Dynamics that trigger/inhibit cluster formation in a one-dimensional granular gas

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Abstract

We present a study of a one-dimensional granular gas of point-like particles not subject to gravity between two walls at granular-temperatures T_- and T_+, with $T_- < T_+$ and submit a physical picture of the mechanism that triggers or inhibits cluster formation. It is known that, depending on the normalized temperature difference $\Delta = (T_+ - T_-)/(T_+ + T_-)$, the system may be completely fluidized, or in a mixed state in which a cluster coexists with the fluidized gas. We devise and explain in detail a method for integrating the one-dimensional dissipative Boltzmann equation in the test-particle limit for the stationary case. The behavior of the system in its fluid phase is dominated by characteristic lines which are trajectories of particles subjected to a force which attracts them to a fixed point. If this point lies between the two walls a cluster forms, if not then the system remains fluidized.

Keywords: Granular; Clustering; Boltzmann equation

1. Introduction

Granular systems have been the focus of much attention due to both the theoretical challenges they present [1] and to the applications of industrial importance that stem

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from the rich phenomena they exhibit (see Ref. [1] and references therein). These systems are characterized by a loss of energy in collisions, and this loss is at the base of many interesting phenomena. Among these, the clustering of particles has drawn much attention [2–5].

In this paper, we present the detailed mechanism that allows us to understand the dynamics—in the quasielastic limit—of a one-dimensional system not subject to gravity between the two thermalizing walls. The paper gives a picture of the dynamics that trigger/inhibit cluster formation. This physical picture is complementary to and clearer than what we presented in Ref. [5]. From the mathematical point of view the system is described using Boltzmann's integro-differential equation and in this article we describe a way to integrate it numerically. It is necessary to perform such integration from the analysis by which the physical pictures emerge.

The system consists of point-like particles, confined in a box of unit length, that interact via collisions that conserve momentum but dissipate kinetic energy. Any particle that reaches a wall is expelled from it with its velocity randomly chosen from a Maxwellian distribution with the "temperature" of that wall. There are no external forces. A cluster may or may not be formed. In our previous article we saw that there are two relevant control parameters: the restitution coefficient which characterizes the collisions and the normalized temperature difference Δ between the walls, $\Delta \equiv (T_+ - T_-)/(T_+ + T_-)$. In the plane of these two parameters there is a *transition line*, shown in Fig. 1: above it the system is a granular fluid that reaches a stationary state while on the other side a cluster forms and, apparently, no stationary solution can be reached, at least in the limit of infinitely many particles. In Ref. [5] we described what happens, while in the present paper we disclose the underlying physical mechanism.

In our previous article, we gave clear evidence that Boltzmann's equation describes faithfully the results of molecular dynamics in the case of the pure fluid phase, even

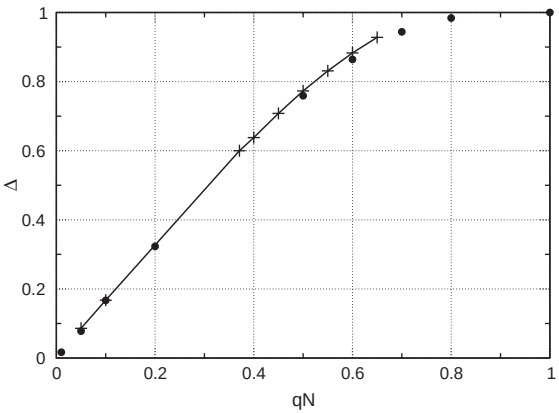

Fig. 1. Molecular dynamics simulations show that the (qN-Δ) plane has a threshold line, above which the system reaches a stationary fluid phase while below it a cluster coexists with a low density gas. See the text for details. It is argued that the clustering phase, in the $N \to \infty$ limit, never reaches a stationary state.

quite close to the transition line. To integrate Boltzmann's equation we used direct-simulation Monte Carlo (DSMC). That method of integration did not help us fully understand the mechanism that triggers/inhibits cluster formation. Here we provide a more direct way of integration, which should stand by itself as a contribution to integrate Boltzmann's integro-differential equation, while yielding an intuitive picture from the understanding of our integration method.

