Heat flux in a vibrated granular gas: the diffusive heat conductivity coefficient

J. Javier Brey* and M.J. Ruiz-Montero*

*Física Teórica. Facultad de Física. Apdo. de Correos 1065. 41080-Sevilla. Spain

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 medium. This temperature inversion is closely related to the existence of the new transport coefficient. Particle simulations using the Direct Simulation Monte Carlo method will be used to compute the transport coefficient, and the results will be compared with theoretical predictions derived from the Boltzmann equation. Finally, the accuracy of a boundary condition requiring the hydrodynamic heat flux to vanish for infinite heights will be discussed.

INTRODUCTION

Steady states of granular materials are obtained when energy is supplied to the system in order to compensate the energy loss in collisions. One of the easiest ways to add energy to a system in experiments is to do so through a vibrating wall. If the vibration is strong enough, the system will be fluidized, and one can expect its behavior to be described by the extension of the Navier-Stokes equations to granular systems. In this work, we will use the hydrodynamical description to study the steady state of an open, vibrated, granular system in presence of gravity. The granular fluid will be modelled as a system of inelastic hard particles, whose collisions are characterized by a constant coefficient of normal restitution α. Besides, we will be interested in the dilute limit, when the Boltzmann equation applies.

A distinctive feature of granular gases as compared to molecular (elastic) ones, is that the expression of the heat flux has to be generalized by including a new term coupling the heat flux and the density gradient. This implies the introduction of a new coefficient, the diffusive heat conductivity μ, that vanishes in the elastic limit. This coupling has been derived by kinetic theory methods [1, 2, 3], and its consequences confirmed in computer simulations [4, 5, 6]. For the particular case of a vibrated granular gas in the presence of gravity, this term implies a peculiar behavior of the temperature profile, that increases with height after a minimum. The existence of the minimum was first derived from the hydrodynamic equations [5], and was confirmed by computer simulations [5, 7, 8], and also in experiments [9]. Here, we will show that the value of the diffusive heat conductivity μ can be obtained from the behavior of the system at the temperature minimum. Then, the value of the transport coefficient will be compared with the theoretical prediction from the Boltzmann equation derived in [2]. Finally, the boundary conditions to be used when solving the hydrodynamic equations will be also discussed.

HYDRODYNAMIC DESCRIPTION

Let us consider a system of N inelastic hard spheres ($d=3$) or disks ($d=2$) of mass m and diameter σ, in presence of a gravitational field $\mathbf{g}=-g\mathbf{e_z}$, where g is a positive constant and $\mathbf{e_z}$ a unit vector in the Z direction. In the hydrodynamic description, the state of the system is completely specified by the local number of particles density, $n(\mathbf{r},t)$, the velocity flow $\mathbf{u}(\mathbf{r},t)$, and the temperature, $T(\mathbf{r},t)$. For a dilute gas, the evolution of these quantities is given by the extension to the inelastic case of the Navier-Stokes equations [2, 10],

$$\frac{\partial n}{\partial t}+\nabla\cdot(n\mathbf{u})=0\,, \tag{1}$$

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$$\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}+\frac{1}{nm}\nabla\cdot\mathscr{P}-\mathbf{g}=0\,, \tag{2}$$

$$\frac{\partial T}{\partial t}+\mathbf{u}\cdot\nabla T+\frac{2}{dnk_B}[\mathscr{P}:\nabla\mathbf{u}+\nabla\cdot\mathbf{q}]+T\zeta=0\,. \tag{3}$$

Here, k_B is the Boltzmann constant, $\mathscr{P}$ is the pressure tensor,

$$\mathscr{P}=p\mathscr{I}-\eta\left[(\nabla\mathbf{u})+(\nabla\mathbf{u})^{+}-\frac{2}{d}\mathscr{I}\nabla\cdot\mathbf{u}\right], \tag{4}$$

where $p=nk_BT$ is the hydrostatic pressure, $\mathscr{I}$ the identity tensor, and η the shear viscosity coefficient. $\mathbf{q}$ appearing in Eq. (3) is the heat flux,

