Scaling Behavior of Granular Particles in a Vibrating Box

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Abstract

Using numerical and analytic methods, we study the behavior of granular particles contained in a vibrating box. We measure, by molecular dynamics (MD) simulation, several quantities which characterize the system. These quantities—the density and the granular temperature fields, and the vertical expansion—obey scaling in the variable \( x = Af \). Here, \( A \) and \( f \) are the amplitude and the frequency of the vibration. The behavior of these quantities is qualitatively different for small and large values of \( x \). We also study the system using Navier-Stokes type equations developed by Haff. We develop a boundary condition for moving boundaries, and solve for the density and the temperature fields of the steady state in the quasi-incompressible limit, where the average separation between the particles is much smaller than the average diameter of the particles. The fields obtained from Haff’s equations show the same scaling as those from the simulations. The origin of the scaling can be easily understood. The behavior of the fields from the theory is consistent with the simulation data for small \( x \), but they deviate significantly for large \( x \). We argue that the deviation is due to the breakdown of the quasi-incompressibility condition for large \( x \).

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1 Introduction

Systems of granular particles (e.g. sand) exhibit many interesting phenomena, such as segregation under vibration or shear, density waves in the outflow through a hopper and a tube, and the formation of heaps and convection cells under vibration \[1, 2, 3, 4\]. These phenomena are consequences of the unusual dynamical response of the systems, many of which are still poorly understood.

Granular particles in motion lose energy due to inelastic collisions of the particles. Thus energy has to be supplied to granular systems from an external source(s) in order to sustain the movement of the particles. We can classify granular systems according to the way in which energy is supplied, or how the systems are agitated. A few common ways to agitate the systems are shear, vibration and body force (e.g. gravity). Here, we consider only vibrational agitation, which is probably one of the most popular method. There are many interesting phenomena associated with the vibrated systems, such as convection cells \[5, 6, 7, 8\], heap formation \[1, 9, 10, 11, 12, 13\], subharmonic instability \[14\], surface waves \[15, 16\] and even turbulent flows \[17\]. The basis for understanding these diverse phenomena is, in our opinion, to understand the state of granular media under vibration. The state is characterized by several fields of the system, for example, the density, velocity and granular temperature fields.

There have been several studies on the state of granular systems under vibration. Thomas et al studied the system in three dimensions, mainly focusing on the behavior of shallow beds \[18\]. Clément and Rajchenbach experimentally measured the density, velocity and temperature fields of a two-dimensional vertical packing of beads \[19\]. They found that the temperature increases monotonically as the distance from the bottom plate is increased. The same system was studied by molecular dynamics (MD) simulation with similar results \[20\]. In a series of simulations and experiments, Luding et al studied the behavior of the one and two dimensional systems \[21, 22, 23\]. They found that the vertical expansion, which is the increase of the center of mass due to the vibration, scales in the variable \(x = A f\). Here, \(A\) and \(f\) are the amplitude and the frequency of the vibration. The expansion behaves as \(x^2\) and \(x^{3/2}\) in one and two dimensions, respectively. The reported shape of the temperature fields is decreasing as the distance from the bottom is increased, in contrast to the previous result \[21, 23\]. In a recent
MD simulation of the three dimensional system, Lan and Rosato measured the density and temperature fields [23]. They compared the results with the theoretical predictions by Richman and Martin [25], and found good agreements. More discussion on the theory will come later. They also found the shape of the temperature field is different for low and high amplitude of the vibration. Finally, an approximate theory was developed for the system in one dimension, which agrees with simulations in the weak and the strong dissipative regime [26].

In this paper, we measure the density, the granular temperature and the expansion for the two dimensional system using MD simulation. We find that not only the expansion, but also the density and the temperature fields, scale in the variable $x$. The behavior of these quantities is qualitatively different for small and large values of $x$. The different shapes of temperature field reported can be due to different values of $x$ used in the measurements. We also study the system using continuum equations developed by Haff [27]. We develop a boundary condition for moving boundaries. We solve the equations for the density and the temperature fields and the expansion of the steady state. We consider only the quasi-incompressible case, where the average separation between the particles is much smaller than the average diameter of the particles. The fields obtained from Haff’s equations show the same scaling as those from the simulations. Furthermore, the origin of the scaling can be traced back to the boundary conditions, and can be easily understood. Also, behaviors of the fields from the theory are consistent with the simulational data for small $x$, but they deviate significantly for large $x$. We argue that the discrepancy is due to the breakdown of the quasi-incompressibility condition for large $x$. Some of these results can also be obtained using the theory by Richman and Martin, which is based on an extension of the Boltzmann equation for inelastic gas [28, 29].

The paper is organized as follows. In Sec. 2, we start from defining the interaction of the particles used in the MD simulations. The geometry and various fields of the system will be discussed. We then present the expansion and the fields obtained by the simulations. Analytic results will be discussed in Sec. 3. The continuum equations for granular material will be given, and simplified for the present system. We then derive a boundary condition for moving walls, and present the solution of the equations. In Sec. 4, we compare the fields obtained by the simulations with those by the theory. Finally, conclusions are given in Sec. 5.
2 Molecular Dynamics Simulations

