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Density waves in granular flow: a kinetic wave approach

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Abstract. — It was recently observed that sand flowing down a vertical tube sometimes forms a traveling density pattern in which a number of regions with high density are separated from each other by regions of low density. In this work, we consider this behavior from the point of view of kinetic wave theory. Similar density patterns are found in molecular dynamic simulations of the system, and a well defined relationship is observed between local flux and local density — a strong indicator of the presence of kinetic waves. The equations of motion for this system are also presented, and they allow kinetic wave solutions. Finally, the pattern formation process is investigated using a simple model of interacting kinetic waves.

Systems of granular particles (e.g. sand) exhibit many interesting phenomena, such as segregation under vibration or shear, density waves in the outflow through tubes and hoppers, and probably most strikingly, the formation of heap and convection cell under vibration [1, 2, 3, 4]. In granular flows through a narrow vertical tube, Pöschel found [5] that the particles do not flow uniformly, but form high density regions which travel as coherent structures with a velocity different from the center of mass velocity. He also reproduced these density waves using molecular dynamics (MD) simulations [5]. However, the motion of these high density regions and the mechanism which is responsible for their formation are not fully understood.

In this paper, we present numerical and theoretical evidence that these density waves are of a kinetic nature [6]. Using MD simulations, we measure the dependence of the particle flux on the density. We find a well-defined flux-density relation — an indication that a kinetic wave theory describes the behavior. A direct measurement of the velocity of these high density regions shows a dependence on the mean density which is in good agreement with the predictions from kinetic wave theory. On the theoretical side, we consider one dimensional equations of motion for the density and the velocity fields in the tube. These equations, together with Bagnold’s law for friction [7], allow kinetic density wave solutions.

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In order to understand the formation of these high density regions, we consider the general problem of interacting kinetic waves. We first show numerically that a system with an initially random density field evolves to a configuration in which neighboring regions have a high density contrast. At the early stage of development, we can show analytically that the density contrast between nearby regions increases linearly with time.

We first discuss the MD simulations of the system, and begin with a brief description of the interparticle force laws that were used in our calculations. The particles interact with each other (or with a wall) only if they are in contact. The force that acts on particle $i$ due to particle $j$ can be divided into two components. The first, $F_{j\rightarrow i}^n$, is parallel to the vector $r \equiv R_i - R_j$, where $R_i$ and $R_j$ are the coordinates of the centers of particles $i$ and $j$ respectively. We refer to this as the normal component. The second component, orthogonal to $r$, is the shear component $F_{j\rightarrow i}^s$. The normal component is given by

$$F_{j\rightarrow i}^n = k_n (a_i + a_j - |r|)^{3/2} - \gamma_n m_e \frac{v \cdot r}{|r|},$$

(1a)

where $a_i (a_j)$ is the radius, and $m_i (m_j)$ the mass of particle $i$ ($j$). Also, $m_e$ is the effective mass $m_i m_j / (m_i + m_j)$, and $v \equiv dr/dt$. The first term in equation (1a) is the Hertzian elastic force, where $k_n$ is a material dependent elastic constant. The second term is a velocity dependent friction term, where $\gamma_n$ is a normal damping coefficient. The shear component is given as

$$F_{j\rightarrow i}^s = -\gamma_s m_e \frac{v \cdot s}{|s|},$$

(1b)

where $s$ is defined by rotating $r$ clockwise by $\pi/2$. The shear force, equation (1b), is simply a velocity dependent friction term similar to the second term in the normal component. Finally, we must specify the interaction between a particle and a wall. The force on particle $i$, in contact with a wall, is given by equations (1) with $a_j = \infty$ and $m_j = \infty$. The choice of the interactions defined by equations (1) is rather typical in the MD simulations of granular material [8]. A detailed explanation of the interaction is given elsewhere [9].

For simplicity, we study granular flows in 2 dimensions and use a fifth order predictor-corrector scheme to integrate the equations of motion, calculating both the positions and velocity of each particle at all times. The tube is modeled by two vertical sidewalls of length $L$ with a separation $W$, and we apply a periodic boundary condition in the vertical direction. Between the sidewalls, particles of radii 0.1 are initially filled with a uniform density of $\rho_0$ (throughout this paper, numerical values are given in CGS unit). The particles begin to move under the influence of gravity, and soon reach a steady state, where the gravitational force is balanced by the frictional force from the interactions with the sidewalls.

