An adiabatic piston in a temperature gradient

J Javier Brey and Nagi Khalil

Física Teórica, Universidad de Sevilla, Apartado de Correos 1065, E-41080 Sevilla, Spain
E-mail: brey@us.es and nagi@us.es

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Abstract. The steady states of two gases of hard spheres or disks separated by an adiabatic piston in the presence of a temperature gradient are discussed. The temperature field is generated by two thermal walls at different temperatures, each of them in contact with one of the gases. The presence of the piston strongly affects the hydrodynamic fields, inducing a jump in its vicinity. A simple kinetic theory model is formulated. Its predictions are shown to be in good agreement with molecular dynamics simulation results. The applicability of the minimum entropy production principle is analyzed, and it is found that it only provides an accurate description of the system in the limit of a small temperature gradient.

Keywords: transport processes/heat transfer (theory), stationary states, kinetic theory of gases and liquids

The adiabatic piston consists of a container filled with a gas that is divided into two compartments by a freely moving adiabatic piston [1]. Usually, the system is isolated and initially prepared with the two gases in both compartments at different independent states. Then, the relaxation to equilibrium is studied. It is observed that the system first converges towards a state of mechanical equilibrium with both gases having the same pressure. Then, the pressure fluctuations that are asymmetrical because the temperatures of the gases are different drive the system very slowly to thermal equilibrium [2]–[6]. Of course, the situation is much more complex and less understood when the system cannot relax to equilibrium due to some imposed external conditions. Very recently, several configurations consisting of granular gases separated by an adiabatic piston have been considered [7]–[9]. Granular gases are inherent non-equilibrium systems, since no equilibrium state is possible for them and, for this reason, they have been intensively
used to investigate many fundamental issues in the context of non-equilibrium statistical mechanics [10, 11]. Nevertheless, it must be realized that the irreversibility in granular gases has an internal origin, and it is not related, in principle, to some imposed boundary or initial conditions, as is the case for molecular systems. Actually, as a consequence of the above, gradients and inelasticity are related in steady granular gases and this leads to a quite peculiar rheological behavior.

The aim of this paper is to study the steady state of two molecular gases separated by an adiabatic piston, when each of the gases is in contact with a thermal wall at a different temperature. Attention will be restricted to the final state of the system, without studying the way in which it is reached. The questions addressed are related to the modification of the hydrodynamic steady profiles because of the presence of the piston and the steady position of the latter.

The system considered is a rectangular \((d = 2)\) or cylindrical \((d = 3)\) container of length \(L_x\). It is divided into two compartments by a movable adiabatic piston of mass \(M\), constrained to remain perpendicular to the axis of the system, taken as the \(x\)-axis. By ‘adiabatic’ it is meant, as usual, that the piston has no internal degrees of freedom and, therefore, it cannot transmit energy when it is at rest. A sketch of the system is given in figure 1. In each of the two compartment there are \(N\) elastic hard disks \((d = 2)\) or spheres \((d = 3)\) of mass \(m\) and diameter \(\sigma\). Collisions between particles and the piston as well as collisions of the particles with the lateral walls of the container are also elastic. Moreover, the motion of the piston occurs without friction with the lateral walls.

The walls of the container located at \(x = 0\) and \(x = L_x\) and perpendicular to the \(x\)-axis are thermal walls with temperatures \(T_{10}\) and \(T_{20}\), respectively. At the microscopic level of description, a thermal wall is modeled by assuming that whenever a particle collides with it, a new velocity is assigned to the particle drawn from a Maxwellian distribution with a second moment defined by the temperature of the wall [12, 13]. More specifically, the velocity distribution of the particles leaving a thermal wall with temperature \(T_{i0}, i = 1, 2\), is given by

\[
P(v) = \theta \left[ (-1)^{i-1} v_x \right] (2\pi)^{-(d-1)/2} \left( \frac{m}{k_B T_{i0}} \right)^{(d+1)/2} v_x \exp \left( -\frac{mv_x^2}{2k_B T_{i0}} \right),
\]  

Figure 1. Sketch of the system considered in this work. The left and right walls are thermal with temperatures \(T_{10}\) and \(T_{20}\), respectively.
where \( \theta(x) \) is the Heaviside step function and \( k_B \) is the Boltzmann constant. At the macroscopic level, it will be assumed that the fluid in the vicinity of a thermal wall has the same temperature as the wall.