2.1 Interaction of the Particles

We start by describing the interactions used in the molecular dynamics simulations. The force between two particles $i$ and $j$, in contact with each other, is the following. Let the coordinates of the center of particle $i$ ($j$) be $\vec{R}_i$ ($\vec{R}_j$), and $\vec{r} \equiv \vec{R}_i - \vec{R}_j$. In two dimensions, we use a new coordinate system defined by two vectors $\hat{n}$ (normal) and $\hat{s}$ (shear). Here, $\hat{n} = \vec{r}/|\vec{r}|$, and $\hat{s}$ is defined as rotating $\hat{n}$ clockwise by $\pi/2$. The normal component $F_{n \to i}^n$ of the force acting on particle $i$ by $j$ is

$$F_{n \to i}^n = k_n(a_i + a_j - |\vec{r}|) - \gamma_n m_e (\vec{v} \cdot \hat{n}),$$  \hfill (1)

where $a_i$ ($a_j$) is the radius of particle $i$ ($j$), and $\vec{v} = d\vec{r}/dt$. The first term is an linear elastic force, where $k_n$ is the elastic constant of the material. The constant $\gamma_n$ of the second term is the friction coefficient of a velocity dependent damping term, $m_e$ is the effective mass, $m_i m_j / (m_i + m_j)$. The shear component $F_{s \to i}^s$ is given by

$$F_{s \to i}^s = -\gamma_s m_e (\vec{v} \cdot \hat{s}) - \text{sign}(\delta s) \min(k_s|\delta s|, \mu|F_{n \to i}^n|),$$  \hfill (2)

where the first term is a velocity dependent damping term similar to that of Eq. (1). The second term is to simulate static friction, which requires a finite amount of force ($\mu F_{n \to i}^n$) to break a contact [30]. Here, $\mu$ is the friction coefficient, $\delta s$ the total shear displacement during a contact, and $k_s$ the elastic constant of a virtual spring. There are several studies on granular systems using the above type of interactions [31]. However, only a few of them [30, 31, 32] include static friction. A particle can also interact with a wall. The force on particle $i$, in contact with a wall, is given by Eqs. (1)-(2) with $a_j = \infty$ and $m_e = m_i$. A wall is assumed to be rigid, i.e. it is not moved by collisions with the particles. Also, the system is under a gravitational field $\vec{g}$. We do not include the rotation of the particles in present simulation. A detailed explanation of the interaction is given elsewhere [33].

The trajectories of the particles are calculated using a fifth order predictor-corrector method. The interaction parameters used in this study are fixed as follows, unless otherwise specified. They are $k_n = 5 \times 10^6$, $k_s = 1 \times 10^4$, $\gamma_n = 1 \times 10^3$, $\gamma_s = 0$ and $\mu = 0.2$. The timestep is taken to be $5 \times 10^{-6}$. This small
timestep is necessary for the large elastic constant used in the simulations. For too small values of the elastic constant, the system loses the character of a system of distinct particles, and behaves like a viscous material. In order to avoid artifacts of monodisperse systems (e.g., hexagonal packing), we choose the radius of the particles from a Gaussian distribution with the mean 0.1 and the width 0.02. The density of the particles is 0.5. Throughout this paper, CGS units are implied.

2.2 Setup for the Simulations

We put the particles in a two-dimensional rectangular box. The box consists of two horizontal (top and bottom) plates which oscillate sinusoidally along the vertical direction with a given frequency and amplitude. The separation between the two plates is chosen to be much larger (10^5 times) than the average radius of the particles, so the particles never interact with the top plate for all the cases studied here. For simplicity, we apply a periodic boundary condition in the horizontal direction.

We start simulation by inserting the particles at random positions in the box. We let them fall by gravity and wait until they lose energy by collisions. We wait for 10^5 iterations for the particles to relax, and during this period we keep the plates fixed. The typical velocity at the end of the relaxation is of order of 10^{-2}. After the relaxation, we start oscillating the plates. We vibrate for about 50 cycles before taking any measurements in order to eliminate any transient effect.

The main quantities we are interested in are density, velocity and granular temperature, which probably are the most basic quantities to characterize the system. In order to measure these fields, we divide the system into rectangular cells of width w and height h. For cell i, we identify the particles whose center lies within the cell, which we label by j = 1, 2, 3..., N_i. Here, N_i is the total number of particles in the cell. The density at cell i, \( \rho_i \), is defined as

\[
\rho_i \equiv \frac{1}{w \cdot h} \sum_{j=1}^{N_i} \pi r_j^2,
\]

where \( r_j \) is the radius of particle j. We define an average of a certain quantity
$A$ in cell $i$, $\langle A \rangle_i$, as

$$\langle A \rangle_i \equiv \frac{\sum_{j=1}^{N_i} m_j A_j}{\sum_{j=1}^{N_i} m_j},$$

where $m_j$ is the mass of particle $j$. Then, the velocity field at cell $i, \vec{v}_i$, is given by

$$\vec{v}_i \equiv \langle \vec{v} \rangle_i,$$

and the granular temperature at cell $i, T_i$ is

$$T_i \equiv \frac{1}{2} (\langle v_x^2 - \langle v_x \rangle_i^2 \rangle_i + \langle v_y^2 - \langle v_y \rangle_i^2 \rangle_i).$$

We also measure the vertical component of the center of mass $y_{cm}$ of the particles, which is an useful quantity to compare with theoretical predictions. In principle, we can calculate $y_{cm}$ from the measured density fields, but the calculation introduces additional sources of uncertainty. We measure the above quantities by averaging over at least three independent runs, where each run is averaged over about 200 cycles of vibrations.

We study the effects of the width $W$ of the vibrating plates on the measured quantities in order to determine the optimal width for the main measurements. We measure the density and the granular temperature fields for $W = 1, 2, 3, 4$, where the height $H$ of the pile is roughly fixed constant by changing the number of particles to be 50, 100, 150, 200. The resulting height is little smaller than 2. Also, we use $w = W$ and $h = 0.2$. Here, the large $w$ is chosen due to the translational symmetry resulted from the periodic boundary condition. We do not find any systematic dependence of the fields on $W$ except that they become less noisy for larger $W$, which is simply due to the larger number of particles contained in a cell. We find $W = 1$ is a good compromise between the quality of data and the computation time. The dependence of the fields on $H$ will be discussed later.

