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Heat flux and upper boundary condition in an open fluidized granular gas

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Abstract. – The transport coefficient coupling heat flux and density gradient in a granular gas is measured by taking advantage of the existence of a minimum in the temperature profile of an open vibrated granular system. The results from particle simulations are found to be in good agreement with the theoretical predictions derived from the Boltzmann equation. The accuracy of a boundary condition requiring the hydrodynamic heat flux to vanish at infinite height is discussed, and shown to be consistent with the simulation data.

When an open granular system is fluidized, in the presence of gravity, by a bottom plate vibrating with small amplitude and high frequency, it reaches a steady situation where the energy lost in collisions is balanced by the energy injected into the system through the vibrating wall. A surprising feature of this steady state is that the granular temperature, defined as proportional to the local average kinetic energy, presents a minimum at a certain height, increasing from there on. This is a result that has been derived theoretically from the Navier-Stokes equations for dilute granular gases modeled as a system of inelastic hard spheres [1], confirmed in computer simulations of the same model [1–3], and also directly observed in experiments [4–6]. Besides, it has been verified [1] that the temperature minimum occurs in a region of the system that is correctly described by the hydrodynamic equations. On the other hand, the existence of an upper region where the gas has to be described as a free-molecule flow, with no collisions, renders far from trivial the boundary condition to be used in a hydrodynamic description.

A peculiar property of granular gases, as compared to molecular (elastic) ones, is that the Fourier law for the heat flux has to be modified by including an additional term that couples the heat flux to the density gradient. This coupling has been derived by kinetic theory methods [7–9], and also observed in molecular-dynamics simulations [10]. A new transport coefficient, usually denoted by μ and that has no analogue in elastic systems, is therefore introduced. As is also the case with the other transport coefficients of a granular fluid, μ depends on the local values of the density and temperature of the system, but also has an explicit dependence on the degree of inelasticity. The existence of this new transport term is closely related with the temperature inversion mentioned above. It implies that the heat flux does not vanish at the temperature minimum, as far as the density gradient is different from zero there. Since to Navier-Stokes order all the contribution to the heat flux at the temperature

minimum comes from the density gradient term, its value there is directly related to the value of the transport coefficient μ.

The aim of this work is to investigate the two mentioned questions. Firstly, the transport coefficient μ will be obtained, as a function of inelasticity, from the properties of the system at the temperature minimum, measured by means of computer simulations of a system of inelastic hard particles. The results will be shown to be in good agreement with the predictions obtained from the Boltzmann equation. Secondly, the accuracy of some fundamental implication following from requiring that the heat flux, as given by the Navier-Stokes equations, vanishes in the limit of very large height will be analyzed.

We consider a dilute system of N hard spheres ($d = 3$) or disks ($d = 2$) of mass m and diameter σ. Collisions between particles are inelastic and characterized by a constant coefficient of normal restitution α. There is a gravitational field acting on the system that has the usual form $\boldsymbol{g} = -g\boldsymbol{e}_z$, g being a positive constant and $\boldsymbol{e}_z$ a unit vector in the direction of the z-axis. The system is confined in a container of section S that is open at the top. Energy is added to the system through a vibrating wall located at the bottom. The amplitude of the vibration is small and the frequency high so that the position of the wall can be approximated as fixed at $z = 0$. A system under these conditions exhibits a steady state with gradients only in the z-direction and vanishing velocity field. The Navier-Stokes equations determining the density n and temperature T are [1]:

$$\frac{\partial p}{\partial z} = -nmg, \tag{1}$$

$$\frac{2}{\mathrm{d}nk_{\mathrm{B}}}\frac{\mathrm{d}q_z}{\mathrm{d}z} + T\zeta^{(0)} = 0. \tag{2}$$