$$\mathbf{q}=-\kappa\nabla T-\mu\nabla n\,, \tag{5}$$

with κ the heat conductivity coefficient, and μ the diffusive heat conductivity. Finally, ζ is the cooling rate associated to the energy dissipation in collisions. The expression for these coefficients reads:

$$\eta=\eta^{*}(\alpha)\eta_0(T),\quad \kappa=\kappa^{*}(\alpha)\kappa_0(T),\quad \mu=\mu^{*}(\alpha)\mu_0(T), \tag{6}$$

$$\zeta\simeq\zeta^{(0)}=\zeta^{*}(\alpha)\frac{p}{\eta_0}, \tag{7}$$

with η_0, κ_0 the Boltzmann elastic values of the viscosity and heat conductivity, $\mu_0=T\kappa_0/n$, while $\eta^{*}(\alpha)$, $\kappa^{*}(\alpha)$, $\mu^{*}(\alpha)$, and $\zeta^{*}(\alpha)$ are dimensionless functions of the coefficient of restitution. Although their expressions will not be given here (they can be found in [2, 10]), it is important to remember that in the elastic limit $\alpha\to 1$, η^{*} and κ^{*} tend to unity, while μ^{*} and ζ^{*} vanish. Besides, both η_0 and κ_0 are proportional to $T^{1/2}$.

Let us consider that energy is supplied to the system through a vibrating wall of size S located at $z=0$. Although the details of the wall movement are not very important here, we will consider that the vibration amplitude is small enough as to approximate the position of the wall as fixed. Also, the wall moves with a sawtooth profile, so particles find it moving upwards with a characteristic velocity. When the energy supplied by the wall compensates the one lost in collisions, the system reaches a steady state. Besides, and because of the symmetry of the problem, we can expect that, once in this state, there will be gradients only in the Z direction. When Eqs. (1)–(3) are particularized for this state, they take the form

$$\frac{\partial p}{\partial z}=-nmg, \tag{8}$$

$$\frac{2}{dnk_B}\frac{dq_z}{dz}+T\zeta^{(0)}=0. \tag{9}$$

Besides, Eq. (8) implies that the heat flux in this case is

$$q_z(z)=-(\kappa^{*}-\mu^{*})\kappa_0\frac{dT}{dz}+\mu^{*}\kappa_0\frac{mg}{k_B}\,. \tag{10}$$

In order to solve these equations, it is convenient to introduce the new dimensionless length scale ξ as:

$$\xi=\sqrt{a}\int_z^{\infty}dz'\frac{1}{\lambda(z')}\,, \tag{11}$$

where $\lambda(z)$ is the local mean free path for hard disks or spheres, $\lambda(z)=[Cn\sigma^{d-1}]^{-1}$, with $C=2\sqrt{2}$ for $d=2$ and $C=\pi\sqrt{2}$ for $d=3$. Let us notice that, when $z\to\infty$, $\xi\to 0$, while ξ takes its maximum value, $\xi_0=\sqrt{a}C\sigma^{d-1}N_z$, with $N_z=N/S$, at $z=0$. The coefficient a appearing in Eq. (11) is a function of the coefficient of restitution and reads

$$a(\alpha)=\frac{32(d-1)\pi^{d-1}}{C^2(d+2)^3\Gamma(d/2)^2}\,\frac{\zeta^{*}(\alpha)}{\kappa^{*}(\alpha)-\mu^{*}(\alpha)}\,, \tag{12}$$

vanishing, therefore, in the elastic limit. In terms of the new scale, the solution to the Navier-Stokes equations is [5]:

$$T^{1/2}(\xi)=\xi^{-\nu}[AI_{\nu}(\xi)+BK_{\nu}(\xi)], \tag{13}$$

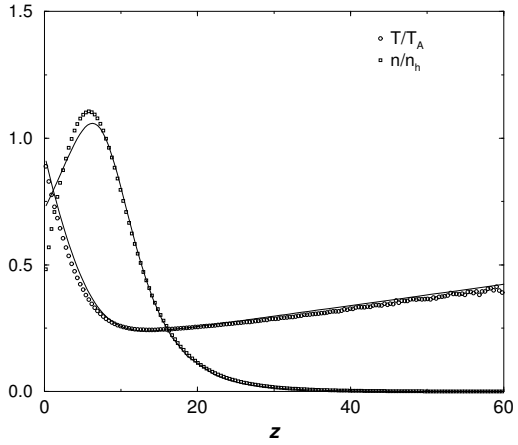

FIGURE 1. Temperature and density profiles for a system of hard spheres with $\alpha = 0.925$, $\xi_0 = 1.92$. The symbols are from the simulations, while the lines are the solution to the hydrodynamic equations, with the arbitrary constants determined from the temperature minimum.

