# Sand as Maxwell's Demon

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We consider a dilute gas of granular material inside a box, kept in a stationary state by vertical vibrations. A wall separates the box into two identical compartments, save for a small hole at some finite height $h$. As the gas is cooled, a second order phase transition occurs, in which the particles preferentially occupy one side of the box. We develop a quantitative theory of this clustering phenomenon and find good agreement with numerical simulations.

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One of the most outstanding features of a gas of granular material is its tendency to spontaneously form highly concentrated regions or clusters [1–4]. So even in its gaseous state it behaves fundamentally different from a molecular gas, which keeps its uniform density. Apart from throwing light on the nonequilibrium properties of a granular gas, this clustering instability is of major technological importance. Imagine a flow of rocks down a chute: whenever a very dense region has formed due to the instability, the rocks may easily get entangled and the flow is stuck.

In a molecular gas collisions are overwhelmingly elastic, so maximizing the entropy requires the equilibrium state to be spatially uniform. In the case of a granular material collisions are inelastic, and entropy is transferred to the microscopic degrees of freedom by the way of heating or through changes in the microstructure. As a result the granular assembly may assume a more ordered state. Qualitatively, the mechanism behind this ordering is that for binary collisions the rate of energy loss grows quadratically with the density, with a volume-fraction dependent correction at high concentrations. This means that a dense region rapidly cools, increasing the density even more according to the equation of state.

Goldhirsch and Zanetti [3] used a hydrodynamic description of a dilute gas or "rapid granular flow" [5–9] to show that this mechanism leads to a long-wavelength instability of a homogeneous assembly of inelastic particles. In the absence of driving the density becomes so high that the equations used in [3] are no longer valid, and indeed any result based on kinetic theory becomes meaningless as the particles eventually come to rest. Another complication is the *inelastic collapse* known to occur inside clusters [4], i.e., an infinity of collisions in finite time. In the experiment described in this Letter, a stationary state is maintained by an external driving. On one hand, this keeps the gas sufficiently dilute so that simple leading order density expansions are applicable throughout. On the other hand, the existence of time-independent solutions without mean flow simplifies the problem tremendously, so that analytical solutions are feasible. As the hydrodynamic instability of [3] is a shear instability with finite mean velocity, it is clearly distinct from the phase separation described here, although the central mechanism of collisional cooling remains the same.

The experiment, first described by Schlichting and Nordmeier [10], consists of a box of base area 12 cm$^2$ and height 20 cm, mounted on a shaker, and filled with $N = 100$ plastic particles of radius $r = 1$ mm (see Fig. 1). The box is separated into two equal parts by a wall which has a narrow horizontal slit at a height $h = 2.3$ cm. When the shaker is operating at full power, the amplitude in vibration is approximately $A = 0.3$ cm and the frequency $f = 50$ Hz. Even if all particles are on one side initially, they rapidly distribute equally to both sides. Lowering the frequency below a critical value of 30 Hz the symmetry is spontaneously broken, and particles settle preferentially on one side. As seen qualitatively in Fig. 1 the wall separates a dilute phase at high temperature from a dense phase a low temperature, meaning that the particles fall to the bottom. In the limit that the hole is so small that its surroundings are virtually undisturbed one expects a discontinuous jump of density and temperature across the boundary.

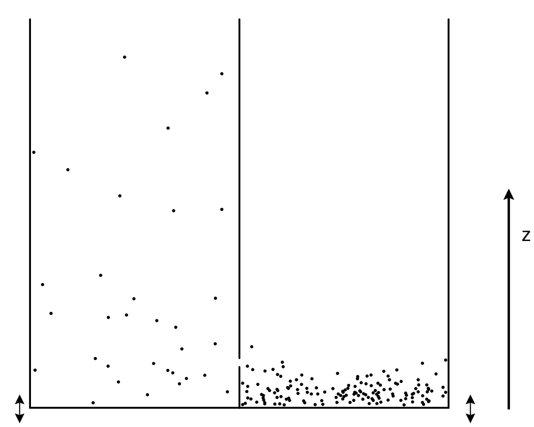


FIG. 1. A drawing of the experimental setup. The two sides of the box are connected by a hole at height $h$. The picture is taken below the bifurcation, so most particles have settled on the right hand side. As a result, the gas sinks to the bottom, reducing the flux.

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The grains thus act as Maxwell's demon [11], who preferentially lets particles pass from left to right or vice versa. As a result, a more ordered state is formed in which most particles are on one side. The demon must then absorb entropy, a role which in our system is assumed by the sand grains. Still another interpretation would be that of a dissipative structure, which in the stationary state is maintained by a flux of entropy [12].