Here, $p = nk_{\mathrm{B}}T$ is the hydrodynamic pressure, k_{B} the Boltzmann constant, $\zeta^{(0)}$ the cooling rate associated with the energy dissipation in collisions, and q_z the heat flux given by

$$q_z = -\kappa\frac{\mathrm{d}T}{\mathrm{d}z} - \mu\frac{\mathrm{d}n}{\mathrm{d}z}\,, \tag{3}$$

where κ is the heat conductivity coefficient and μ another transport coefficient. Explicit expressions for κ, μ, and $\zeta^{(0)}$ have been derived from the inelastic Boltzmann equation by using the Chapman-Enskog procedure in the first Sonine approximation, and have the form [1, 11]

$$\kappa = \kappa^*(\alpha)\kappa_0(T), \qquad \mu = \mu^*(\alpha)\mu_0(T), \qquad \zeta^{(0)} = \zeta^*(\alpha)\frac{p}{\eta_0}\,, \tag{4}$$

with η_0 and κ_0 denoting the Boltzmann elastic values of the viscosity and the heat conductivity (both proportional to $\sqrt{T}$), $\mu_0 = T\kappa_0/n$, and $\kappa^*(\alpha)$, $\mu^*(\alpha)$, and $\zeta^*(\alpha)$ being dimensionless functions of the coefficient of restitution. The explicit expressions of all these quantities are given in refs. [1, 11]. In the elastic limit $\alpha \to 1$, κ^* tends to unity while μ^* and ζ^* vanish.

In [1] it was shown that the temperature profile solution of eqs. (1) and (2) has a minimum T_m at a certain height z_m, lying well inside the region in which the hydrodynamic description applies. This is because the density there is not very small yet and, therefore, the local Knudsen number is not too large. In fact, the temperature minimum z_m is not far from the maximum of the density profile. Using eq. (1), eq. (3) can be rewritten as

$$q_z(z) = -(\kappa^* - \mu^*)\kappa_0\frac{\mathrm{d}T}{\mathrm{d}z} + \mu^*\kappa_0\frac{mg}{k_{\mathrm{B}}}\,. \tag{5}$$

At the temperature minimum, this equation reduces to

$$q_z(z_m) = \mu^* \kappa_0(T_m) \frac{mg}{k_B} . \tag{6}$$

It is important to remark that the validity of eq. (6) does not rely on any particular boundary conditions, but only on the accuracy of eqs. (1) and (2) to describe the stationary state reached by the system, and more concretely the minimum of the temperature profile.

To check the above theoretical prediction and compute the coefficient μ^*, we have performed computer simulations of a system of inelastic hard particles. As we are interested in the dilute limit, we used the Direct Simulation Monte Carlo (DSMC) method [12]. The reason why we choose this method over the molecular-dynamics one, which was employed in ref. [1] to study the same state, is that the DSMC method allows to exploit the symmetry of the system in the transversal direction, making the simulations much more efficient, and avoiding the development of the transversal instabilities that have been observed in wide systems [13, 14]. Besides, we have verified that results obtained by molecular dynamics and by DSMC show no differences as far as the density in the molecular-dynamics simulations stays small enough.

We have investigated both two- and three-dimensional systems. The wall at the bottom vibrates with a sawtooth profile and a velocity v_W, so particles that collide with the wall always find it with this positive velocity. Collisions of the particles with the vibrating wall are elastic. The system is divided into horizontal layers of height Δz_c, chosen smaller than the local mean free path. In all the cases, the initial state has been homogeneous, filling the system up to a given height, with a Gaussian velocity distribution of zero mean and arbitrary temperature. From this state, the system evolves to a stationary situation. Then, the relevant quantities are computed, and the results averaged over different times. Besides, several realizations of the simulations were made in order to improve the statistics. We will use the mass of the particles, m, as the unit of mass, the initial homogeneous mean free path, λ_h, as the unit of length, and the initial temperature, $T(0)$, as the unit of temperature. Besides, we will take $k_B = 1/2$, so $2k_BT(0)$ defines the energy unit. All the simulations we will report correspond to a fixed value of $g = 0.01$, and the velocity of the vibrating wall was chosen so that the system was fluidized, *i.e.*, the density did not become too large in any region. Simulations then show that the hydrodynamic profiles scale with v_W^2, so changing the vibrating velocity does not affect their qualitative shape. Different values of the restitution coefficient have been considered and, for each of them, several values of $N_z \equiv N/S$, proportional to the number of mono-layers in the z-direction at rest, were studied.

As an example, in fig. 1, the temperature and density profiles for $d = 3$, $\alpha = 0.925$ and $N_z\sigma^2 = 4.05$ are shown. It is seen that the temperature has a minimum at a certain height, increasing from there on. The density profile exhibits a maximum, and it is observed in all the simulations that the temperature minimum occurs at a larger height than the density maximum, although not so far from it as to show up once the density is too low. It is worth mentioning that, in order to observe the density maximum, N_z has to exceed a certain threshold that depends on the inelasticity [1]. In all the simulations reported here, this condition was satisfied. Similar profiles are obtained for other values of the parameters.