In the following, attention will be restricted to steady states in which the gases on both sides of the piston are very dilute, so that they verify the local equation of state \( p_i = n_i k_B T_i \), where \( p_i, n_i, \) and \( T_i \), are the local pressure, number density, and temperature of the gas in compartment \( i, i = 1, 2 \). Also, in the steady states considered, only gradients of the hydrodynamic fields in the \( x \) direction are present.

The hydrodynamic Navier–Stokes equation for the velocity field, when applied to the above steady states, implies that the pressure must be uniform in each container. In addition, mechanical equilibrium of the piston requires that the pressures on both faces be the same,

\[
p_1 = p_2 = p. \tag{2}
\]

The energy balance in each container reads

\[
\frac{\partial}{\partial x} q_{x_i} = 0, \tag{3}
\]

where \( q_{x_i} \) is the heat flux along the \( x \) direction in compartment \( i \). According to the Fourier law,

\[
q_{x_i} = -\kappa(T_i) \frac{\partial T_i}{\partial x}. \tag{4}
\]

The thermal conductivity \( \kappa(T) \) in the dilute limit being considered is

\[
\kappa(T) = \frac{d(d+2)}{16(d-1)} \Gamma(d/2) \pi^{-(d-1)/2} k_B \left( \frac{k_B T}{m} \right)^{1/2} \sigma^{-(d-1)}. \tag{5}
\]

From equations (3)–(5) it follows that

\[
\frac{\partial^2 T_i^{3/2}}{\partial x^2} = 0, \tag{6}
\]

and so

\[
T_i^{3/2}(x) = a_i x + b_i, \tag{7}
\]

with \( a_i, b_i \) constants. But stationarity also requires that the heat flux be the same in both compartments, since otherwise the energy of the piston could not be constant. Then, \( q_{x1} = q_{x2} \) and using the Fourier law this leads to

\[
a_1 = a_2 = a. \tag{8}
\]

Now the boundary conditions at the thermal walls, \( T_1(0) = T_{10} \) and \( T_2(L_x) = T_{20} \), are imposed, to get

\[
T_1^{3/2}(x) = a x + T_{10}^{3/2}, \tag{9}
\]

\[
T_2^{3/2}(x) = -a (L_x - x) + T_{20}^{3/2}. \tag{10}
\]

Equation (9) holds for \( 0 < x < x_P \), and equation (10) for \( x_P < x < L_x \), where \( x_P \) is the steady position of the piston.

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The boundary conditions associated with the piston must also be introduced. Then, expressions for the energy flux between the piston and the two gases are needed. This flux appears as a consequence of the velocity fluctuations of the piston [6, 14]. Assuming that they are Gaussian in the steady state, something that is confirmed with very good accuracy by the numerical simulations, in the limit $m/M \ll 1$ it is obtained that the energy flux from the piston to the gas in compartment $i$ is given by [8]
\[ Q_i \approx -2 \left( \frac{2mk_BT}{\pi} \right)^{1/2} \frac{T_i(x_P) - T_P}{T_i^{1/2}(x_P)} M, \] (11)
where $T_P$ is the temperature parameter of the piston, defined from the second moment of its velocity distribution, and the temperature $T_i(x_P)$ is to be understood as the temperature of the gas in compartment $i$ in the limit $x \to x_P$ taken from inside the gas. Stationarity of the piston yields $Q_1 + Q_2 = 0$, i.e.
\[ \frac{T_1(x_P) - T_P}{T_1^{1/2}(x_P)} = \frac{T_2(x_P) - T_P}{T_2^{1/2}(x_P)} \] (12)
or
\[ T_P = [T_1(x_P)T_2(x_P)]^{1/2}. \] (13)
The limits of equations (11) and (13) for a system of infinite length have been also derived in [3]. A second condition at the piston follows from the continuity of the energy flux, implying that
\[ q_{x1}(x_P) = -Q_1. \] (14)
Use of equations (4) and (11) yields
\[ T_2^{1/2}(x_P) - T_1^{1/2}(x_P) = C \frac{\alpha}{\beta}, \] (15)
where
\[ C \equiv \frac{d(d+2)2\Gamma(d/2)\pi^{-(d-2)/2}k_B M}{48\sqrt{2}(d-1)m\sigma^{d-1}}. \] (16)
The last needed condition is that the number of particles in each compartment is fixed to $N$, so it must be
\[ S_P \int_0^{x_P} dx n_1(x) = S_P \int_{x_P}^{L_x} dx n_2(x) = N, \] (17)
where $S_P$ is the area ($d = 3$) or length ($d = 2$) of the piston and, therefore, also the section of the container. Employing the local equation of state and equations (9) and (10), the above conditions (15) and (17) are seen to be equivalent to
\[ T_1^{1/2}(x_P) + T_2^{1/2}(x_P) = T_{10}^{1/2} + T_{20}^{1/2} \] (18)
and
\[ T_1^{1/2}(x_P) = T_{10}^{1/2} + D \frac{\alpha}{\beta}, \] (19)
Equations (15), (18), and (19) form a closed set of equations for the unknown $T_1(x_P)$, $T_2(x_P)$, and $a/p$. Solving it gives