### 2.3 Measurement of the Expansion

We now discuss the quantities obtained as described previously. We start from the vertical expansion of the pile $y_{exp}$, defined as the difference in the vertical center of mass $y_{cm}$ during and before vibration. Since the expansion can be expressed as an integral involving the density field, $y_{exp}$ can be used as a number representative of the density field. In Fig. 1, we show $y_{exp}$ measured.
for various values of the amplitudes $A$ and the frequencies $f$ of the vibration \[34\]. Here, the width $W = 1$ and the number of particles $N = 50$. Note that the expansion is plotted against a scaling variable $x = Af$. For the entire range of variable $x$, we do not find any systematic deviation from the scaling behavior except that the lowest frequency data ($f = 20$) seems to be slightly off. This scaling behavior was first measured in the simulations by Luding \textit{et al} \[21, 22, 23\]. For intermediate values of $x$, our data is also consistent with the $x^{3/2}$ behavior proposed by Luding \textit{et al} \[22\]. However, for small and large values of $x$, our data shows deviations from the behavior. The pattern of the deviation is not affected by changing the values of the elastic constant $k_n$ (to $10^6$ and $5 \times 10^5$). The scaling behavior and the deviation will later be discussed in more detail.

Since we are concerned about the possibility that $y_{cm}$ is dominated by a few top particles isolated from the main part of the pile, we also try an alternative definition of the expansion. We sort the particles in a box according to their vertical coordinates. We then define $y_{center}$ as the vertical coordinate of the center of the particle which is the ($N/2$)-th in the list. Here, $N$ is the total number of particles in the box. The quantity $y_{center}$ still contains the meaning of the center of mass, but is now not dominated by a few particles. We find that, in contrast to our worries, the expansions using $y_{center}$ behave essentially the same way as those using $y_{cm}$. We thus use the definition using $y_{cm}$ from now on.

2.4 Measurement of Density and Temperature

We discuss the density $\rho(y)$ and the granular temperature $T(y)$ fields. First, we study the behavior of the fields at the bottom plate, i.e., in the lowest cell ($y = 0$). These values are, as we shall see later, easier to compare with theoretical predictions than the entire fields. In Fig. 2 (a), we show the density $\rho(y = 0)$ vs $x$ for various values of $A$ and $f$. Here, we find the same scaling behavior as the expansion $y_{exp}$ (Fig. 1). This is not surprising considering the relation between the expansion and the density field. We also find the same scaling behavior for the temperature. The square root of $T(y = 0)$ is plotted against the scaling variable $x$ in Fig. 2(b). Although there are larger fluctuations, the same scaling is still apparent. Also, the decay of $T(y = 0)$ for large $x$ is partly due to a dip in the density near the bottom plate.
We then proceed to study the entire $y$-dependent fields. In Fig. 3, we show the density field $\rho(y)$ for several values of $A$ and $f$. Here, the value of $x$ is fixed to be 3 and 10 in Fig. 3(a) and (b), respectively. In the figures, the quality of scaling is poorer than those shown previously (Figs. 1 and 2). However, the quality of scaling will be improved by discarding the lowest frequency data ($f = 20$). The density field plotted against $y/y_{\text{exp}}$ was also shown to collapse into a single curve [23], which is consistent with above scaling, since $y_{\text{exp}}$ scales in $x$. The situation is not much different for the temperature field $T(y)$. In Fig. 4(a) and (b), we show the square root of $T(y)$, where $x$ is again fixed to be 3 and 10, respectively. Here also, the quality of scaling is not great, and will be improved by ignoring the $f = 20$ data. Putting aside the deviations at low frequencies, it is not entirely clear from these data that either the density or the temperature field exhibits more than an approximate scaling.

One interesting point is the shape of the temperature field. For large values of $x$, the field $T(y)$ is a monotonically decaying function of the height $y$ (as shown in Fig. 4(b)). As one decreases $x$, a local maximum begins to appear. In Fig. 4(a) one can see an maximum is starting to form around $y = 2$. As one decreases $x$ further, the maximum becomes more and more pronounced. The above observation can explain the different shapes of $T(y)$ reported by several experiments and simulations on the granular systems. In experiments of the two dimensional system, a local maximum is always present in the $T(y)$ field [19]. In contrast, $T(y)$ is found to be monotonically decaying in simulations of the one dimensional systems [21, 23]. Other simulations of the system in three dimensions also report monotonic decay of the temperature field. In the three dimensional simulations, however, changes of the shape of the field for smaller amplitudes were noted, although were not systematically studied [24].

We conclude this section by presenting the dependence of $y_{\text{exp}}$ on the total height $H$ of the pile. We change the total height by varying the number of particles $N$ and keeping the width $W$ fixed. We keep the previous value of $W = 1$. In Fig. 5, we show the scaled expansion for $N = 50, 100, 150$ and for several values of $A$, where $f$ is fixed to 100. The expansion is scaled by $50/N$, where the factor 50 is used to keep the $N = 50$ data unchanged. In the figure, we find a reasonable collapse of the curves. There seems to be no systematic deviation, although the data for large $x$ seems to be slightly off. The scaling is first found by Luding et al [21].
In this section, we have presented the data from the MD simulations. The expansion as well as the density and the granular temperature fields exhibit scaling in the variable $x$, but the quality of the scaling for the fields is worse than that of the expansion. Also, the lowest frequency data seems to deviate from the scaling. In the next section, we present a continuum theory of granular material which can explain the origin of the observed scaling.