The experimental findings are easily reproduced by a numerical simulation of the event-driven type [13]. To reduce the numerical effort we use a two-dimensional simulation, where the particles are represented by smooth and hard disks. Upon collision, the normal velocity is reduced according to $v_n' = -ev_n$, where $e$ is the coefficient of restitution. To minimize wall effects, which are not essential to our problem, all wall collisions are assumed to be elastic. The top is left open. For simplicity, the bottom of the container is taken to move in a sawtooth manner, such that a colliding particle always finds it to move upward with velocity $v_b = Af$. In addition the amplitude $A$ of the vibration is assumed to be very small compared with the mean free path, so that the bottom is effectively stationary. In summary this means that the $z$ component of the velocity of a particle colliding with the bottom is changed according to $v_z' = 2v_b - v_z$.

The transition is best characterized by the asymmetry parameter $\epsilon = (\bar{N}_{\ell/r} - \bar{N}/2)/\bar{N}$, where the overbar denotes the number of particles relative to the half-width of the container. Figure 2 shows the average value of $\epsilon$ as function of $h$ for $\bar{N} = 225$ as circles, which exhibits a behavior typical of a second order phase transition as $h$ is raised above a critical value. This is not surprising since the present nonequilibrium transition is associated with a

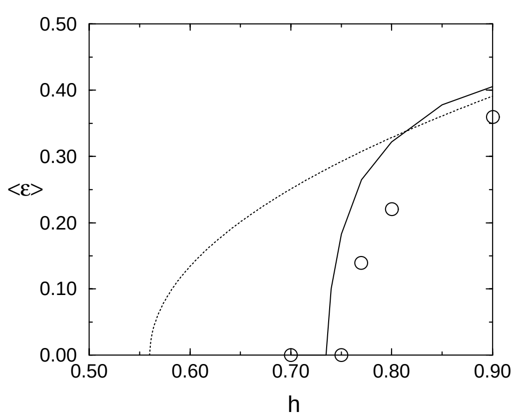


FIG. 2. The bifurcation of the asymmetry $\epsilon$ as function of the height $h$. The circles represent numerical simulations with $N = 360$ particles in a box of half-width 1.6, averaged over time. The particles are circular disks of radius $r = 0.01$ and coefficient of restitution $e = 0.95$. The velocity of the bottom is $v_b = 0.149$, acceleration of gravity is $g$, and mass $m$ is normalized to one. The full line is the result of the theory presented in this paper; the dotted line comes from a simplified bifurcation analysis.

spontaneous breaking of the symmetry between left and right [14].

To treat the transition theoretically, we observe that the condition of stationarity is that the total flux between the two compartments is zero, i.e., the fluxes going from one side to the other cancel:

$$F_{\ell\to r}(h) = F_{r\to\ell}(h)\,. \qquad (1)$$

A nonsymmetric solution of (1) becomes possible because the flux $F$ is no longer a monotonously increasing function of the number of particles as it would be in equilibrium. Another hallmark of a nonequilibrium system is that the stationary state is described by a flux balance (1), while the temperature on either side of the hole is not equal, as it would be in thermal equilibrium.

In the limit that the connecting hole is small, it remains to find the density and temperature distribution in a one-dimensional column of a vibrated granular assembly, from which we calculate the flux of particles leaving a compartment at the height of the hole $h$. In the next few paragraphs the left and right hand sides of the problem is first treated separately as a one-dimensional column of gas in a gravitational field. We compute the profiles using a continuum theory, then we compare with numerical simulations of a gas of smooth, inelastic disks. Knowledge of the one-dimensional profiles will then allow us to look for solutions of (1). We show that (1) has a single solution for strong driving or small $h$, but two asymmetric solutions become stable as the driving is lowered or $h$ is increased. A simplified analytical theory shows that the transition is controlled by a single combination of the input parameters. Finally, we study the effect of fluctuations.

*One-dimensional column.*—The problem of a vertically vibrated granular gas in a gravitational field has recently been treated in a number of papers [15–17]. Equations of motion for the number density $n(z)$, pressure $p(z)$, and granular temperature $T(z)$ can be found from conventional kinetic theory [5,6]. The position $z$ is measured from the bottom of the container and the granular temperature is defined as $T = \langle v^2 \rangle / d$, where $d$ is the dimension of space and $v$ is the velocity of a particle. This definition of temperature is customary for granular media, but differs from the usual molecular temperature, which is recovered by formally setting $k_B = m$. Now the stationary equations become in the dilute limit

$$p = mnT, \qquad \partial_z p = -mgn\,,$$
$$\kappa \partial_z [T^{1/2} \partial_z T] = (2\kappa/3) \partial_z^2 T^{3/2} = Dn^2 T^{3/2}. \qquad (2)$$