$$T^{1/2}_1(x_P) = T^{1/2}_{10} + D \frac{T^{1/2}_{20} - T^{1/2}_{10}}{2D + C},$$

(21)

$$T^{1/2}_2(x_P) = T^{1/2}_{20} - D \frac{T^{1/2}_{20} - T^{1/2}_{10}}{2D + C},$$

(22)

$$\frac{a}{p} = \frac{T^{1/2}_{20} - T^{1/2}_{10}}{2D + C}.$$ 

(23)

The only remaining task is to identify $a$ (or $p$) and the steady position of the piston $x_P$. By means of equations (9) and (10) it is found that

$$a = \frac{T^{3/2}_1(x_P) - T^{3/2}_2(x_P) - T^{3/2}_{10} + T^{3/2}_{20}}{L_x},$$

(24)

$$x_P = \frac{L_x[T^{3/2}_1(x_P) - T^{3/2}_{10}] - T^{3/2}_2(x_P) - T^{3/2}_{10} + T^{3/2}_{20}}{T^{3/2}_1(x_P) - T^{3/2}_2(x_P) - T^{3/2}_{10} + T^{3/2}_{20}}.$$ 

(25)

Therefore, as a consequence of the presence of the piston, the slope $a$ of the temperature profile decreases as compared with its values in a gas without a piston, being the same the temperatures of the two thermal walls.

To check the accuracy of the above theoretical predictions, molecular dynamics (MD) simulations of a system of hard disks ($d = 2$) have been performed, using an event driven algorithm [15]. The number of particles in each of the two compartments is $N = 100$ and the size of the system is $L_x = 2S_P = 100\sigma$. The values of $M/m$ and $T_{20}/T_{10}$ have been varied as indicated below. All the simulations started with the piston located in the middle of the system ($x_P = L_x/2$) and the particles homogeneously distributed in each compartment. After a short transient time, of the order of a few collisions per particle, a steady state was always reached. Then, density and temperature profiles of the gases in both compartments as well as the position and velocity distributions of the piston were measured. To identify the hydrodynamic profiles, the system was divided into 20 layers of the same width, parallel to the piston. Moreover, the average quantities have been averaged over time (typically 200 registers) and also over a given number of trajectories (typically 50).

In figure 2, the steady temperature and density profiles are plotted for a system with $M/m = 10$ and $T_{20}/T_{10} = 1.5$. The profiles for a system with the same value of the mass ratio $M/m$, but with a much larger temperature ratio, $T_{20}/T_{10} = 5$, are given in figure 3. The symbols are MD results, while the solid lines are the theoretical predictions obtained above. The vertical line indicates the average position of the piston. A fairly good agreement is observed. It is important to realize that the hydrodynamic fields in the vicinity of the average position of the piston are much influenced by the fluctuations of the latter, that are not accounted for in the simple model developed here.

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Figure 2. Steady temperature (blue crosses and solid line) and density (red circles and solid line) profiles. The symbols are MD simulation results for a two-dimensional system of $2N = 200$ hard disks with $L_x = 2S_p = 100\sigma$, $M/m = 10$, and $T_{20}/T_{10} = 1.5$. The solid lines are the theoretical predictions derived in the main text.

Figure 3. The same as figure 2, but now with $T_{20}/T_{10} = 5$.