3 Analytic Results

3.1 Basic Equations

The system of granular particles needs an external agitation(s) in order to sustain the movement of the particles. Without such an agitation, the motion of the particles will be suppressed because of the constant energy loss resulting from inelastic collisions of the particles. Many granular systems with an external agitation, including the system of granular particles in a vibrating box, can loosely be described as inelastic gas. A particle in such a system constantly moves. It assumes a ballistic trajectory until it collides with another particle or, if there is, a wall of the container. After the collision, the particle again moves ballistically. Such movement is analogous to those of particles in a gas. Motivated by the analogy, tools used to develop the kinetic theory of gas have been adapted to study granular systems. One such effort is to extend the Boltzman equation to an inelastic gas [28, 29]. In this approach, the time evolution of the fields (velocity, density and granular temperature) is written in terms of an integral involving all possible collisions, namely the Boltzman integral. Another approach, due to Haff, is to develop equations of motion very similar to the Navier-Stokes equations [27]. However, the coefficients in the equations, e.g. viscosity, are no longer constant, but now functions of the fields. Both approaches are not yet complete, and they contain assumptions whose validities have yet to be checked. Haff’s approach seems to be less rigorous; for example, the dependence of the coefficients on the fields are derived based only on intuitive arguments. On the other hand, the equations one has to solve in Haff’s approach are much simpler. Despite its simplicity, known solutions for a few systems using Haff’s approach do not significantly differ from those using the other method [27, 29]. In this paper, we will follow Haff’s approach.
The equations of motion developed by Haff consist of mass, momentum and energy conservation. The mass conservation equation is

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \vec{v}) = 0,$$

where \(\rho\) and \(\vec{v}\) are the density and the velocity fields, respectively. The equation (7) is exactly the same as that of the Navier-Stokes equations. Next is the \(i\)-th component of the momentum conservation equation,

$$\rho \frac{\partial}{\partial t} v_i + \rho (\vec{v} \cdot \nabla) v_i = \frac{\partial}{\partial x_i} [\frac{1}{2} \rho v^2 + \frac{1}{2} \rho T] + \frac{\partial}{\partial x_j} [\eta (\frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j})] + \rho g_i,$$

where summation over index \(j\) is implied. The coefficients \(\lambda\) and \(\eta\) are viscosities which will be determined later. Also, \(p\) is the internal pressure, and \(g_i\) is the \(i\)-th component of the gravitational field. The form of Eq. (8) is again the same as that of the Navier-Stokes equations. However, the coefficients as well as the internal pressure are now functions of the fields instead of being constant. The last of the equations of motion is energy conservation,

$$\frac{\partial}{\partial t} (\frac{1}{2} \rho v^2 + \frac{1}{2} \rho T) + \frac{\partial}{\partial x_i} [(\frac{1}{2} \rho v^2 + \frac{1}{2} \rho T)v_i] = -\frac{\partial}{\partial x_i} (pv_i)$$

$$+ \frac{\partial}{\partial x_i} [\lambda (\vec{v} \cdot \vec{v}) v_i] + \frac{\partial}{\partial x_i} [\eta (\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}) v_j]$$

$$+ \rho v_i g_i$$

$$+ \frac{\partial}{\partial x_i} [K \frac{\partial}{\partial x_i} (\frac{1}{2} \rho T)] - I.$$

Here, \(T\) is the granular temperature field defined in Eq. (6), \(K\) is the “thermal conductivity,” and \(I\) is the rate of dissipation due to inelastic collisions [32]. Also, the summation over repeated indices is implied. Although the form of Eq. (9) is somewhat different from that of the Navier-Stokes equations, the equation can still be easily understood. The left hand side of Eq. (9) is simply the material derivative of the total kinetic energy, where the total kinetic energy is divided into the convective part (involving \(\vec{v}\)) and the fluctuating part (involving \(T\)). On the right hand side of the equation, the first three lines are simply the rate of work done by the internal pressure,
viscosity and gravity, respectively. The term involving $K$ is the rate of energy transported by “thermal conduction.” The term $I$, which is a consequence of inelasticity of the particles, is responsible for many unique properties of granular material.

We now discuss the above coefficients which are yet to be determined. The relations of these coefficients to the fields are derived based on intuitive arguments. Also, the derivation assumes that the density is not significantly smaller than the closed packed density, i.e., the system is almost incompressible. The relation for the internal pressure is

$$p = td\rho \frac{T}{s}, \quad (10)$$

where $t$ is an undetermined constant, $d$ is the average diameter of the particles. The variable $s$, which is roughly the gap between the particles, is related to the density by

$$\rho \equiv \frac{m}{(d+s)^3}, \quad (11)$$

where $m$ is the average mass of the particles. Then, the viscosity $\eta$ is given as

$$\eta = qd^2 \rho \frac{\sqrt{T}}{s}, \quad (12)$$

where $q$ is an undetermined constant. In a similar way, the thermal conductivity is found to be

$$K = rd^2 \frac{\sqrt{T}}{s}. \quad (13)$$

Here again, $r$ is an undetermined constant. Finally, the rate of dissipation is

$$I = \gamma \rho \frac{T^{3/2}}{s}. \quad (14)$$

Also, $\gamma$ is an undetermined constant. One can notice the viscosity $\lambda$ is left undetermined. This is due to the fact that in the range where these relations are valid, the term containing $\lambda$ is negligible, and is dropped from the calculation.
3.2 Equations for Particles in a Vibrating Box

