Kinetic Theory for 1D Granular Gases

Rosa Ramírez and Patricio Cordero

Departamento de Física, Facultad de Ciencias Físicas y Matemáticas
Universidad de Chile, Santiago 3, Chile. e-mail: rosa@cecam.fr

Abstract. The Boltzmann like equation for a dissipative 1D granular gas, can be regarded, in the thermodynamic limit, as that of a simple particle inside a viscous medium - viscosity produced by the dissipative collisions with the rest of the particles. Analytical perturbative solutions can be found for this equation. We find that for low dissipative regimes, there is excellent agreement between our theoretical predictions for the macroscopic fields, and the measurementes from molecular dynamics simulations.

1 Introduction

Even if one dimensional granular systems are not totally realistic, they may reproduce several of the phenomena observed in higher dimensions [1–5]. They have also the advantage that both theory and molecular dynamic simulations are considerably easier to understand.

Our aim is to study within the frame of kinetic theory, a system of N inelastic point particles of mass $m = 1$ restricted to move under the action of gravity g in a 1D box of height L and bouncing on a base which we have chosen to behave as a thermal wall. The interaction between these particles is modeled by the inelastic collision rule $c_1' = q\,c_1 + (1-q)\,c_2$ and $c_2' = (1-q)\,c_1 + q\,c_2$ where the constant restitution coefficient is $r = 1 - 2q$. To describe this quasielastic system we write down a Boltzmann's like kinetic equation . The low dissipation thermodynamic limit ($N \to \infty$, $q \to 0$ with qN finite) leads to a highly simplified equation. Further assuming that qN is a small parameter, analytical perturbative solutions arround the elastic case can be found for this equation, that is, the stationary state for the quasielastic system is simply a distortion of the elastic stationary state. In other words, we study the regime in which the trajectories of the particles are only slightly modified by the dissipative collisions as shown in fig. 1. The elastic case—our reference system—deserves some comments.

A 1D system of elastic point particles is tantamount to a non-interacting system. In fact, relabeling the particles involved after each collision corresponds to a system of particles passing through each other without ever interacting. This leads to some important consequences. First, Liouville's distribution function for the N particle system is simply the product of the N one-particle distribution functions $F^{(N)}(\boldsymbol{z}_1 \cdots \boldsymbol{z}_N) = F^{(1)}(\boldsymbol{z}_1) \cdots F^{(1)}(\boldsymbol{z}_N)$ hence Liouville's equation exactly reduces to Boltzmann's equation: there are

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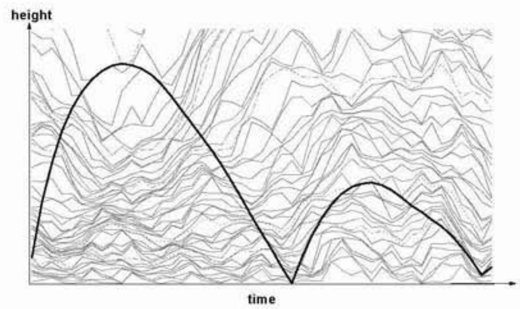

Fig. 1. Movement of one particle in the background of the rest of them for a quasielastic open system on a hot wall.

no particle-particle correlations at all. Second, due to the absence of any interaction between particles, the only way for the velocity distribution to evolve from a given initial condition is by the effect of the boundaries. Stochastic boundary conditions are absolutely necessary to define a stationary velocity distribution independent of the initial condition.

For this reason we will choose at the bottom a stochastic boundary defined in the same way as a thermal wall: any particle hitting the bottom wall will forget its velocity and will take a new one with a probability

$$W(c) = 2\,\frac{c}{\sqrt{2T_0}}\,e^{-c^2/2T_0} \tag{1}$$

T_0 being a temperature with dimensions of velocity squared. This boundary condition does not create any correlation and it destroys any one that the inelastic dynamics could create.

A conservative 1D system with such boundary condition will reach a Maxwellian distribution function in the stationary state—the trajectories of the test particles (relabeled after each collision) are just parabolas with different energies taken from the base and they do not see each other. In our quasielastic case, these parabolas are slightly modified as shown in Fig. 1, so that a perturbative expansion around the Maxwellian distribution is justified.