To fix notation, if c_1 and c_2 are the velocities of two particles that are about to collide, their velocities after the collision are $c_1' = qc_1 + (1-q)c_2$ and $c_2' = (1-q)c_1 + qc_2$. Here $q = (1-r)/2$, where r is the usual restitution coefficient. For the elastic case ($q = 0$) the particles simply exchange velocities. Since the grains are point-like, the elastic case is then indistinguishable from a system in which the particles do not interact. More explicitly, the point-like character of the grains allow us to exchange their identities after the collision, giving the collision rules $c_2' = qc_1 + (1-q)c_2$ and $c_1' = (1-q)c_1 + qc_2$. Thus, when $q = 0$ the velocities are unaffected, and when q is small the velocities barely change, yielding a system of weakly interacting particles, whose relative velocities decrease at every interaction.

The one-dimensional granular system is being excited from the two walls, generally at different temperatures T_- and T_+. Particles emerging from the walls act as a *wind* pushing the particles away from them. One could picture the effect of this wind as an effective *repulsive force* which pushes the particles away from the walls. If the temperature difference between the walls is large enough, the repulsive force associated to the hotter wall prevails over the force associated to the colder wall across the system. Therefore in this case the overall effect is a net force everywhere pointing toward the colder wall, much like how gravity acts in a gas, always pointing to the base. If, on the contrary, the temperature difference is not large enough, there is a point in the system where the two repulsive forces cancel each other, producing an equilibrium point—a particle at rest in this point would tend to remain at rest—about which a cluster grows. As the cluster absorbs particles the density of the surrounding gas decreases, and the equilibrium point may shift in time.

In the limit $N \to \infty$, but keeping qN fixed, the one-dimensional Boltzmann equation transforms into the test-particle equation [3,4,6]

$$\partial_t f + c\partial_x f = qN\partial_c(Mf), \quad M(x,c) \equiv \int_{-\infty}^{\infty} f(x,c')(c-c')|c-c'|\,\mathrm{d}c' \,. \tag{1}$$

Since the equation is nonlinear, we must define explicitly the normalization

$$\int_0^1 \int_{-\infty}^{\infty} f(x,c)\,\mathrm{d}c\,\mathrm{d}x = 1 \,. \tag{2}$$

The system is confined in a box of unit length, and the particles may have any velocity: $(x,c) \in [0,1] \times (-\infty,\infty)$. Particles reaching a wall immediately bounce back so that the velocity distribution of expelled particles is a Gaussian distribution at the temperature of that wall, which corresponds to choosing wall kernels without memory and without a delay time (see Ref. [7])

$$f(0, c>0) \propto \mathrm{e}^{-c^2/2T_-}, \quad f(1, c<0) \propto \mathrm{e}^{-c^2/2T_+} \,. \tag{3}$$

The temperatures at both walls are chosen so that the system temperature for the perfectly elastic case is $T_0 = \sqrt{T_- T_+} = 1$. We will always take $T_+ \geqslant T_-$. The missing constants in Eq. (3) are determined by Eq. (2) and by imposing that there is no flow across the walls:

$$\int_{-\infty}^{\infty} c f(x_{\text{wall}}, c)\, \mathrm{d}c = 0 \,. \tag{4}$$

2. The fluidized stationary case

In a stationary situation, Eq. (1) may be rewritten as follows:

$$c\partial_x f - qNM\partial_c f = qNf\partial_c M \,. \tag{5}$$

The coefficient $-qNM$ multiplying $\partial_c f$ plays the role of a force (per unit mass) and it is what we have called *wind*. It is the effective acceleration of a particle at x with velocity c. When we are reasonably close to the solution, M will not depend on the detailed form of f. Thus, if we have a trial distribution f_n, we may consider M and $\partial M/\partial c$ as given functions of x and c, and then we may solve Eq. (5) for the distribution f_{n+1}. Seen in this light, close to the solution, Eq. (5) is approximately a linear partial differential equation that can be analyzed as a hyperbolic equation for f_{n+1} since M, defined in terms of f_n, is known. Thus, we obtain an iterative method that converges to the solution of Eq. (5), at every step integrating a hyperbolic equation.