The results for the dependence of the steady position of the piston $x_P$ on the mass ratio $M/m$ are shown in figure 4. Three different values of the ratio of the temperatures of the two thermal walls have been considered, as indicated in the inset. As the mass ratio increases, the position of the piston tends to a constant value. A similar behavior is observed for the temperature of the piston, shown in figure 5. In both cases, there is again a fairly good agreement between the simulation results and the theoretical prediction from the model proposed here.

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Figure 4. Steady position of the piston $x_P$ as a function of the mass of the piston $M$. Three values of the ratio of the temperatures of the two thermal walls have been considered, as indicated. The values of $L_x$ and $N$ are the same as in figure 2. The symbols are MD simulation results while the solid lines are the predictions derived in the main text.

Figure 5. The same as figure 4, but now the plotted quantity is the temperature of the piston divided by the temperature of the cold wall.

It seems worth investigating whether the steady state reached by the system considered here can be described by means of a minimum entropy production rule. The entropy production function $P$ of the system is [16, 17]

$$P = S_P \int_0^{x_P} dx q_{x1}(x) \frac{dT_1^{-1}(x)}{dx} + S_P \int_{x_P}^{L_x} dx q_{x1}(x) \frac{dT_2^{-1}(x)}{dx} - Q_1 \left[ \frac{1}{T_P} - \frac{1}{T_1(x_P)} \right] + Q_2 \left[ \frac{1}{T_2(x_P)} - \frac{1}{T_P} \right], \quad (26)$$

where the possible discontinuity of the temperature at the piston has been taken into account. In this expression, the relations given in equations (2), (9), (10), and (17) are assumed to be known since they correspond to boundary conditions. Moreover, the limit
of small temperature gradients will be considered in the following. Define
\[
T_m \equiv \frac{T_{10} + T_{20}}{2}, \quad \theta \equiv \frac{T_{20} - T_{10}}{2T_m},
\]
and introduce the scaled temperature deviations \(\tau_1\), \(\tau_2\), and \(\tau_P\) by
\[
T_1(x_P) = T_m + \theta \tau_1, \quad T_2(x_P) = T_m + \theta \tau_2, \quad T_P = T_m + \theta \tau_P. \tag{28}
\]
When these expressions are substituted into equation (26) and an expansion in powers of \(\theta\) is carried out, it is obtained that
\[
P(\tau_1, \tau_2, \tau_3) = 6\left(2mk_B\right)^{1/2}S_P \left[ \frac{2D}{\pi^{1/2} M L_x T_m^{3/2}} \left\{ 2D[\tau_1^2 + \tau_2^2 - 2(\tau_1 + \tau_2)\tau_P + 2\tau_P^2] 
\right. 
\right. 
+ C[\tau_1^2 + \tau_2^2 + 2T_m(\tau_1 - \tau_2 + T_m)] \theta^2 + \mathcal{O}(\theta^4) \right]. \tag{30}
\]
The values of \(\tau_1\), \(\tau_2\) and \(\tau_3\) minimizing this expression for small \(\theta\), namely neglecting terms of order \(\theta^4\) and higher, are
\[
\tau_1 = -\frac{CT_m}{C + 2D}, \quad \tau_2 = -\tau_1, \quad \tau_P = 0. \tag{31}
\]
Using these values, it is easily seen that
\[
x_P = \frac{L_x}{2} \left( 1 - \frac{C + D}{C + 2D} \theta \right), \quad \rho = \frac{2N k_B T_m}{L_x S_P}, \tag{32}
\]
\[
a_1 = a_2 = \frac{6D}{C + 2D} \frac{T_m^{3/2}}{L_x}. \tag{33}
\]
These results agree with the lowest order expansion in \(\theta\) of equations (23)–(25), as can be easily verified. On the other hand, it is also easily seen that the condition that the entropy production \(P\) is minimum is not equivalent to the hydrodynamic theory developed here outside of the limit of small temperature gradients, leading to results that strongly disagree with the numerical simulations.

In summary, it has been shown that the presence of the adiabatic piston introduces a strong discontinuity of the hydrodynamic profiles, increasing their slope in both compartments. Moreover, the simple model presented here, based on the energy balance, reproduces quite well the molecular dynamics simulation results. A minimum entropy production requirement only holds in the limit of small temperature differences. Although we are not aware of any realization of a situation similar to the one considered here, the effects discussed should be observable in experiments, by extending the devices used to investigate the relaxation to equilibrium \([18]–[20]\).

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