Vol. 32 (2001) *ACTA PHYSICA POLONICA B* No 12

THE ENIGMATIC PISTON*

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(Received September 24, 2001)

The use of ensemble theory to describe systems in thermal equilibrium is justified by the fact that it explains a large variety of experiments. The theoretical understanding, as embodied in the work of Boltzmann and Gibbs, is based on the assumption that all microscopic states with the same energy occur with equal *a priori* probability. Efforts to explain this assumption or to avoid it by using the microscopic equations of motion, are doomed to fail, because of the extreme complexity of these equations. In the present paper, however, we consider a system for which this complexity is reduced to a minimum. It consists of a finite one-dimensional tube, filled with an ideal gas, in which a piston forms an adiabatic separation between the two parts. Analytical and numerical investigation of this system reveals a very slow approach to a final state in which the piston still performs some non-chaotic motion, which is probably related to the formation of shock fronts. The general question of how much complexity is needed for a system to approach thermal equilibrium is, however, still an open problem.

PACS numbers: 05.70.Ln, 05.45.Pq

1. The problem

1.1. The Boltzmann-Gibbs point of view

A perennial source of confused discussions is the paradox that, on the one hand, the equations of motion of a system, consisting of a large number of particles, are invariant under time reversal, whereas, on the other hand, it is clear that all macroscopic systems approach an equilibrium state, so that a preferred time direction seems to exist.

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[*] Presented at the XLI Cracow School of Theoretical Physics, Zakopane, Poland, June 2–11, 2001.

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Although a century ago the misunderstanding giving rise to this paradox, was cleared up by Boltzmann and Gibbs, we believe it worthwhile to repeat the main line of their argument. In this we follow Uhlenbeck and Ford [1].

For an ideal gas all macroscopic properties of the system are determined by the distribution of N points in the μ-space of a single particle. This space is divided into a large number $M \ll N$ of cells of size $\omega_1, \cdots, \omega_M$ and a macroscopic state of the system is then specified by giving the numbers $n_1, \cdots, n_M$ of points in each of these cells. The sizes ω_i are determined by the resolving power of the measuring instruments. To a given set $\{n_1, \cdots, n_M\}$ corresponds a large number of microscopic states. The volume in $\mathit{\Gamma}$-space covered by these states is equal to

$$W(n_1, \cdots, n_M) = \frac{N!}{n_1! \cdots n_M!} \omega_1^{n_1} \cdots \omega_M^{n_M} \, .$$

The distribution which maximises this volume is proportional to the respective cell sizes and is given by

$$\overline{n}_i = A \omega_i \mathrm{e}^{-\beta \varepsilon_i} ,$$

where ε_i is the energy of a particle in cell i and A and β are fixed by the requirement that the total number of particles and the total energy are given quantities. For states $\{n_1, \cdots, n_M\} = \{\overline{n}_1 + \Delta n_1, \cdots, \overline{n}_M + \Delta n_M\}$ close to this maximum state, the corresponding volume in $\mathit{\Gamma}$-space can be calculated and is found to be equal to

$$W(n) = W(\overline{n}) \, \mathrm{e}^{-N \left\langle (\Delta n_i / \overline{n}_i)^2 \right\rangle} \, .$$

The macroscopic states for which the exponential factor is not smaller than a fixed number between zero and unity, are called equilibrium states. They form a small set in the sense that the numbers $\Delta n_i / \overline{n}_i$ are on the average of the order of $1/\sqrt{N}$. Nevertheless, the total of all these states corresponds to microscopic states which cover almost all of phase-space.

Therefore, any initial state in phase-space which is not an equilibrium state in the above sense, will, barring exceptional cases, very quickly enter this equilibrium region, never, or hardly ever, to leave it again.

The above considerations should not, of course, be considered as a proof of Boltzmann's ergodic hypothesis, which says that

> a mechanical system's trajectory in phase-space will spend *equal times* in regions of *equal phase-space measure* [2].

Also Gibbs' ensemble theory for systems in which interactions are not neglected, has no foundation based on Hamilton's equations of motion. At this point we want to quote Van Kampen [3], who argues that

> The introduction of an ensemble, and the related description in terms of probability, cannot be justified on *a priori* ground, but only by appealing to experience.