Hyperbolic equations can be integrated using the notion of characteristic curves [8]. We dedicate a few words to the method, applied to our case, since some readers may not be familiar with it. Hyperbolic equations can be reduced to integrating a set of ordinary differential equations in an independent variable s. The family of curves $(x(s), c(s), f(s))_P$, for different starting points P, forms the parameterized form of the solution to the original equation. The ordinary differential equations have as right-hand sides the coefficients of the partial derivatives in the original equation. In the present case, the characteristic curves satisfy

$$\frac{\mathrm{d}x}{\mathrm{d}s} = c, \qquad \frac{\mathrm{d}c}{\mathrm{d}s} = -qNM(x,c), \qquad \frac{\mathrm{d}f}{\mathrm{d}s} = qNf\partial_c M(x,c) \,. \tag{6}$$

In simple words, our integro-differential equation is treated as if it were a quasi-linear partial differential equation and, since real characteristics exist, it is possible to integrate along these lines dealing with a set of ordinary differential equations. More specifically, given a distribution f_n (which implies that we know M_n and $\partial_c M_n$), we calculate f_{n+1} by solving $c\partial_x f_{n+1} - qNM_n\partial_c f_{n+1} = qNf_{n+1}\partial_c M_n$ through numerical integration of Eqs. (6) along the characteristics. After the integration we normalize f_{n+1} to one, and then use f_{n+1} to calculate f_{n+2}. In this way we eventually reach a fixed point.

If in the first two of Eqs. (6) the parameter s is seen as time, these are the equations of motion of a particle with position x, velocity c subject to a force $F \equiv -qNM(x,c)$. This force is very much like a simple viscous force: for large velocities $F \propto -|c|c$ and when M is small, $F \propto -(c - V_w(x))$, vanishing when c takes a value $V_w(x)$ that we

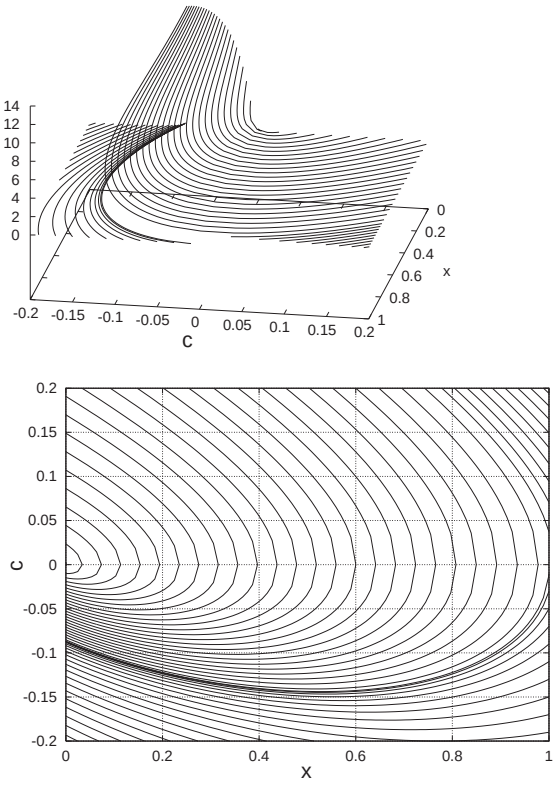

Fig. 2. Top: the distribution function $f(x,c)$ for the case $qN = 0.35$ and $\Delta = 0.6$. Bottom: the projection of the characteristic curves into $(x–c)$ space for the same case.

comment on later. The three equations (6) together determine the characteristic curves (x, c, f), as already pointed out in Refs. [3,4]. The projection of any characteristic line on the (x, c) plane corresponds to the phase–space trajectory of a *test particle* crossing the system.

There are two types of characteristics in Fig. 2: those that begin a $x = 0$ associated to the boundary condition $T = T_-$ and those that begin at $x = 1$ associated to the boundary condition $T = T_+$. The solution is in general discontinuous along the separatrix of these two types of curves. Since our numerical algorithm integrates along these characteristics, it never crosses the discontinuity; every step deals with a smooth function.

3. The wind velocity function and the clustering regime

As mentioned before, the line $M = 0$ defines a velocity V_w as a function of x that can be regarded as the local velocity of the wind, since, as seen in Eq. (6b), $\mathrm{d}c/\mathrm{d}s = 0$

on this line. In Fig. 2 this line lies in the region $c < 0$, that is $V_w(x) < 0$ for all x, meaning that in that case the wind is blowing to the left throughout the system.