2 Kinetic Equation and Boundary Conditions

To describe the inelastic system we define the velocity $v_T = \sqrt{2\,T_0/m}$ and the length $L_T = \frac{T_0}{m\,g}$ which corresponds to the length scale of significant variations of the density in the elastic case. Besides we use the Froude number $Fr = L/L_T = \frac{m\,g\,L}{T_0}$ to describe the adimesional height of the system. If L is much larger than L_T, namely $Fr \to \infty$ the system will resemble an open system. On the contrary, if $Fr \ll 1$ the system will behave almost as if there was no gravity and the density and other fields will be nearly homogeneous. We will see both limits in Sec. 4.

We define a dimensionless distribution function for the stationary state $F(\hat{x}, \hat{c}) = L_T\, v_T\, f(x, c)$ normalized as

$$\int_0^{Fr} d\hat{x} \int_{-\infty}^{\infty} d\hat{c}\, F(\hat{x}, \hat{c}) = 1 \tag{2}$$

where the dimensionless position $\hat{x}$ and velocity $\hat{c}$ are $\hat{x} = x/L_T$ $\hat{c} = c/v_T$. Using these variables the collision term in Boltzmann's equation can be written as an expansion in the small parameter q [3] leading to

$$\left(\hat{c}\,\frac{\partial}{\partial \hat{x}} - \frac{1}{2}\,\frac{\partial}{\partial \hat{c}}\right) F(\hat{x}, \hat{c}) = N \sum_{k=1}^{\infty} \frac{q^k}{k!}\, \frac{\partial^k}{\partial \hat{c}^k} \left[M_k(\hat{x}, \hat{c}, ht)\, F(\hat{x}, \hat{c})\right] \tag{3}$$

where

$$M_k(\hat{x}, \hat{c}) = \int_{-\infty}^{\infty} |\hat{c} - \hat{c}'|\, \left(\hat{c} - \hat{c}'\right)^k\, F(\hat{x}, \hat{c})\, d\hat{c}' \tag{4}$$

Multiplying and dividing this right hand side by N^k—so that there is a factor $(qN)^k/(k!\,N^{k-1})$—and taking the limit $N \to \infty$ keeping qN fixed, (this is what we call the *hydrodynamic limit*), the kinetic equation becomes simply

$$\left(\hat{c}\,\frac{\partial}{\partial \hat{x}} - \frac{1}{2}\,\frac{\partial}{\partial C}\right) F(\hat{x}, \hat{c}) = qN\, \frac{\partial}{\partial \hat{c}} \left[M(\hat{x}, \hat{c})\, F(\hat{x}, \hat{c})\right] \tag{5}$$

where $M(\hat{x}, \hat{c}) \equiv M_1(\hat{x}, \hat{c})$. Equation (5) is the *hydrodynamic limit of Boltzmann's equation for a granular system in 1D*. In principle this equation is valid for any finite value of the parameter qN provided N is large enough. The collision term for a test particle in the original Boltzmann equation is replaced by an effective friction produced by the collisions with the rest of the particles. In this sense equation (5) represents a particle passing through a viscous fluid—viscosity produced by dissipative collisions—and suffering the corresponding acceleration, as observed for example in Fig. 1. Piasecki has already dealt with the idea of a particle moving inside a viscous medium [7]. We claim that Eq.(5) is the one which represents exactly the viscosity of this granular medium in the hydrodynamic limit.

As we can see the adimensional problem in the hydrodynamic limit depends solely on the Froude number, *Fr*, via the normalization condition and on qN via the kinetic equation. The boundary conditions we are about to use do not depend either on *Fr* nor on qN. If a boundary condition with two different temperatures at the bottom and top walls is used, then a third dimensionless parameter would come in. Since we are not going to deal with such case the only two dimensionless parameters that determine the stationary state of the system are *Fr* and qN.

3 The Quasielastic Regime

Although the kinetic equation is valid for any finite value of qN the following formalism is valid only in the *quasielastic regime* characterized by $qN \ll 1$. In this limit we look for solutions of the form

$$F(\hat{x},\hat{c}) = F^{(0)}(\hat{x},\hat{c}) + qN\,F^{(1)}(\hat{x},\hat{c}) + (qN)^2 F^{(2)}(\hat{x},\hat{c}) + \dots \tag{6}$$

where $F^{(0)}$ is the solution for the elastic case.