The heat flux as a function of height for some of the simulations, namely for values of the parameters $d = 2$, $\alpha = 0.95$, and $N_z\sigma = 10.61$, 8.84, and 7.07, is shown in fig. 2. In fact what we have plotted is f_μ defined as $f_\mu = k_B q_z/mg\kappa_0$, as a function of $z - z_m$. Equation (6) implies that μ^* is given by the value of f_μ at $z = z_m$, which must be independent of N_z. In agreement with the theoretical prediction, although f_μ, for given α, depends on N_z, its value at $z = z_m$ is the same in all the cases.

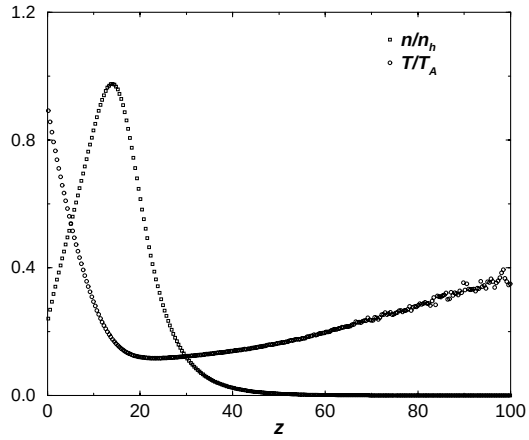

Fig. 1 – Temperature and density profiles for a three-dimensional system with $\alpha = 0.925$, $N_z\sigma^2 = 4.05$ as obtained from the simulations. The temperature has been scaled with an arbitrary temperature, $T_{\rm A}$, and the density with the initial, homogeneous value, $n_{\rm h}$.

Figures 3 and 4 display the coefficient μ^* for $d = 3$ and $d = 2$ as a function of α. The symbols are the results of the simulations, employing the method described above. For each value of α, at least three different values of the number of monolayers N_z have been considered. Moreover, different realizations of the "experiment" have been run in each case in order to get the error bars. They are seen to increase as the coefficient of restitution decreases. This might be due to the coupling between gradients and inelasticity that is characteristic of steady states of granular systems, and that makes it necessary to go beyond the Navier-Stokes order when the inelasticity is large. The solid lines in figs. 3 and 4 are the theoretical predictions for μ^* obtained in refs. [8] and [11]. The agreement between the theoretical prediction and the results of the simulation is quite good, even for the lowest values of α investigated. It could be argued that such an agreement is not surprising, as the theoretical prediction uses

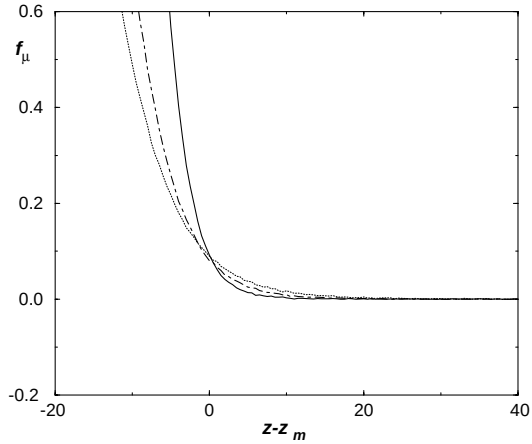

Fig. 2 – Heat flux divided by $T^{1/2}$ for $d = 2$, $\alpha = 0.95$ as a function of $z - z_m$, z_m being the position of the temperature minimum in each case. The solid line corresponds to a number of monolayers $N_z\sigma = 10.61$, the dotted line to $N_z\sigma = 8.84$, and the dot-dashed one to $N_z\sigma = 7.07$.