We now apply Haff’s equations to the system being considered in the present paper—granular particles under vibration. Since the general solution of the problem using Haff’s equations are too difficult to obtain analytically, we introduce several constraints which simplify the equations. First, we only study steady state properties of the system. In order words, we are interested in only the time averaged quantities. Since there is no net flow of particles in the steady state, the time averaged values of $\vec{v}$ is zero, which greatly simplifies the equations. The second simplification is resulting from the horizontal periodic boundary conditions we imposed. Due to the boundary condition, there is no significant variation of the fields along the horizontal direction. As a result we only have to deal with a one dimensional equation instead of two or three dimensional ones. The third condition is incompressibility, which is a little bit tricky. Incompressibility implies, strictly speaking, that the density $\rho$ is constant. Due to the relation between $\rho$ and $s$ (Eq. (11)), $s$ also has to be constant. Here, we are interested in the situation where $s$ is much smaller than $d$, but still non-zero. In such cases, the variation of the density can be ignored, but not the variations of the variables that depends directly on $s$. We call this condition quasi-incompressibility.

The simplified equations for the pile of granular particles under vibration are then

$$\frac{d}{dy} v = 0,$$

(15)

$$\frac{d}{dy} p + \rho g = 0,$$

(16)

and

$$\frac{1}{2} \rho \frac{d}{dy} \left[ K \frac{d}{dy} T \right] - I = 0.$$

(17)

Here, all the fields are averaged over time, so they are not functions of time, but of spatial coordinate $y$ only. We thus replace partial derivatives in the equations with ordinary derivatives. Note that the first equation is automatically satisfied. Substituting the relation for the internal pressure Eq. (10) to Eq. (18), we obtain

$$\frac{d}{dy} \left( s\frac{T}{s} \right) = -\frac{g}{td},$$

(18)
whose solution is

$$\frac{T}{s} = -\frac{g}{td}(y - y_0),$$  \hspace{1cm} (19)$$

where $y_0$ is a constant which will be discussed later. Substituting Eq. (19) to Eq. (17), we obtain

$$\frac{d^2}{dy^2} \sqrt{T} + \frac{1}{y - y_0} \frac{d}{dy} \sqrt{T} - \frac{\gamma}{rd^2} \sqrt{T} = 0,$$  \hspace{1cm} (20)$$

which is a linear differential equation for $\sqrt{T}$. We make a change of variable,

$$z \equiv \frac{y - y_0}{\ell},$$  \hspace{1cm} (21)$$

where $\ell$ is defined as $\sqrt{r/\gamma} \, d$. By inserting the new variable to Eq. (20), we arrive at the final form of the equation

$$\frac{d^2}{dz^2} \sqrt{T} + \frac{1}{z} \frac{d}{dz} \sqrt{T} - \sqrt{T} = 0.$$  \hspace{1cm} (22)$$

The solutions the equation are the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$. However, $K_\nu(z)$ has a singularity at the physical region, and can not be a part of the solution. The solution is, therefore,

$$\sqrt{T} = A \, I_\nu(z),$$  \hspace{1cm} (23)$$

where $A$ is a constant yet to be determined. The result obtained so far is identical to that of Haff [27]. We now discuss our contribution to the problem, which concerns the boundary conditions.

### 3.3 Boundary Condition

One of the areas which are yet to be completed in Haff’s theory is boundary conditions. For example, what is the boundary condition one has to impose for the temperature field $T$ and the velocity field $\vec{v}$ at the bottom of a vibrating box? The boundary conditions for fixed walls have been developed based on energy conservation across the boundary [36]. We will show that a boundary condition for moving walls can also be derived from the similar condition of energy conservation. As noted in [36], there are two energy flows
near a boundary. One is the thermal conduction, and the other is the energy transfer by collisions between the particles and the boundary. Energy conservation implies that the rate of energy transferred by the conduction has to be equal to that by the collisions. We consider an horizontal boundary vibrating vertically, like the bottom plate of a vibrating box. The rate of the thermal conduction per area at the boundary is given as

\[ \frac{1}{2} K \rho \frac{d}{dy} T \big|_{y=0}, \quad (24) \]

where \( y = 0 \) is the average vertical coordinate of the boundary. To calculate the rate of energy transferred by the collisions, consider a particle colliding with the boundary. If convection is absent, the movement of the particle is resulted from the fluctuation. The typical velocity due to the fluctuation is \( \sqrt{T} \). The velocity of the particle after the collision will depend on the velocity of the boundary at the moment of the collision. Here, we assume that the phase of the vibration at which the collision occurs is random—an assumption whose validity will be discussed later. In such cases, the typical velocity of the wall is \( v_w = Af \). The amount of energy transferred in one collision is

\[ \frac{1}{2} m [T(1 - e_w^2) - (1 + e_w^2)v_w^2], \quad (25) \]

where \( e_w \) is the coefficient of restitution between a particle and the wall. The rate of energy transfer per area is Eq. (25) multiplied by the frequency of collisions \( T/s \) divided by the area of contact \( d^2 \). Here, we again use the quasi-incompressibility. Equating this rate to Eq. (24), and use the definition of \( K \) (Eq. (13)), we obtain

\[ T(1 - e_w^2) - (1 + e_w^2)v_w^2 = \frac{rd}{a} \frac{d}{dy} T, \quad (26) \]

where \( a \) is an undetermined constant. The method used to derive the above boundary condition can be extended to a case where the boundary is moving horizontally, and even to a case with both horizontal and vertical motions.