If correct, this statement should put a stop to all further research into the foundations of equilibrium statistical mechanics. There are, however, other fundamental problems, related to how fast a many-particle system approaches equilibrium. There is hope that these problems can be better understood by studying the rôle of chaotic dynamics, which are discussed, among others, by Dorfman [2] and by Zaslavsky [4].

Another way of gaining understanding is to study special systems in which the amount of complexity is reduced to a minimum, so that analytical methods can be applied.

An example of such a model-system will be studied in the present paper. The model will be described in the next section, in which we will also discuss the relation with a peculiar, widely known problem in thermodynamics.

1.2. Two experiments

As an introduction we will first discuss

1.2.1. Rüchardt's experiment [5]

This is an experiment for determining the ratio C_P/C_V of a gas. The apparatus consists of a 60 cm precision bore glass tube, attached vertically to a 10 litre glass jug. A tightly fitting steel ball of about 10 gram is allowed to fall in the tube. The enclosed volume of gas acts as a cushion, on which the ball bounces up and down. Although the oscillations are damped by friction inside the tube, the period of the oscillations can still be measured, and from this it is then possible to calculate C_P/C_V.

For the one-dimensional case we show how the equation of motion for the position $x(t)$ of the ball can be derived, assuming that the gas under the ball is at all times in thermal equilibrium, described by the pressure $P(x)$ and the temperature $T(x)$ and neglecting the friction inside the tube. We also assume that the system is thermally isolated from its surroundings. Using the thermodynamic relations for an ideal gas between energy, pressure and temperature in an adiabatic process

$$U(x) = \frac{1}{2}NkT(x) \qquad \text{and} \qquad P(x) = -\frac{dU}{dx} = -\frac{1}{2}Nk\frac{dT}{dx}\,,$$

and the ideal gas law

$$P(x) = Nk\frac{T(x)}{x}\,,$$

we see that the temperature should satisfy

$$\frac{dT}{dx} = -2\frac{T(x)}{x}\,.$$

The solution of this equation is

$$T(x) = T(x_0)\left(\frac{x_0}{x}\right)^2\,,$$

where x_0 is the position of the ball at time $t = 0$. The equation of motion of the ball becomes

$$M\frac{d^2x}{dt^2} \;=\; -Mg + P(x) = -\frac{dV}{dx}$$

with

$$V(x) \;=\; Mgx + \frac{1}{2}NkT(x_0)\left(\frac{x_0}{x}\right)^2\,.$$

The constant pressure from the outside has been included in the term $-Mg$. This equation describes an oscillatory motion between x_- and x_+, with a period equal to

$$\mathcal{T} = \sqrt{2\,M}\int\limits_{x_-}^{x_+}\frac{dx}{\sqrt{V(x_\pm) - V(x)}}\,.$$

The calculation can be repeated for the three-dimensional case, and the resulting period turns out to be in good agreement with the experimental value.

At this point we want to remark that the undamped periodic motion of the ball is a result of the existence of a velocity independent potential. There is, however, reason to doubt that the true motion of the ball is periodic. In order to show the evidence for this doubt, we have performed a numerical calculation of the motion of the ball for the case where the gas is replaced by a single particle of mass $m = 0.2\,M$, which bounces elastically between the ball and the bottom of the jug, conserving energy and momentum on each collision with the ball. When plotting the position and the velocity of the ball at each moment this particle hits the bottom, we obtain the picture shown in figure 1. This Poincaré-section of four orbits illustrates the fact that a large portion of the total phase-space is filled by a single orbit. Each of the three other orbits describes a quasi periodic motion of the system. For a mass ratio $m/M = 0.465$ the region containing quasi periodic orbits has practically shrunk to zero and all of phase-space is filled by a single orbit. Therefore, in this case the system is ergodic and the microcanonical ensemble can be used to calculate the velocity distribution $f(v)$ of the particle. The result $f(v) \sim (v_{\max}^2 - v^2)^{3/2}$ is in complete agreement with the distribution obtained by monitoring the particle velocity over a large number of collisions in a numerical simulation. During this time the motion of the ball is very erratic. It is, therefore, not unreasonable to expect that, if the single particle is replaced by a large number of gas particles, but with a total mass which is not changed, the motion of the ball will turn out still to be very erratic. Later it will turn out that this is indeed the case. This is different from the smooth behaviour which was found while analysing Rüchardt's experiment. However, the same erratic behaviour is also expected for the gas molecules, which supports the assumption of thermodynamic equilibrium made in discussing Rüchardt's experiment. This assumption led to a smooth periodic motion of the ball. We, therefore, have arrived at a paradoxical situation. One of the purposes of the present paper is to explain the origin of this paradox.