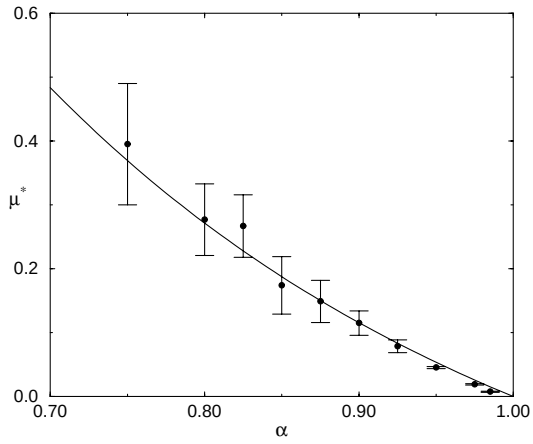

Fig. 3

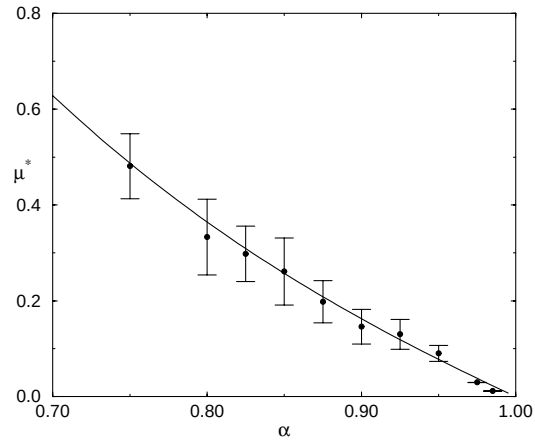

Fig. 4

Fig. 3 – Scaled transport coefficient μ^* for a system of inelastic hard spheres. The symbols are from the simulations while the solid line is the theoretical prediction derived in refs. [8] and [11].

Fig. 4 – The same as in fig. 3, but for a system of hard disks.

the Boltzmann equation as starting point, and the DSMC method is designed to mimic the properties of a low-density flow. Nevertheless, it should be remembered that the simulation method does not assume any of the hypotheses and approximations introduced in the theory (validity of hydrodynamics, gradient expansion, Sonine expansion).

Equation (5) has been used also in [3] to measure the coefficient μ in a system of hard disks by means of molecular-dynamics simulation. Nevertheless, the analysis there is different from the one reported here. The authors assume that there is a hydrodynamic region where the heat flux is negligible and, therefore, the temperature profile is linear. Moreover, they neglect in their analysis μ^* in the first term on the right-hand side of eq. (5), then restricting themselves to first order in $1-\alpha$. The upper boundary condition to be used when solving the hydrodynamic equations for the system is not trivial due to the existence of a collisionless region. Of course, the net energy flux must vanish in that region, as observed in fig. 2. Nevertheless, the question is whether this can be translated into an effective boundary condition for the hydrodynamic equations, by requiring that q_z as given by eq. (5) vanishes in the limit $z \to \infty$. To address this point, we start from the general solution of eqs. (1) and (2) [1],

$$T(\xi)^{1/2} = [AI_\nu(\xi) + BK_\nu(\xi)]\xi^{-\nu}, \tag{7}$$

$$n(\xi) = \frac{mg\xi^{1+2\nu}}{k_{\mathrm{B}}C_d\sigma^{d-1}\sqrt{a(\alpha)}[AI_\nu(\xi) + BK_\nu(\xi)]^2}, \tag{8}$$

where A and B are arbitrary constants, and I_ν and K_ν denote the modified Bessel functions of first and second kind, respectively. The dimensionless length scale ξ is defined by

$$\xi = \sqrt{a(\alpha)}\int_z^\infty \frac{\mathrm{d}z'}{\lambda(z')}, \tag{9}$$

$\lambda(z) \equiv (C_d n\sigma^{d-1})^{-1}$, with $C_d = 2\sqrt{2}$ for $d=2$ and $C_d = \pi\sqrt{2}$ for $d=3$, being the local mean free path. Finally $a(\alpha)$ and $\nu(\alpha)$ are given by

$$a(\alpha) = \frac{32(d-1)\pi^{d-1}\zeta^*}{C_d^2(d+2)^3\Gamma(d/2)^2(\kappa^*-\mu^*)}, \qquad \nu = \frac{\mu^*}{4(\kappa^*-\mu^*)}. \tag{10}$$

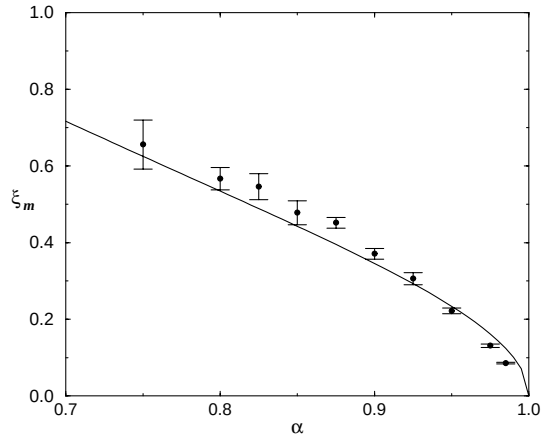

Fig. 5 – Position of the temperature minimum in the scaled variable ξ as a function of the restitution coefficient for a system of inelastic hard spheres. The solid line is the numerical solution of eq. (15), while the symbols are from the simulation.