When $F(\hat{x},\hat{c})$ is replaced back in (5) we find a set of equations for each order of the distribution function. Each $F^{(s)}(\hat{x},\hat{c})$ follows an equation of the form

$$\left(c\,\frac{\partial}{\partial x} - \frac{1}{2}\,\frac{\partial}{\partial c}\right) F^{(s)}(\hat{x},\hat{c}) = J_{(s)}\left[F^{(s-1)}(\hat{x},\hat{c}), F^{(s-2)}(\hat{x},\hat{c}), \dots, F^{(0)}(\hat{x},\hat{c})\right] \tag{7}$$

where $J_{(s)}\left[F^{(s-1)}(\hat{x},\hat{c}), \dots, F^{(0)}(\hat{x},\hat{c})\right]$ is a function representing the collision term at order s and it only contains lower order functions.

We impose the normalization condition (2) so that at each order

$$\int_{-\infty}^{\infty} d\hat{c} \int_0^{Fr} d\hat{x}\; F^{(s)}(\hat{x},\hat{c}) \,= \delta_{0s}. \tag{8}$$

Each $F^{(s)}$ must also satisfy a boundary condition at the bottom $|\hat{c}|\,F^{(S)}(\hat{x} = 0, \hat{c} > 0) = w(\hat{c})\,R_s$, where $w(\hat{c}) = 2\,\hat{c}\,e^{-\hat{c}^2}$ is the dimensionless version of W in (1), while the condition at the elastic top wall is $F^{(s)}(\hat{x} = Fr, \hat{c}) = F^{(s)}(\hat{x} = Fr, -\hat{c})$.

With this scheme the set of equations (7) can be solved exactly starting from $F^{(0)}$—this is the elastic solution –and following recursively up to the desired order [5].

This perturbative solution is valid at any position near or far from the walls since it is the kinetic equation with its corresponding microscopic boundary that is being solved.

4 Results

The open system: The stationary state of the open system ($Fr = \infty$) is determined by qN alone. The function corresponding to the elastic case is just a Maxwellian $F^{(0)} = \frac{1}{\sqrt{\pi}} e^{-(\hat{x}+\hat{c}^2)}$ and the first and second order corrections modify this function as shown in Fig. 2 where the theoretical distribution functions up to zeroth, first and second order evaluated at the bottom $\hat{x} = 0$ with $qN = 0.2$ are compared with the measured distribution function. Interpreting the system as one in which particles pass through each other loosing some energy in the process it can be said that particles coming out

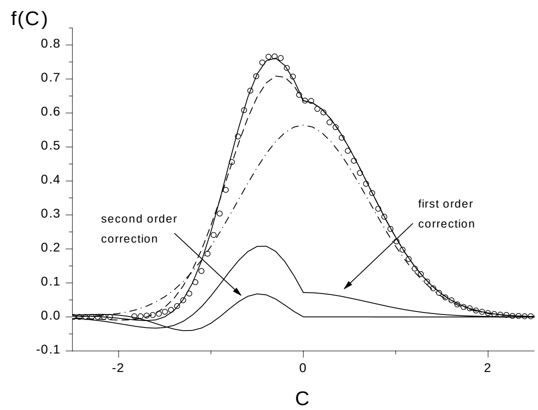

Fig. 2. The distribution function normalized to 1 at $\hat{x} = 0$ evaluated to zeroth (dot-dashed line), first (dashed line) and second order (solid line) are seen in this figure for $qN = 0.2$ and $N = 200$. Circles are the simulational results.

from the base have a vanishing most probable velocity, namely $F(C > 0)$ is maximum at $C = 0$, just like a Boltzmann distribution, while particles coming down are in principle accelerated, but the friction with the background (the rest of the particles) produces an effect similar to a "limit velocity" and $F(C < 0)$ has a maximum away from the origin. Moving away from the base the history of all particles tends to be comparable regardless of the sign of their velocity and the distribution function tends to be more and more symmetric.