In figure 1, we show the time evolution of the density and the velocity fields for $L = 15$ and $W = 1$, measured at every 5 ms. At a given time, we divide the tube into 15 vertical regions of equal length, and measure the density and the average velocity in each region. These fields are displayed as a vertical strip of square boxes, where each box corresponds to a region in the tube. The grayscale of the box is proportional to the value of the field in that region. The parameters we used in this simulation are $k_n = 1.0 \times 10^6$, $\gamma_n = \gamma_s = 5.0 \times 10^2$, with the time step $5.0 \times 10^{-5}$. The initial density $\rho_0$ is 25 particles per unit area. In the figure, we find (1) a region of large density fluctuations is formed out of the initially uniform system, (2) the fluctuations seem to travel with almost constant velocity (different from the center of mass velocity), and (3) there seems to be strong correlation between the density and the velocity fields. These findings remain true for the simulations we have performed with different values of $\gamma$, $k_n$ and $\rho_0$, except when $\rho_0$ is very small, where a steady state is not reached. These traveling density patterns were first observed in the simulations by Pöschel [5].
In order to quantitatively study the correlation between the density and the velocity fields, we measure the local particle flux as a function of the local density in the following manner. Once the system has reached a steady state, we measure the mean velocity $v_i$ and the density $\rho_i$ in region $i$. The flux $j(\rho)$ for a given density $\rho$ is then taken to be $\rho \cdot \langle v(\rho) \rangle$, where $\langle \rangle$ is a time average over all regions which had a particular density $\rho$. The flux-density curve, obtained by averaging over 10,000 iterations, are shown in figure 2. Here, the parameters are the same as those of figure 1. The fact that a well-defined flux-density curve exists suggest that the density waves (traveling density fluctuations) are kinetic in nature. Furthermore, the flux-density curve for the granular flow resembles that of a traffic flow, which is considered as a prime example of the systems which shows kinetic waves [6].

One additional piece of evidence that the density waves are of a kinetic nature is their dependence on the initial density $\rho_0$. The theory of kinetic waves predicts [6] that small density fluctuations in a uniform density background $\rho_0$ travel with a velocity

$$U(\rho_0) = \left. \frac{dj(\rho)}{d\rho} \right|_{\rho=\rho_0},$$

which is the slope of the flux-density curve at the mean density. We thus expect a large negative velocity for small $\rho_0$, a decrease to zero velocity at $\rho_0 \approx 15$, with an increasingly large positive velocity as $\rho_0$ is increased further. To check this, we measure the wave velocities for several values of $\rho_0$ (keeping all other parameters fixed as above). Writing the mean density $\rho_0$ and the measured velocity $U(\rho_0)$ as $(\rho_0, U(\rho_0))$, we find $(10.0, -41 \pm 2)$, $(15.0, 5 \pm 9)$, $(18.7, 12 \pm 11)$ and $(22.5, 113.0 \pm 4)$, which are all consistent with the above prediction.

We now consider the theoretical aspect of the density waves. Consider the equations of

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Fig. 1. — Time evolution of (a) density and (b) velocity fields. These simulations were done with a tube of width $W = 1$ and length $L = 15$. Fields at a given time are shown as a vertical line of small boxes. The grayscale of each box is proportional to the value of the density or velocity in that region of the tube. Regions of high density are formed, and travel with almost constant velocity.
Fig. 2. — Local flux as a function of local particle density. This curve was found for a tube with width \( W = 1 \) and length \( L = 15 \), obtained by time averaging. The parabolic shaped curve resembles the flux-density relation in traffic flows.

motion which govern the time evolution of the density \( \rho(x, t) \) and the velocity \( v(x, t) \) fields for a granular flow in a vertical tube. The first equation is that of mass conservation

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0, \tag{3a}
\]

and the second is a momentum conservation equation

\[
\rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial x} = F(x, t), \tag{3b}
\]

where \( F(x, t)dx \) is the total amount of force acting on the particles in a region \( [x, x + dx] \). The force \( F(x, t) \) has three contributions — gravity, internal pressure, and friction from the sidewalls. The exact form of the internal pressure and the friction is not known. Here, we use Bagnold’s law, which is believed to be valid in the grain inertia regime [7]. Therefore, the force \( F(x, t) \) is

\[
F(x, t) = -\rho g W - \text{sign}(v) \rho_B f_{xy}(p)v^2 - D \frac{\partial}{\partial x}[\rho_B f_{xx}(p)v^2] \tag{4}
\]

Here, \( g \) is gravitational acceleration, \( \rho_B \) the density of the material which forms the particles, \( p \) the packing fraction (\( \rho = \rho_B p \)) and \( D \) is the diameter of the particles. We assume the thickness of the shear layer to be of order of \( D \). Also, \( f_{xx} \) and \( f_{xy} \) are geometry dependent functions, which contain the information about the density dependence of the forces.