Both are monotonically decreasing functions of α, vanishing in the elastic limit. By differentiation of eq. (7) it follows that the position of the temperature minimum ξ_m is given by the solution of

$$AI_{\nu+1}(\xi_m) = BK_{\nu+1}(\xi_m). \tag{11}$$

Using eqs. (7)-(9) and the properties of the Bessel functions, it is an easy task to rewrite eq. (5) for the heat flux in the explicit form

$$q_z = A(\kappa^* - \mu^*)\frac{2mg\kappa_0}{k_{\mathrm{B}}T^{1/2}}\left[I_{\nu-1}(\xi) - \frac{B}{A}K_{\nu-1}(\xi)\right]\xi^{1-\nu}. \tag{12}$$

Taking into account the limiting forms of $I_{\nu-1}(\xi)$ and $K_{\nu-1}(\xi)$ for $\xi \to 0$, it follows that the heat flux in the limit of very large heights (small ξ) is given by

$$q_z = A(\kappa^* - \mu^*)\frac{2mg\kappa_0}{k_{\mathrm{B}}T^{1/2}}2^{-\nu}\left[\frac{2}{\Gamma(\nu)} - \Gamma(1-\nu)\frac{B}{A}\right] \tag{13}$$

and the requirement that this quantity vanishes leads to the relation

$$\frac{B}{A} = \frac{2}{\Gamma(\nu)\Gamma(1-\nu)}\,, \tag{14}$$

i.e. the ratio of the two constants is given by a function of α only. A test of the above relation, and therefore, of the validity of the boundary conditions that the heat flux vanishes at $z \to \infty$, follows by using it into eq. (11). This leads to a closed equation for ξ_m involving only the parameter ν, being independent of the other relevant parameters (number of monolayers, gravity, and vibration velocity):

$$I_{\nu+1}(\xi_m) - \frac{2}{\Gamma(\nu)\Gamma(1-\nu)}K_{\nu+1}(\xi_m) = 0. \tag{15}$$

In fig. 5, ξ_m obtained from the simulations is plotted as a function of α in the three-dimensional case. The solid line is the solution of the prediction given by eq. (15). Again,

for each value of the restitution coefficient, several values of N_z were considered and it was found that, apart from the statistical noise, the position of the minimum was effectively independent of other parameters than α. The value of ξ_m is a monotonic decreasing function of α, vanishing in the elastic limit. The agreement between the simulation results and the prediction of the Navier-Stokes equations together with the mentioned boundary condition is very good. Similar results are found for two-dimensional systems. This provides a strong support to the validity of the assumed boundary condition, as well as a global test of the validity of the hydrodynamic description.

A vanishing heat flux implies a constant temperature gradient, as follows from eq. (5). Nevertheless, some care is needed when using this latter property for practical applications. We have required the heat flux to vanish in the limit $z \to \infty$, which implies $T \to \infty$, and identifying this asymptotic regime in experiments or computer simulations can be an almost impossible task. In fact, a careful analysis of the spatial scales in the system shows that in the relevant hydrodynamic region the temperature increases according with a law of the form $\mathrm{d}T^{3/2}/\mathrm{d}z = \text{const}$ [1]. The difficulties to identify the linear asymptotic region of the temperature profiles are well exemplified by the results shown in fig. 1.

In summary, by exploiting the existence of a minimum in the temperature profile of an open fluidized granular gas, we have measured the transport coefficient coupling heat flux and density gradient. The agreement between the simulation results and the theoretical predictions based on a hydrodynamic description provides a strong evidence for the validity of the latter, even well beyond the quasi-elastic limit. This also applies to the boundary condition to be imposed to the temperature field, namely that the hydrodynamic heat flux must vanish at large height.

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