We now apply the above boundary condition to the problem of the vibrating box. First, note that the modified Bessel function \( I_o(z) \) can be approximated as

\[ I_o(z) \sim \frac{\exp(z)}{\sqrt{2\pi z}}, \quad (27) \]
for $z > 0$. The expression is actually an asymptotic form of $I_o(z)$ for $z \gg 1$, but it still is a good approximation even for small values of $z$. By applying the boundary condition Eq. (26) to the solution Eq. (23) with the approximation Eq. (27), we obtain

$$A^2 = \frac{1}{I_o^2(-y_o/\ell)} \frac{(1 + e_w)^2}{1 - e_w^2 - (2rd/a\ell)} \frac{v_w^2}{(1 - \ell/2y_o) v_w^2}$$

where a new variable $B$ is introduced. Substituting for $A$ in the solution Eq. (23), we now arrive at the final form of the solution for the temperature field

$$\sqrt{T}(y) \simeq B v_w \frac{y}{y_o - y} \exp(-y/\ell),$$

where we use the property $I_o(-z) = I_o(z)$. Besides the prefactor $B$, the above result is the same as that obtained by Haff who simply assumed that $\sqrt{T}$ at the boundary is $v_w$ [27]. The temperature field decays exponentially with decay length $\ell$ as one moves away from the bottom plate. Note that it has a singularity at $y = y_o$, which is an artifact resulting from the fact that Haff’s theory is not valid near the top part of the pile. In other words, the theory is based on the picture that the state of the system is gaseous. Near the top of the pile, however, the particles do not collide frequently, but assume ballistic trajectories [27]. On the other hand, Eq. (23) is still valid for $y$ not very close to $y_o$, since the gaseous picture is valid for that ranges of $y$. Thus, the behavior of $T$ to increase again for large $y$ is a physical effect, not an artifact. A word about $y_o$. One can see $y_o$ is still left undetermined. According to Eq. (19), the condition to determine $y_o$ is that the internal pressure vanishes at $y = y_o$. However, since the solution we have obtained is not valid at $y = y_o$, we can not impose the condition to determine $y_o$.

Having determined $T(y)$, we now determine the density field, represented here by the separation $s(y)$. Inserting the solution of $T(y)$ into Eq. (19), we obtain

$$s(y) \simeq \frac{t^2 d^2 \rho_o}{g} B^2 v_w^2 \frac{y_o}{(y_o - y)^2} \exp(-2y/\ell),$$

where $\rho_o$ is the density of the pile at rest. The separation $s$ also decays exponentially as one moves away from the bottom plate, then increases for
large values of $y$, similar to $T(y)$. Also, the above expression for $s$ is not valid in the neighborhood of $y = y_0$. Finally, we consider the expansion $y_{\text{exp}}$. The expansion can be written as

$$y_{\text{exp}} \simeq \frac{1}{d} \int_{0}^{y_0} s(y)dy$$

$$\simeq \frac{\ell^2 d \rho}{2gh_o} B^2 \ell v_w^2.$$  

4 Discussion

4.1 Condition for the Gaseous State

In the previous section, we have obtained analytic results for the vibrating box problem using Haff’s theory. There are several assumptions made in the construction of the theory as well as in the derivation of the solution. In this section, we check the validity of the solution, and in turn the assumptions, by comparing with the results obtained by the MD simulations.

Before making the comparison, we check the condition under which the system is regarded as gaseous. We consider that the system is gaseous if the particles in the system stay afloat for the most part of time colliding with each other. Therefore, for the gaseous system, the vibration should provide enough input to make the particles float. In other words, the collisional force caused by the bottom plate should be large enough to overcome the pressure due to the gravity. Consider a particle at the bottom of the box, where the pressure is the greatest. The typical change of momentum during a collision of the particle with the bottom plate is $mv_w$, where $m$ is the mass of the particle, and $v_w$ is the typical velocity of the plate. Here, we choose $v_w$ to be $2\pi Af$, the maximum velocity of the plate. We then consider the frequency of such collisions. We argue that the particle collides roughly once during one period, at least for the small amplitudes of the vibration. It will be later shown that the system becomes gaseous at a small value of the amplitude, so the above estimation seems to be reasonable. The total force generated due to the collisions is of order of $2\pi mAf^2$. On the other hand, the force on the particle due to gravity is of the order of $mgn$, where $n$ is the number of layers in the pile. Then, the condition for the gaseous system becomes that the ratio $F$ of the collisional force to the gravitational force to be much larger
than one. The ratio $F$ is essentially the Froude number. The condition can be written as
\[ F \sim \frac{\Gamma}{2\pi n} \gg 1, \] (32)
where $\Gamma$ is $4\pi^2 A f^2 / g$, the maximum acceleration of the plate scaled by that of the gravity. Thus, the acceleration of the bottom plate, not the velocity, is relevant in determining the condition for the system to be gaseous.

We check the condition also by MD simulation. At a given time, we measure the total number of pairs of particles in contact with each other. We average the number over 200 periods of the vibration. The system is gaseous, if the averaged number of pairs $N_p$ is much smaller than the total number of particles $N$. Here, we use the criterion that $N_p < 0.1 N$ for the system to be gaseous. We choose the width $W = 1$ and $N = 50$. For several frequencies, we increase the amplitude $A$ until $N_p/N$ becomes less than 0.1. We obtain, for each $f$, an interval of $A$ containing the value at which $N_p/N = 0.1$. The intervals are $[0.06, 0.08]$, $[0.01, 0.02]$ and $[0.003, 0.004]$ for $f = 20, 50, 100$, respectively. The corresponding intervals of $\Gamma$ are $[0.97, 1.29]$, $[1.01, 2.01]$ and $[1.21, 1.61]$. The acceleration at which the system becomes gaseous is roughly constant, which is consistent with the above argument. We now study the height dependence of the condition. We fix the frequency $f = 100$ and the width $W = 1$, and vary $N$ to 100 and 150. By using the same criterion, we find the intervals of $\Gamma$ to be $[2.41, 3.22]$ and $[4.03, 5.64]$ for $N = 100$ and 150, respectively. The acceleration needed for the gaseous system is consistent with a linear increase in $N$, which is again in agreement with the above argument. One thing to note is that $\Gamma$ to make the system gaseous is fairly close 1 for $N = 50$. For the values of $\Gamma$ used in the simulations of the preceding section, the system is always gaseous. Also, $N_p$ for large amplitudes $A \sim 0.1$ is essentially zero, which will be further discussed later.