The effects of dissipation over density: The zeroth order density $n_0(\hat{x})$ decreases exponentially, and since $qN \leq 0.1$ deviations from this behavior should be small. Dissipation prevents particles from reaching the heights they would in the conservative case implying that the system has a smaller effective height. Consequently the density tends to be higher near the base although corrections due to dissipation have not a maximum on the base but at some distance over the it. This suggests that for higher values of qN (too high for our theoretical description to be valid) a drop floating on a vapor would be formed in the system as, in fact, we have seen in simulations.

Effects on the granular temperature and the heat flux: In Fig. 3 the temperature profile is shown for three values of qN. The zeroth order temperature profile is the straight line $T = 1/4$ in all three cases. The effect of dissipation is to produce a $T(\hat{x})$ with negative gradient and this is already predicted by the negative first order correction. Figure 3 also shows that the temperature reaches an asymptotic value that our formalism predicts to be $T(\hat{x} \sim \infty) \approx 1/4 - qN(1 - qN)/2$ which coincides with what we observe. At $\hat{x} = 0$ there is a temperature gap: the temperature of the system does not coincide with the imposed value $T_0 = 1/4$.

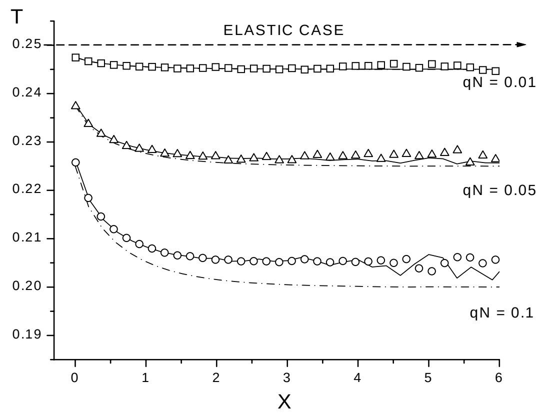

Fig. 3. Temperature profiles for $qN = 0.01$ (squares), $qN = 0.05$ (triangles) and $qN = 0.1$ (circles). The solid (dot-dashed) line is the predicted dimensionless temperature up to second (first) order.

In our case this *temperature slip* at the base is $\delta T \approx qN(1 - qN/2)/4$ which is also the observed gap. This thermal slip at the wall is a well known effect when the system has an externally imposed temperature gradient, but in granular systems δT is due to the dissipative collisions, namely, it is an intrinsic property of the system and it does not vanish with increasing density, but it rather increases.

The heat flux Q—the flux of energy entering through the base and being dissipated in the bulk—has an *analytic* expression to first order in q,

$$Q(\hat{x}) = qN \int_{-\infty}^{\infty} dC \, \frac{C^3}{2} \, F(\hat{x}, C) = \frac{qN}{\sqrt{2\pi}} \, e^{-2\hat{x}} \, . \tag{9}$$

An elastically closed system: The perturbative solution for our system with an elastic wall at height L (dimensionless height $\hat{x} = Fr$) has the form

$$F(\hat{x}, \hat{c}) = \lambda \left(F^{(0)}(\hat{x}, \hat{c}) + qN\lambda \, F^{(1)}(\hat{x}, \hat{c}) + (qN\lambda)^2 \, F^{(2)}(\hat{x}, \hat{c}) + \cdots \right) \tag{10}$$

where the prefactor $\lambda = 1/(1 - e^{-Fr})$ determines the system's density scale. The method to recursively construct the solution is the same one seen in Sec. 3 except that in this case the two boundary conditions have to be imposed [6]. The quasielastic condition for the system is in this case $qN\lambda \ll 1$, namely, not only qN but also λ will determine the behavior of the stationary state. We can see at left in Fig. 4 the corrections to the density profile for a fixed qN value and different values for λ (or Fr). The agreement with theory is quite good even though the shape of the corrections vary widely for the different values of the Froude number conisdered. For small Fr the correction is almost symmetric about $\hat{x} = \frac{1}{2} Fr$ where it has a maximum. As Fr gets larger the maximum of $n_1(\hat{x})$ moves down until it reaches the base and disappears. The correction develops a minimum high up and it moves down as Fr grows.