Comparing the *wind velocity function* $V_w(x)$ for different fluidized solutions, it is observed that they are all negative, but they approach $c = 0$ as we near the transition line in Fig. 1. Our integration algorithm does not converge when the transition line is reached. In Fig. 1 the plus signs show the lowest values of Δ for each value of qN before our algorithm becomes unstable. The circles show the lowest values of Δ for each qN before a cluster is detected in a molecular dynamics simulation of $N = 1000$ particles. The plus signs are joined by a line to guide the eye.

Our molecular dynamics simulations show that below the transition line particles, on the average, move in trajectories like those shown in Fig. 3. The wind velocity function crosses the c-axis at some point x_0 and the phase–space trajectories spiral around this point. In fact, the transition line is defined by the condition that the $M = 0$ line touches for the first time the c axis, and this takes place when $x = x_0 = 0$, that is,

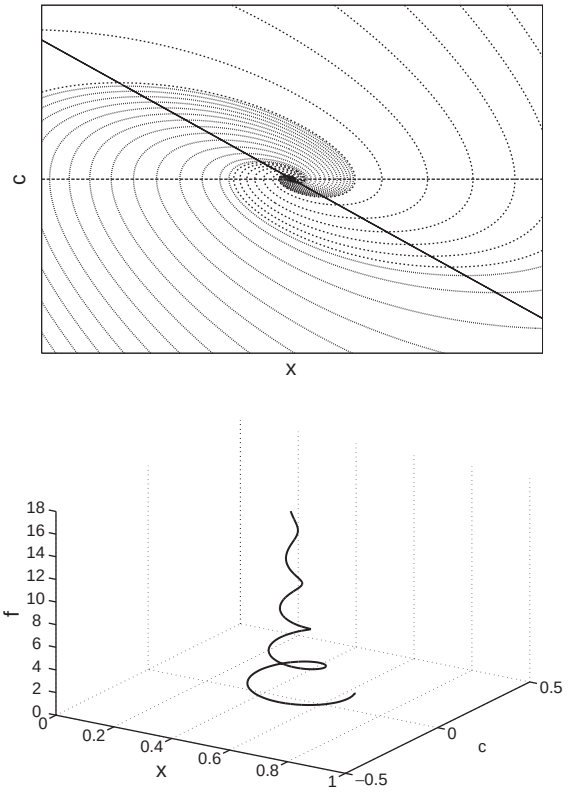

Fig. 3. Top: the trajectories of particles in (x–c) space when there is a *wind* whose velocity (function of x, represented by an almost straight diagonal line in the figure) vanishes at some point. Bottom: one trajectory in (x–c–f) space spiraling around the point where the wind vanishes.

$M(x=0,c=0)=0$, namely $V_w(0)=0$. Varying Δ, this equation has one solution for each value for qN. The set of such solutions is the transition line.

Fig. 3 is a sketch of what would happen to the characteristics around the intersection point: they would spiral around it. Meanwhile, since $\partial_c M > 0$ in that vicinity, we have that f is increasing along the curve. In other words, in (x,c,f)-space the characteristic curve becomes increasingly vertical, with f increasing sharply along it. If in the fluid case the function $V_w(x)$ is prolonged beyond the physical box, it vanishes at some point x_0 and the extension of the (x,c) trajectories would be seen to spiral about such unphysical point. Hence, that fixed point x_0 always exists, and the transition occurs when x_0 enters the box.

4. Conclusions

We have integrated the dissipative Boltzmann equation in the quasielastic limit integrating ordinary differential equations at every step. Part of them are equations of motion of a particle subjected to a *wind* with velocity $V_w(x)$, function of the net dissipation qN and the normalized temperature difference Δ. For the system to be completely fluidized the wind must not vanish at any point. As Δ decreases, V_w decreases in magnitude, first vanishing at the colder wall, where the cluster first forms. For smaller Δ the cluster detaches from the wall, with the characteristic curves winding around it and the surrounding areas becoming more rarefied, yielding a non-steady state.

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