4.2 Scaling of Density and Temperature

We compare the expansion $y_{\text{exp}}$ measured by the MD simulations with that predicted by the theory. Measured values of $y_{\text{exp}}$, as shown in Fig. 1, exhibit good scaling for the variable $x = A f$ with no systematic deviation for the entire range of $x$. The scaling is exactly what is predicted by the theory in Eq. (31). The theory also predicts $y_{\text{exp}}$ is inversely proportional to the rest height of the pile $H$ for fixed $A$ and $f$, which is certainly consistent
with the data presented in Fig. 5. On the other hand, $y_{\text{exp}}$ should behave as $x^2$ according to the theory, but the data (Fig. 1) is consistent with the behavior only for small values of $x$ (up to $\sim 2$). For larger values of $x$, $y_{\text{exp}}$ definitely increases slower than $x^2$. The situations for the density $\rho(y)$ and granular temperature $T(y)$ fields are very similar. The value of the fields at the bottom plate ($y = 0$) shows good scaling for $x$ (Fig. 2), as again predicted in Eqs. (29) and (30). The value of $T(0)$ from the simulations increases for small $x$, reaches a maximum around 4, than decays, very different from the $x^2$ behavior given by Eq. (29). The behavior is again consistent with the prediction only for small values of $x$. For the density field, we recall the relation between the separation $s$ and the density $\rho$, which is

$$\frac{s(0)}{d} \simeq \left( \frac{\rho_o}{\rho(0)} \right)^{1/3} - 1,$$

where $\rho_o$ is the density of the rest pile. In Fig. 6, we plot $\rho(0)^{-1/3}$ against $x^2$. The resulting curve, as predicted in Eq. (30), should be straight. The curve is indeed straight, but only for small values of $x$. For large $x$, the curve increases slower than linearly.

All three quantities we have studied behave in a similar manner. They all scale in the variable $x$, they are all consistent with the theory for small values of $x$, and they all deviates from the predicted behavior as $x$ is increased. Furthermore, the value of $x$ where they start to deviate seems to be roughly the same ($x = 2 \sim 3$). We recall that one of the assumptions in deriving the solution in the previous section is quasi-incompressibility, which implies that the separation $s$ is much smaller than $d$, the average diameter of the particles. However, as shown in Fig. 2(a), the density of the pile becomes the half of a packed density for $x \sim 3$, which is in violation of the assumption. The system can not be treated as quasi-incompressible for values of $x$ larger than about 3. Since the point where the quasi-incompressibility breaks down seems to coincide to the point where the deviation from the theory starts, we strongly suspect that the deviations are resulted from the breakdown. Furthermore, if the deviation is due to the breakdown, it is clear why the relevant variable for the breakdown is $x$, not $\Gamma$ or other variable. The breakdown occurs when $s$ is comparable to $d$, and $s$ scales in the the variable $x$. Thus, the breakdown occurs at a specific value of $x$.

We now consider the behavior of the entire density and temperature fields. The density field $\rho(y)$, as shown in Fig. 3, roughly scales in $x$ and has one
maximum, both of which are consistent with Eq. (30). The temperature field $T(y)$ also scales in $x$, but displays qualitatively different shapes (Fig. 4) depending on $A$. For small $A$, the field has a local maximum around $y = 2$, while the maximum disappears for larger $A$. On the other hand, the maximum is always present in the prediction of the theory Eq. (29). We study the condition for the change of the shape. For given $f$, we increase $A$ until the local maximum disappears. We obtain intervals of $A$ containing the value at which the maximum disappears. They are $[0.10, 0.15], [0.04, 0.06]$ and $[0.019, 0.020]$ for $f = 20, 50, 100$, respectively. The corresponding intervals of $x$ for the different frequencies are roughly the same. We thus face a familiar situation—the behavior of $T(y)$ is consistent with the theory for small $x$, but deviates for large $x$. Furthermore, the value of $x$ at which $T(y)$ deviates from the theory is about 2, which is again consistent with the previous argument.

4.3 Beyond Incompressibility

Since we argue quasi-incompressibility is valid only for modest range of $x$, one might wonder why we do not relax the condition. The simple answer is that the system of equations becomes too complicated. We now consider the changes needed in order to relax the quasi-incompressibility. The three equations Eqs. (7)-(9) are written in general form, and do not need any modification. The relations of $p, \eta, K, I$ to the fields Eqs. (10)-(14) as well as the boundary conditions Eq. (26) have to be modified. It is not these modifications themselves, but the complexity of the resulting equations, that makes the analytic solution too difficult to obtain. A word about the regime of validity. The range of $x$ where the quasi-incompressible theory is valid depends on $H$ the rest height of the pile. For $H = 2$, which corresponds to the system of about 10 layers, the theory is valid until $x$ reaches about 3. As we increase $H$, the range of validity also increases. Since a typical experiment of granular system involves several tens or more layers, the quasi-incompressible theory can describe quite large range of $x$, and we hope many interesting phenomena occur within the regime of validity.