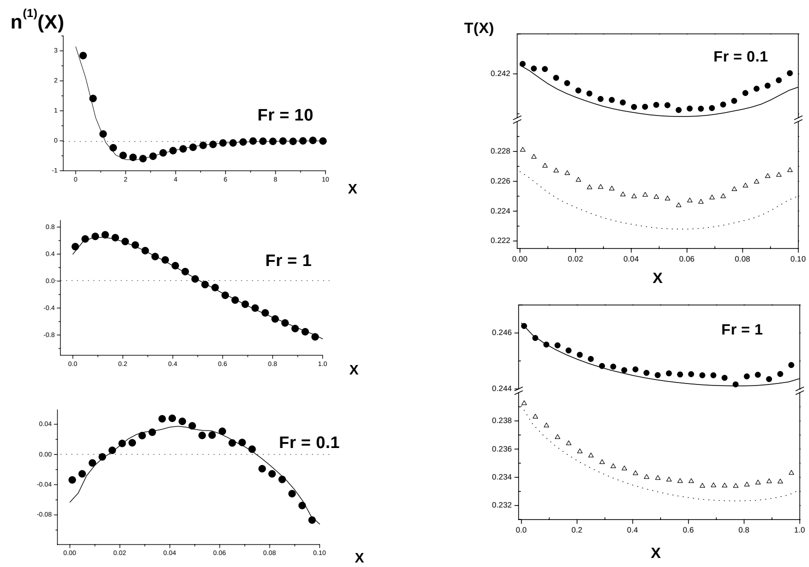

Fig. 4. At left, density corrections due to dissipation for different Froude numbers. At right, the temperature profile for two values of the Froude number with $qN = 0.01$ (dots) and $qN = 0.03$ (triangles). If Fr is small enough T shows a minimum even though the only source of energy is at the bottom. In both cases lines are the theoretical predictions while symbols are the measured data from MD simulations.

The temperature profile: When $Fr \gg 1$ few particles reach the top wall and the behavior of the profile tends to that of the open system observed in Fig. 3. Taking smaller values of Fr the temperature profile eventually develops a minimum near the top. The position of this minimum approaches the mid height as Fr gets smaller, being approximately in the middle of the box when $Fr = 0.1$ as shown in Fig. 4.

In spite of this minimum, notice that the heat flux, which at first order reads,

$$Q(\hat{x}) = \frac{qN}{\sqrt{2\pi}\,\left(1 - e^{-Fr}\right)^2}\,\left(e^{-2\hat{x}} - e^{-2Fr}\right) \tag{11}$$

decreases monotonically with height, being zero at $\hat{x} = Fr$, as it should be due to the elastic wall that closes the system.

Namely, the energy coming from the base heats the system near the top more than it heats the region immediately underneath. This remarkable effect is a boundary effect, in the sense that the upper wall is needed to observe such a quasi-elastic regime. For an open system, in the quasi-elastic limit $qN \ll 1$ this kind of temperature profile does not exist.

Conclusions

The problem of a 1D granular gas can be understood as the problem of *one particle* passing through a viscous medium. In this work we analyzed the system in the hydrodynamic limit in which the properties of the system are independent of the number of particles. In this context we have pointed out the effective acceleration this only particle suffers due to dissipative collisions.

Due to dissipative interactions, the granular gas needs an energy injection to reach a stationary time independent state. This energy enters as a boundary condition in the kinetic theory and, in the case of a 1D granular gas, determines completely the quasi-elastic regime.

For an open system, the only parameter entering the problem is the factor qN. In this case we predict, among other results, that there exists a temperature slip at the hot wall which does not decrease with density and which is of the same order as the gradients produced by dissipation. This implies that the standard hydrodynamic boundary condition for the temperature (temperature of the system at the wall equals the imposed temperature) is not suitable for these kind of systems not only for the 1D system but also for higher dimension ones.

Any other boundary in the system plays a role as important as the energetic boundary. We have predicted and observed an inverse heat flux (from colder to hotter zones) just by including an elastic upper wall. Although there have been observed inverse heat fluxes in very low density systems in higher dimensions [8] which could be due to a dissipative bulk effect, our case corresponds mainly to a boundary effect.

Although some of properties of 1D systems are generalizable to two or three dimensional systems, we have to point out that there exists a crucial fact which makes the 1D case special: the velocity distribution function is completely determined by the boundary conditions. Then, some of the 1D results we present here could qualitatively be extended to higher dimensions in the case of Knudsen gases, or even standard gases but just near the boundaries.

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