$$n(\xi) = \frac{mg\xi^{1+2\nu}}{Ck_B\sigma^{d-1}\sqrt{a(\alpha)}\left[AI_\nu(\xi)+BK_\nu(\xi)\right]^2}, \tag{14}$$

where I_ν and K_ν are the modified Bessel functions of first and second kind, and A and B are constants to be determined from the boundary conditions. The parameter ν is

$$\nu(\alpha) = \frac{\mu^*(\alpha)}{4[\kappa^*(\alpha)-\mu^*(\alpha)]} > 0, \tag{15}$$

In the limit $\xi \to 0$ ($z \to \infty$) $I_\nu \to 0$, while $K_\nu \to \infty$ [11]. Nevertheless, this does not imply that the constant B has to be taken identically equal to zero, as there is nothing unphysical in the fact that T diverges as far as the density decreases fast enough as to guarantee that the local kinetic energy density goes to zero in that limit. Besides, it is clear that the hydrodynamic description will not be valid for very large heights, as the density will have decayed to very small values, and the local Knudsen number will be very small. Then, we will keep the B constant different from zero.

The presence of the term proportional to K_ν in the temperature profile implies that it has a minimum located at $\xi = \xi_m$ given by

$$AI_{\nu+1}(\xi_m) - BK_{\nu+1}(\xi_m) = 0, \tag{16}$$

and the temperature T_m at the minimum is

$$T_m^{1/2} = \xi_m^{-\nu}\left[AI_\nu(\xi_m)+BK_\nu(\xi_m)\right]. \tag{17}$$

Then, if hydrodynamics is valid in the vicinity of the temperature minimum, the constants A and B can be determined from the measured temperature profiles. It has been also shown [5] that the density has a maximum at $\xi = \xi_n$ that is approximately given by the solution of the equation:

$$I_\nu(\xi_n) - 2\xi_n I_{\nu+1}(\xi_n) = 0, \tag{18}$$

which can be solved numerically for each value of α. Let us just comment that ξ_n takes values of the order of unity. Of course, in order to observe the density maximum in an experiment the number of particles in the system has to be large enough so that $\xi_0 > \xi_n$. If this condition is not fulfilled, the density will decay monotonically with height.

In order to check the above hydrodynamic description, computer simulations for two and three dimensional systems by using the Direct Simulation Monte Carlo method (DSMC) [12] have been performed. This method is particularly suited for this problem as we are interested in the low density limit, and as it allows to exploit the symmetry of the system in the transversal direction. In Fig. 1 the steady density and temperature profiles for a system of hard spheres have been plotted. The density has been scaled with the initial, homogeneous density, while the temperature is scaled with some arbitrary value. Space is measured in units of the initial, homogeneous, mean free path. The values of the

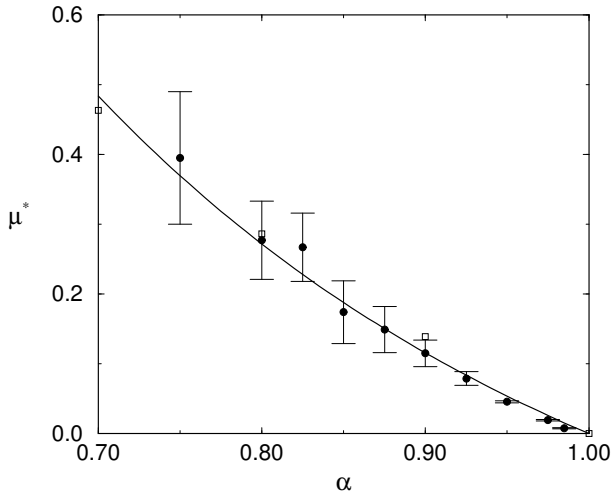

FIGURE 2. Reduced transport coefficient μ^* as a function of α for a system of hard spheres. The solid line is the theoretical prediction derived in [2], and the circles the results from the simulation of a vibrated system. The squares are also simulation results but using a Green-Kubo expression for μ.