The first equation is the usual equation of state; the second is the force balance, where $-mg$ is the force on a single particle. The third equation is the balance of heat flux and dissipation due to inelastic collisions. As usual, the thermal conductivity $\kappa T^{1/2}$ is proportional to the average particle velocity. In the simplest possible model of hard and smooth particles the energy loss in one collision is proportional to $(1 - e^2)T$ on the average. Together with the number of collisions being proportional to $n^2 T^{1/2}$ this explains the form of the loss term on the right hand side of the third equation (2).

We will consider the two-dimensional case of circular disks of radius $r$, for which the coefficients are found to be [6] $\kappa = \pi^{-1/2} m/r, D = 4\pi^{1/2} mr(1 - e)$. Next, we have to supply boundary conditions. In the derivation of (2) it has been assumed that the velocity distribution is nearly Maxwellian, and making the same assumption for the velocity distribution at the boundary allows us to calculate the rate of energy input per unit width (or unit area in 3D) to

$$Q = mn[v_b T(0) + \sqrt{2/\pi}\, v_b^2 T(0)^{1/2}]. \qquad (3)$$

We will see below that the first term in (3) dominates, the second typically being smaller by a factor of 10 in our simulations. The two boundary conditions for $z = 0$ become

$$p(0) = -gm\bar{N}, \qquad Q = -\kappa T^{1/2} \partial_z T(0), \qquad (4)$$

where the first equation comes from integrating the force balance. The second equation balances the energy input with the heat flux out of the bottom according to (2).

Since (2) is of third order, another boundary condition is needed for a unique solution. The missing third condition is found by observing that (2) allows for a solution of the form $T^{3/2}(z) = cz + b$ and $n(z)$ decaying exponentially for large $z$, as expected on physical grounds. In that case $c$ must be zero to prevent $T$ from becoming negative or infinity. This is the desired third condition, and solutions are easily found by shooting for a temperature profile which is asymptotically constant. The resulting temperature and density profiles are shown as dotted lines in Fig. 3 for a typical set of parameters, from which it is seen that the temperature is mostly constant apart from a boundary region.

This suggests an even simpler theory [16] where the temperature is assumed to be constant, which allows us to calculate the profiles in closed form. Namely, at constant temperature the density is an exponential and $T_\infty$ is found from a balance of the energy input and dissipation:

$$n(z) = \frac{g\bar{N}}{T_\infty} e^{-gz/T_\infty}, \qquad T_\infty = \left(\frac{2mv_b}{D\bar{N}}\right)^2. \qquad (5)$$

Here we have neglected the second term of (3) in favor of the first. This as well as the form of the profiles (5) is asymptotically correct for $e \to 1$. The resulting profiles are the dashed lines in Fig. 3. Evidently, the present theory is more accurate, but the constant temperature solution has the great merit of simplicity and still contains the essentials.

Next we assess the quality of the predictions of continuum theory by comparing with a numerical simulation as described above (solid lines). The agreement is quite good, but gets worse if the number of particles is reduced, and deteriorates even more in three dimensions. The reason is that even for the parameters of Fig. 3 the temperature changes significantly over the length of the mean free path. As a result, the distribution of the $v_z$ velocities of particles hitting the bottom deviates significantly from a Maxwell-Boltzmann distribution at $T(0)$.

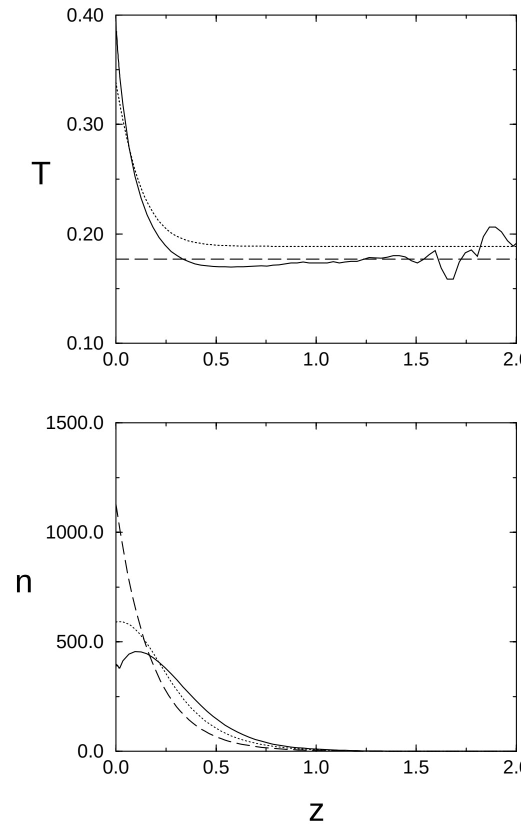


FIG. 3. Temperature and density profiles of $N = 320$ grains in a box of width $w = 1.6$. All other parameters are the same as in Fig. 2. The full line is the result of a particle simulation, the dotted line is the present theory, and the dashed line is (5).