The uniform density solution of equation (3) with the force given by equation (4) is

\[
\rho(x, t) = \frac{\rho_B \rho_o}{\sqrt{\rho_o g W / f_{xy}(\rho_o)}} \]

\[
v(x, t) = -\sqrt{\rho_o g W / f_{xy}(\rho_o)} \tag{5}
\]

If we add small density fluctuation \( \rho = \rho_o + dp \) in the uniform density flow, the fluctuation
travels with a velocity

\[ U(p_0) \simeq -\frac{1}{2} \sqrt{p_0 g W/f_{xy}(p_0)} \cdot \frac{3f_{xy}(p_0) - p_0 df_{xy}(p_0)/dp}{f_{xy}(p_0)}, \]

which is given by equation (2). Equations (5) and (6) are exactly what one expects if the kinetic wave theory is to apply – uniform flow is a solution to the equations of motion, and density fluctuations travel with a density dependent velocity.

Thus, it is clear then that the motion of the density pattern can be understood by applying the ideas of kinetic wave theory. However, this basic formalism only describes the motion of a pre-existing density pattern. It does not explain the observation that regions with large density contrasts are being formed out of the uniform background. Our simulations show that the large scale density pattern begins as a collection of small fluctuations in the density. These small fluctuations grow in time and a pattern emerges in which large density contrasts exist between neighboring regions. The evolution to such a state can be understood by considering the system as set of interacting kinetic waves. A detailed treatment of the general problem of interacting kinetic waves can be found elsewhere [11]; in this paper, we present only the results from a simple model for the pattern evolution process in sand flowing down a tube.

Consider the early stages of the flow in which the density of sand is nearly uniform at \( \rho \approx \rho_0 \). Because of the roughness of the grains, the roughness of the walls or from the stochastic nature of the inelastic collisions, small density fluctuations appear in the system. In the interacting density wave approach, we treat the fluctuations as a set of distinct density regions with interfaces whose velocities are determined by a discrete form of equation (2). In this case, the interface separating a region of density \( \rho_1 \) from a region with density \( \rho_2 \) moves with a velocity, \( U(1, 2) \), given by

\[ U(1, 2) = \frac{j(\rho_1) - j(\rho_2)}{\rho_1 - \rho_2}, \]

which is the kinetic wave theory result for interfacial velocities involving finite density differences [6]. In the case that the difference between \( \rho_1 \) and \( \rho_2 \) is very small, the equation becomes equation (2). The evolution of the system is determined by the motion of the interfaces and, as shall be shown, the nature of their interactions leads to a final state in which large density contrasts occur.

In the computational and analytic results that follow, we choose a specific form for the density fluctuations in the system. In our model, the initial positions of the interfaces are taken as a set of \( N_0 \) points placed randomly on the interval \([0, L]\), with regions between successive interfaces being assigned a density randomly in the range \([\rho_0 - W, \rho_0 + W]\). The principal virtues of this model are its simplicity and the fact that there are no correlations in the initial state which might influence the final structure. A more realistic model for the fluctuations of the system would require a microscopic understanding of each specific source of noise.