parameters of the simulations were $\alpha = 0.925$, $\xi_0 = 1.92$. The symbols are the results of the simulations: as predicted, the density shows a maximum, while the temperature exhibits a minimum, increasing from there on. The continuous lines are the theoretical prediction, with A and B determined from the temperature minimum. The agreement is very good, confirming the validity of hydrodynamics in the temperature minimum region. The same qualitative results are achieved for other values of the parameters both in the two and three dimensional cases, as far as the coefficient of restitution is not too low. Due to an intrinsic coupling between gradients and inelasticity in this steady state, retaining only up to the Navier-Stokes order in the Chapman-Enskog expansion may be not enough for small values of α.

THE HEAT FLUX

In the steady state of a granular material, the heat flux is given by Eq. (11). At the temperature minimum, as the derivative of T vanishes, we have

$$q_z(z_m) = \mu^* \kappa_0(T_m) \frac{mg}{k_B} . \tag{19}$$

Then, the computation of the heat flux at the temperature minimum provides a direct measurement of the scaled diffusive heat conductivity coefficient, μ^*. It must be pointed out that Eq. (19) only requires the validity of the hydrodynamic description, and no additional condition has to be introduced. In Fig. 2 we have plotted the coefficient μ^* as a function of α for a system of hard spheres. The solid line is the theoretical prediction derived in [2] by using the Chpaman-Enskog expansion from the Boltzmann equation. The circles are the results of the simulation using Eq. (19). The error bars are obtained by giving different values to the parameter ξ_0 and the velocity of the vibrating wall. The agreement between theory and simulation is quite good, even at the lowest values of α investigated. Nevertheless, it must be said that, for those values, the shape of the profiles begin to show discrepancies from the theoretical prediction derived here. This is the reason of the large error bars for the lowest values of α, and for not having considered smaller values of this parameter. Finally, we have also included in the figure the results of independent DSMC simulations where μ^* was computed by means of Green-Kubo expressions derived in Ref. [13] (squares). The agreement is again very good. It could be argued that it is not surprising to obtain a good agreement between the results of the DSMC simulation and a theoretical description derived from the Boltzmann equation. Nevertheless, it must be remembered the the theoretical derivation requires given hypothesis and approximations (validity of hydrodynamics, gradient expansions, Sonine expansion) that are not assumed at all by the simulation method.

It is important to stress that the fact that the heat flux does not vanish at the temperature minimum is a direct proof of the existence of the coupling between heat flux and density gradient. Besides, Fig. 2 shows that, although $\mu^* \to 0$ in the elastic limit, its contribution cannot be neglected as α goes beyond the quasi-elastic limit.

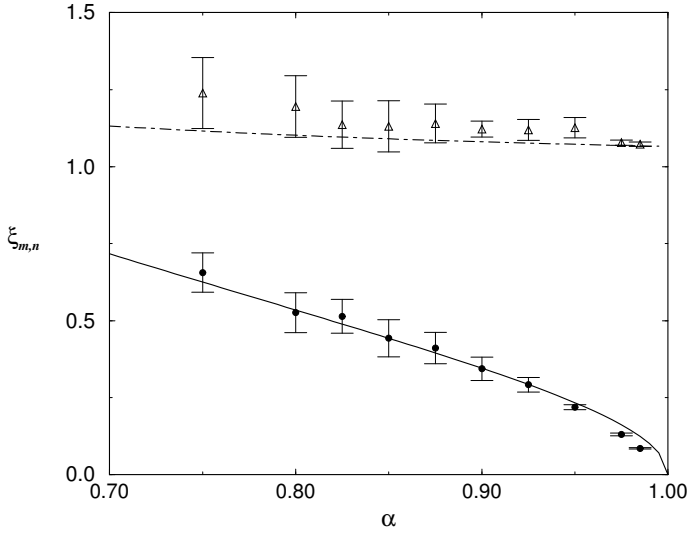

FIGURE 3. Position of the temperature minimum ξ_m and of the density maximum $\xi_n$in the three dimensional case. The lines are the theoretical prediction (solid line for ξ_m, dot-dashed line for ξ_n. The symbols are the results of the DSMC simulations.