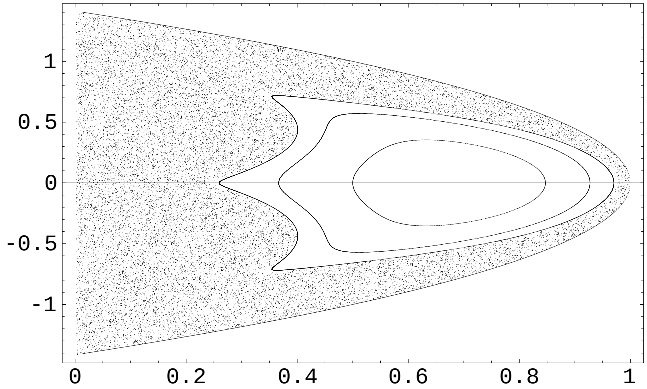

Fig. 1. Phase plot of the ball for $m/M = 0.2$.

It is related to a similar problem, about which in recent times quite a few publications have appeared, and which we will call the problem of Callen's piston.

1.2.2. Callen's experiment

In his book on thermodynamics [6] Callen calls attention to a situation which he denotes as a "uniquely delicate problem". The Gedankenexperiment is sketched in figure 2. Two gases are separated by a movable adiabatic piston. In equilibrium the pressures and temperatures on the left will be equal to those on the right, and the equations of state will then determine the position of the piston.

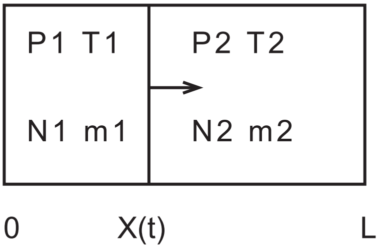

Fig. 2. Callen's piston.

Callen notices, however, that thermodynamics only predicts the correct mechanical equilibrium, $P_1 = P_2$, but that other parameters are largely undetermined. For instance, temperatures and volumes of the two compartments depend on the details of the viscous processes by which the piston dissipates its kinetic energy, but these processes do not belong to the realm of thermodynamics.

The problem which therefore arises, may be illustrated for the case of one dimensional ideal gases, although viscosity is absent there. At time $t = 0$ when the piston is released in the position x_0 with zero velocity, the internal energies, temperatures, pressures and volumes of the two gases are given. Under the assumption that the gases stay in thermal equilibrium during the motion of the piston, the ideal gas laws then determine the values of these quantities at later times. In particular the pressures become

$$P_1(x) = P_1(x_0)\left(\frac{x_0}{x}\right)^3 \quad \text{and} \quad P_2(x) = P_2(x_0)\left(\frac{L-x_0}{L-x}\right)^3 .$$

The motion of the piston then follows from

$$M\frac{d^2x}{dt^2} = P_1(x) - P_2(x) .$$

From this it can be shown that the piston is only in a stable position when from the outset the pressures are equal and the temperatures are chosen such that $P_1 = \frac{N_1kT_1}{x_0} = \frac{N_2kT_2}{L-x_0} = P_2$. Only for equal densities the temperatures to the left and to the right will be equal. It, therefore, shows, and this was Callen's main observation, that thermodynamics is not sufficient to understand why in general only that state is realised for which not just the pressures, but also the temperatures of the two gases are equal.