It is also necessary to choose a form for the flux curve \( j(\rho) \). We have taken the parabolic form

\[ j(\rho) = J_0 \frac{\rho}{R} \left(1 - \frac{\rho}{R}\right), \]

where \( R \) is the density at which no flow occurs, and \( J_0 \) is one quarter of the maximum flux of the system. This curve was chosen for several reason. The first is that its simplicity eases some of the hardships of analytical calculations. The second reason is that for density fluctuations over a sufficiently small range, the true flux response can be approximated by this form (with \( R \) and \( J_0 \) being fitting parameters). And finally, it is a first approximation to the form observed for the \( j(\rho) \) observed in figure 2.
Numerical simulation of this system is a very straight-forward exercise. The values of the densities in two adjacent regions determine the velocity of the associated interface. Consider three successive density regions A, B and C. During the course of the simulation, the interface A-B may encounter the interface B-C. This indicates that all of the mass that was inside region B has been completely "swallowed up" by the regions A and C. In this case, the interfaces A-B and B-C are replaced by a single A-C interface. The velocity of this interface can be calculated from the densities in regions A and C. Thus, it is a matter of tracking all of the interfaces, checking for collisions, and when they occur, replacing the two old interface with a single new one. Therefore, this technique does not allow for any density values other than those initially present, and the number of interfaces is always decreasing. For convenience, the simulations were done using periodic boundary condition.

The first set of results shown below are from a simulation in which there are 400 interfaces initially placed randomly in the interval [0,1] (i.e. $L = 1$). We also choose the values $J_0 = 1$ and $R = 1$. The densities are chosen at random from the interval $[0.3,0.8]$ (i.e. $\rho_0 = 0.55R$, $W = 0.25R$). Figure 3a shows the initial density configuration, while figure 3b shows the system after a time $t = 0.486$ (where time is measured in the units of $RL/J_0$), and there are only 33 interfaces which remain along the interval. The system has evolved to a state in which the density contrast is very high between neighboring regions, and this behavior was observed for all values of $\rho_0$ and $W$.

This increase in the density contrast can be characterized quantitatively in the following way. Let the density of each region be $\rho_i$, with $i$ indexing the different regions, and $N(t)$ be the number of regions at time $t$. Define the quantity

$$M(t) \equiv \frac{1}{N(t)} \sum_{i=1}^{N(t)} |\rho_i - \rho_{i+1}|,$$

where $\rho_{N(t)+1} \equiv \rho_1$. The larger the value of $M(t)$ the larger the density contrast between neighboring regions. Figure 4 shows the quantity $M(t) - M(0)$ averaged over 10 simulations with $N_0 = 10,000$ interfaces. At early times, there is a linear increase in $M(t)$ with a crossover to a nearly constant value at late times.

At early times, it is possible to calculate $M(t)$ analytically and the results are shown as the dotted line in figure 4. In this regime, the changes in $M(t)$ are dominated by the interaction of interfaces whose movements are determined by the initial configuration of the system. The
Fig. 4. — Contrast, $M(t)$, as function of time, $t$. The solid line shows the results from averaging over 10 simulations with $N(0) = 10,000$, and densities chosen in the range $[0.3, 0.8]$. At early times, the increase in contrast is linear and at long times it becomes a constant. The dashed line shows the results from an analytical calculation of the short time behavior.

calculation averages over all possible configurations of the initial random densities and interfaces, determines the time at which each interface collision occurs and how much that collision changes the value of $M(t)$. In this regime, the agreement with the simulation is good. It is also possible to show exactly that $M(0) = 2W/3$. At later times, after there have been many collisions between interfaces, the structure of the system depends on the nature of the earlier evolution. Thus, this long time behavior is much more difficult to calculate. The results from the calculation described above break down in this regime because the distribution of density regions is no longer that of the initial random distribution.

At long times $M(t) \approx 2W$. Thus, the density contrast at long times is, on average, as large as the largest density contrasts present in the initial configuration. It turns out that the interacting kinetic waves do not create large contrasts. Rather, the interfaces from the initial distribution which survive are those that have a very large density contrast [11]. Thus, while the noise in the system may provide a variety of such contrasts, the interacting kinetic waves will destroy all but the very largest.

This paper outlines a kinetic wave approach to understanding the density patterns observed in sand flow along a vertical tube (many of the details omitted here can be found in references [10, 11]). However, these ideas certainly do not constitute a complete theory for the patterns observed in the experimental system. The role that the flow of air plays in this process [12], as well as the sources of noise in the system, are certainly not well understood. Further experimental investigation of these issues would be most enlightening. From a theoretical point of view, it is not clear whether the frictional force at the wall and the internal pressure obey Bagnold's law. While this form has been observed in the sheer cell geometry [7, 13], there has been no direct measurement of the frictional force for gravity driven flow. Finally, it is known that the interface between two regions of differing densities may not be a stable
structure [6], and that diffusive effects may strongly influence the long time behavior of a system of interacting kinetic waves.

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