*Bifurcation.*—Returning to the original stability problem, the *flux* through a hole of area $S$ is found to be $F = Sn(h)\sqrt{T(h)/2\pi}$. Using this formula, and solutions of (2)–(4) to find the profiles, one can look for solutions of (1) subject to the constraint $\bar{N} = \bar{N}_\ell + \bar{N}_r$ that the total number of particles is conserved. Figure 2 shows the solution of (1) as a function of $h$ for $\bar{N} = 225$ as the solid line, in good agreement with numerical simulations. Even more insight can be gained by computing the fluxes according to the simplified solution of (5), where the temperature is assumed constant over one-half of the container. From (5) we find the average flux $F_{\ell\to r} = F_0 \bar{N}_\ell^2 \exp(-a\bar{N}_\ell^2)$, where $F_0$ is a constant and $a = 4\pi ghr^2(1 - e)^2/v_b^2$. The equation of motion for $\epsilon$ thus reads

$$\partial_t \epsilon = F_0 N[(\epsilon - 1/2)^2 e^{-\mu(\epsilon - 1/2)^2} - (\epsilon + 1/2)^2 e^{-\mu(\epsilon + 1/2)^2}] + \xi, \qquad (6)$$

where $\xi$ is a noise term which comes from fluctuations in the flux that will be considered later. The vanishing of the angular brackets, which means that the two fluxes are equal, is controlled by the parameter

$$\mu = 4\pi(gh/v_b^2)(r\bar{N})^2(1 - e)^2 \tag{7}$$

alone. If $\mu > 4$, the equation $[\cdots] = 0$ has three roots and the two asymmetric solutions become stable. Not surprisingly, broken symmetry is favored for large inelasticity $1 - e$ and particle densities $r\bar{N}$, but also if the combination $gh/v_b^2$ gets large. Small $h$ implies that the hole is near the bottom, which allows for a ready exchange of the low-temperature "condensate" with the other side. Strong external driving corresponds to large $v_b$, which also tends to restore the symmetric state. Just above the bifurcation the asymmetric solutions are described by $\langle\epsilon\rangle = \pm\sqrt{3(\mu - 4)/16}$, which is included as the dashed line in Fig. 2. While there is an offset between the simplified theory and the simulation, it does describe the form of the bifurcation fairly well using the single parameter $\mu$.

To estimate the amplitude of the noise term in (6) we assume that the particles passing through the hole are uncorrelated. This means that if $\langle\Delta\rangle$ is the average number of particles passing from left to right in a given time interval, then $\langle(\Delta - \langle\Delta\rangle)^2\rangle = \langle\Delta\rangle$. On a coarse-grained time scale this is equivalent to saying that $\xi$ in (6) is uncorrelated Gaussian white noise [18], with the second moment given by

$$\langle\xi(t)\xi(t')\rangle = F_0[(\epsilon - 1/2)^2 e^{-\mu(\epsilon-1/2)^2} + (\epsilon + 1/2)^2 e^{-\mu(\epsilon+1/2)^2}]\delta(t - t'). \tag{8}$$

Note that the constant $F_0$ can be eliminated by rescaling time, so the strength of the noise is controlled by the total number of particles alone. By considering the fluctuations around the local minimum to Gaussian order, we find [18] $\sqrt{\langle(\epsilon - \langle\epsilon\rangle)^2\rangle} = [4N(\mu - 4)]^{-1/2}$. Adjusting this formula to the critical value of $\mu_{cr} = 5.4$ found from simulation this gives $\sqrt{\langle(\epsilon - \langle\epsilon\rangle)^2\rangle} = 0.045$ in reasonable agreement with numerical simulations. Of course, Eqs. (6)–(8) also allow for a more detailed analysis of transitions between the two asymmetric states and many more questions relating to the critical fluctuations typical of a second order transition. This will be considered in more detail in future publications.

In conclusion, hydrodynamic equations are a very valuable tool to describe a dilute granular gas. The greatest problem lies in the formulation of the boundary conditions. The clustering instability can be understood in terms of a very simple experiment, which we model in a static, one-dimensional description.

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