One also might wonder why the scaling predicted by the theory is valid even in the regime where the quasi-incompressible theory is no longer valid. The only place where the external parameters $A$ and $f$ come to the system is the boundary condition. The boundary condition, as previously discussed, is a consequence of energy conservation. Even in the general situation of
a compressible system, the boundary condition is obtained by equating two energy fluxes. One is the energy transferred by collisions between the particles and the wall, which is a function of the velocity of the wall. Now, the velocity is proportional to $Af$, but the other flux term does not depend on $A$ or $f$, but on the fields of the system. Thus, it is not surprising to see the scaling for the variable $Af$ holds even for the compressible systems.

We finish the section by discussing two behaviors previously mentioned. As noted in Sec. 2.3, the expansion $y_{exp}$ seems to increase faster near the largest value of $x$. This may be explained as follows. As $A$ is increased for fixed $f$, the system becomes more expanded, and the number of interparticle collisions decreases. For sufficiently large $A$, it is be possible that a particle in the system hardly interact with other particles, and it mainly interacts with the bottom plate [37]. This is supported by the measurement of the average number of pairs $N_p$ in contact, discussed in Sec. 4.1. We find that $N_p$ is essentially zero near the largest values of $A$. If we completely ignore the interparticle interaction, it is straightforward to show that $y_{exp} \sim x^2$. Thus, $y_{exp}$ has to increase faster for large $x$, which is consistent with the data (Fig. 1). However, it is not clear, without further detailed study, that above mechanism is actually operating. Also, note that the mechanism predict scaling for variable $x$. The behavior of $y_{exp}$ was shown to depend on properties of the sidewall [22, 23]. It was shown that $y_{exp}$ behaves as $x^{3/2}$ for entire range of $x$ with inelastic sidewalls, while it deviate from the behavior with elastic ones (no energy loss).

The other problem I want to discuss is the deviation from the scaling for very small values of $f$. In Secs. 2.3 and 2.4, we find nagging deviations from the scaling of the expansion, the density and the temperature field for $f = 20$ data. One possible way to explain them is to consider the way the boundary condition is imposed. In constructing the boundary condition, we assume that particles collide with the bottom plate at random phase of the vibration. We thus assume the “thermal motion” is much larger than the convective motion. For low enough frequencies, however, the particles have enough time to dissipate their thermal fluctuations, so the assumption may not be valid. In such cases, the convective motion of the particle dominates, and one can no longer think of the system as particles with random motion.
5 Conclusion

We study the behavior of granular particles contained in a vibrating box. Using MD simulation, we show that several quantities which describe the system—the density and the temperature fields as well as the expansion—obey scaling in the variable $x = Af$. The behavior of these quantities is qualitatively different for low and high values of $x$. We also study the system using continuum equations developed by Haff. We develop a boundary condition for moving boundaries, and apply at the bottom plate of the box. We solve for the density and the temperature fields of the time averaged steady state of the system. Here, we are limited to the quasi-incompressible case, where the average separation between the particles is much smaller than the average diameter of the particles. The fields obtained from Haff’s equations show the same scaling as the simulational counterparts. The behaviors of the fields from the theory are consistent with the simulational data for small $x$, but they deviate significantly for large $x$. We argue that the discrepancy is due to the fact that the quasi-incompressibility condition we impose is not valid for large $x$.

In this paper, we have showed that Haff’s theory, even with many assumptions, seems to describe the system reasonably well in the quasi-incompressible case (small $x$). It goes without saying that the current study is only a very small step towards the understanding of the system, and the following are what we consider important things yet to be understood. The quality of the simulational data needs to be improved in order to convincingly demonstrate the scaling. For example, it is not certain from Figs. 3 and 4 that $\rho(y)$ and $T(y)$ obey strict scaling or an approximate one. Also, the improvement is necessary for quantitative comparison of the fields from the theory with from simulations. Next is the validity of Haff’s theory in the compressible regime (large $x$). As discussed in Sec. 4.3, due to the complexity of the problem in the regime, it may be too difficult to obtain a closed form analytic solution of the problem. However, with perturbative or approximate methods, one might be able to get some information. Also, one can numerically solve Haff’s equations, and compare the results with MD simulations. Another issue to be understood are time dependent properties of the system. In this paper, we have studied only steady state properties, which averages out the variations of the fields during one period of the vibration. Time dependent properties can be studied by perturbation from the steady state \[38\]. And
of course, Haff’s theory has to be applied to other systems to find the power and limitation of the theory.

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Figure Captions

Fig. 1: The expansion $y_{exp}$ for several values of the amplitudes $A$ and the frequencies $f$ of the vibration. We find the expansion exhibits good scaling behavior with variable $Af$.

Fig. 2: (a) The density and (b) the square root of granular temperature at the bottom plate for various values of $A$ and $f$ of the vibration. Here, we find that the same scaling as the expansion holds.

Fig. 3: The density field for various values of $A$ and $f$. Here, value of $Af$ is fixed to be (a) 3 and (b) 10. We find that the same scaling as the expansion $y_{exp}$ seems to hold. However, the quality of scaling is poorer.

Fig. 4: The square root of the granular temperature field for various values of $A$ and $f$. The value of $Af$ is fixed to be (a) 3 and (b) 10. We again find poorer scaling similar to the density field (Fig. 3).

Fig. 5: The scaled expansion vs $Af$ for $N = 50, 100, 150$ and for several values of the amplitude. All the curves seems to collapse to a single curve.

Fig. 6: Plot of $\rho(0)^{-1/3}$ against $x^2$ calculated from Fig. 2(a). The curve is straight for small values of $x$, and deviates from the linear behavior for large $x$. 
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