. For columns containing a mixture of grain masses, $\overline{m}$ represents the average grain mass. The data in Fig. 11 collapse nicely onto a single curve indicating the validity of Eq. (18) not just for perfect columns, but also for columns with mass inhomogeneities.

It should be noted that there are substantial differences between the behaviors of the columns containing mass defects and those containing voids. A void cannot be thought of as a defect of zero mass. Treating voids in this way leads to the prediction that the sound speed increases as grains are removed from the column — a result in direct contrast to the numerical simulations. Removing a grain from the system not only reduces the density of the column, but leads to the loss of the corresponding intergrain contacts.

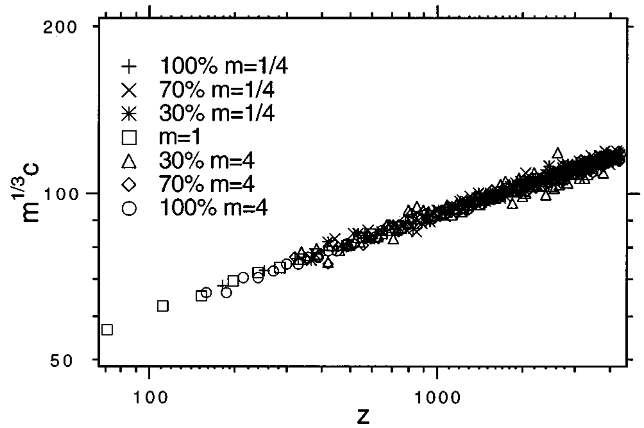

FIG. 11. Mass-scaled speeds of vertical disturbances in granular columns with mass defects for $n=5/2$ in the limit of weak perturbations. Legend refers to the fraction of $m=1$ grains that have been replaced by mass defects.

IV. SUMMARY AND CONCLUSION

In this article we have reported our results from extensive molecular dynamics based studies on the problem of sound and shock propagation in one- and two-dimensional granular columns. Our key findings are (1) we recover and generalize the $c \propto z^{1/6}$ scaling law usually obtained using Hertzian contact theory for vertical sound propagation at large depths from particle dynamics studies; (2) we extend this result to include columns with small (as defined by the upper limit of ϵ) void fractions, $c \propto (1-\epsilon)z^{1/6}$, $0 \leqslant \epsilon \leqslant 0.125$; (3) we discuss the case of propagation of a large amplitude perturbation; and (4) we study the problem of sound propagation in a column with random bimodal mass distribution.

This work demonstrates that present day computational power allows one to carry out detailed analysis of sound and shock propagation in dry granular media in both small and large length scales. Thus both the small length scale physics associated with the structural details of the granular media and their elastic properties can be extracted from this kind of an approach. Because of the fact that the elastic properties can be extracted from this study in which sound and shock propagation is strongly influenced by the gravitational field, one may anticipate that most of the features of $c(z)$ reported here will also be found in pristine three-dimensional columns. However, it is important to note that for imperfect three-dimensional columns, say due to the presence of voids and mass impurities, the details of sound and shock propagation could be different and hence three-dimensional columns need to be studied separately [26].

To our knowledge, much remains to be done experimentally in terms of addressing the issues (2)–(4) above. Our model uses periodic boundary conditions in the horizontal direction and it has been assumed all along that in the simulation cell, the depth far exceeds the width. This latter feature in turn allows the pressure to increase with depth instead of rapidly reaching saturation as might be the case with a very wide granular bed. The results presented here are therefore applicable to dry granular columns such as columns of dry sand (or perhaps to a situation with negligible static friction). We would like to encourage our experimentalist colleagues to probe the effects of voids and impurities on sound and shock propagation in granular columns and explore the validity of our results for real systems. Such research may in turn allow us to better understand sound and shock propagation in granular columns and perhaps also in granular beds. The problem of backscattering of disturbances from shallow impurities and voids can also lead to insights into possible ways of detecting buried inclusions via acoustic probes [19]. Such insights can be helpful in developing special acoustic probes for studying the position distribution of buried land mines and similar inclusions in dry granular soil.

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