Eq. (19) provides the heat flux at the temperature minimum. A general expression for q_z valid at any position can be obtained when the solution given by Eq. (14) is substituted in Eq. (11), and it reads

$$q_z = A(\kappa^* - \mu^*)\frac{2mg\kappa_0}{k_B T^{1/2}}\left[I_{\nu-1}(\xi) - \frac{B}{A}K_{\nu-1}(\xi)\right]\xi^{1-\nu}. \tag{20}$$

Let us consider now the limit $z \to \infty$ or, equivalently, $\xi \to 0$. Taking into account the asymptotic behavior of the modified Bessel functions, it follows that, for very large heights is given by:

$$q_z = A(\kappa^* - \mu^*)\frac{2mg\kappa_0}{k_B T^{1/2}}2^{-\nu}\left[\frac{2}{\Gamma(\nu)} - \Gamma(1-\nu)\frac{B}{A}\right]. \tag{21}$$

If we require that the heat flux vanishes for very large heights, we get the relation

$$\frac{B}{A} = \frac{2}{\Gamma(\nu)\Gamma(1-\nu)}, \tag{22}$$

i.e. the ratio of the two constants is given by a function of α alone. Taking into account the behavior of the Γ function, $\mu^* = 0$ (i.e. $\nu = 0$) implies $B = 0$, and the temperature would be constant for large heights. If we introduce the above relation into the equation that determines the position of the temperature minimum, Eq. (16), we get a closed equation for ξ_m:

$$I_{\nu+1}(\xi_m) - \frac{2}{\Gamma(\nu)\Gamma(1-\nu)}K_{\nu+1}(\xi_m) = 0. \tag{23}$$

Then, the position of the temperature minimum in a vibrated system in the scaled space variable is a function only of the coefficient of normal restitution, independent of the other relevant parameters of the system (number of particles, gravity and vibration velocity).

In Fig. 3 the position of the temperature minimum ξ_m in the three dimensional case is plotted as a function of α. The symbols are the results of the DSMC simulation, while the solid line is the solution of Eq. (23). The agreement is very good, supporting the use of the above mentioned boundary condition to solve the hydrodynamic equations. It must be noticed that the validity of this boundary condition is not at all clear, as it is imposed in the very large heights region, i.e., once the density has decayed to very small values and the hydrodynamic description is not valid. Of course, the heat flux must vanish in that region, but the question is whether this can be translated into an effective boundary condition for the hydrodynamic equations. For instance, a vanishing heat flux implies a constant temperature gradient whose value is directly related to ν. But identifying the asymptotic region where this linear behavior is achieved is

very difficult in practical applications, because of the failure of hydrodynamics to describe the upper region of the system [6]. Here we have shown that the condition of vanishing flux at large heights translates into a condition *inside* the hydrodynamic region, so it can be clearly tested.

We have also included in Fig. 3 the position of the density maximum, ξ_n. The dot-dashed line is the theoretical prediction given by the solution of Eq. (18), while the triangles are the results of the simulations. The agreement is again quite good, although some discrepancies appear for the lowest values of α studied. The reason for this might be that Eq. (18) is not exact [5], and is in fact obtained for $\nu \ll 1$, while for $\alpha = 0.7$, $\nu \sim 0.14$. Nevertheless, it must be noticed the weak dependence on α of ξ_n as compared to ξ_m. In fact, for the values of the coefficient of restitution considered in the simulations $\xi_n \sim 1$.

In conclusion, hydrodynamics provides a very useful tool to study non-homogeneous steady states of granular systems. Nevertheless, this hydrodynamic description has distinctive characteristics that cannot be guessed from the one of molecular fluids. In particular, a new transport coefficient, the diffusive heat conductivity, has to be introduced. In this work we have shown that this new transport coefficient has relevant consequences in the hydrodynamic profiles, so it cannot be neglected in the description of granular flows.

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