All non stationary solutions of the equation of motion are undamped periodic oscillations around the point

$$x = \overline{x} = \frac{L}{1+\gamma} \quad \text{with} \quad \gamma = \left(\frac{P_2(x_0)}{P_1(x_0)}\right)^{1/3}\frac{L-x_0}{x_0} .$$

For small amplitudes we find that the square of the frequency is equal to

$$\omega^2 = \frac{3N_1 k T_1(\overline{x})}{M} \frac{L}{\overline{x}^2(L-\overline{x})} \,. \tag{1}$$

As in the case of Rüchardt's experiment, we see no tendency of the system to approach equilibrium. The piston, as well as the temperatures and pressures, keep oscillating. Also adding dissipation terms to the equations of motion of the gas and of the piston does not help, because the final position of the piston, and therefore the temperatures, turn out to depend on the piston's initial position.

An appeal to ensemble theory does not improve the situation. Distributing the total energy E as the sum of E_1 and E_2 over the two gases and considering the position x of the piston as an external parameter, we can calculate the entropy, *i.e.*, the logarithm of the microcanonical partition function $Z(E_1, x)$ by standard methods:

$$\ln Z(E_1, x) = \frac{N_1}{2} \ln E_1 + \frac{N_2}{2} \ln(E - E_1) + N_1 \ln x + N_2 \ln(L-x) + \cdots \,,$$

where we have omitted terms which are independent of E_1 and x. By considering E_1 and x as independent variables we easily find the values of E_1 and x for which $\ln Z(E_1, x)$ reaches its maximum. This occurs when E_1 and x satisfy the equations

$$\frac{N_1}{E_1} = \frac{N_2}{E - E_2} \quad \text{and} \quad \frac{N_1}{x} = \frac{N_2}{L-x} \,,$$

which amounts to saying that in equilibrium the pressures and the temperatures will be equal. This seems to solve the problem of the indeterminacy of the temperatures.

However, the variables E_1 and x are not independent, because, due to the adiabatic constraint, the relations

$$dE_1 = -P_1 dx \quad \text{and} \quad d(E - E_1) = -P_2\, d(L-x)$$

exist, where $P_1 = \frac{2E_1}{x}$ and $P_2 = \frac{2(E-E_1)}{L-x}$. From these only the equality of the pressures can be deduced; separate conclusions on temperatures and volumes cannot be drawn. This is in agreement with the fact that under the adiabatic constraint $d \ln Z = 0$ identically, as in Callen's demonstration.

The controversies around Callen's piston have been discussed by Curzon and Leff [7], who also give references to older literature. Gruber [9] discusses more recent developments.

The above considerations show that on the basis of pure thermodynamic theory it cannot be understood why also the temperatures on both sides of the adiabatic piston should become equal. An important assumption has been, however, that during the process the system went through a series of states which were always equilibrium states. This assumption will be questioned in the present paper by developing a model which is closer to kinetic theory. Other models of this type have been discussed in the recent literature [8-15]. A comparison with our work will, however, be postponed until the last section.

2. The continuum limit

Our goal is to derive a macroscopic description of the behaviour of the gas and of the piston, in the limit where N_1 and N_2 tend to infinity. This can, however, not be the usual thermodynamic limit, in which simultaneously the size of the system grows indefinitely, while the particle masses are kept constant. In this case the correlations between recollisions, which are essential for the establishment of equilibrium, would be lost.

Instead we now consider the case in which the size L of the container is fixed and the masses N_1m_1 and N_2m_2 of the gas to the left and to the right are comparable to the mass M of the piston. This piston mass, as well as the total energy, will also be kept fixed when $N = N_1 + N_2 \to \infty$. The mass of the gas particles will tend to zero, however.

This is called the continuum limit. It can be formally characterised by taking Boltzmann's constant $k \to 0$. As was explained in great detail by Compagner [16], this is the proper limit for the description of a thermodynamic system when macroscopic dependencies on space and time are present. All microscopic fluctuations are suppressed.

At any time the state of the system is given by specifying the position $X(t)$ and the velocity $V(t) = \frac{dX(t)}{dt}$ of the piston and also the coordinates and velocities of the gas molecules. Since, however, the number of molecules goes to infinity and since these molecules have no mutual interaction, the state of the gas is actually completely described by two distribution functions $f_1(x,v,t)$ and $f_2(x,v,t)$. Here $f_1(x,v,t)\,dx\,dv$ is the fraction of all molecules on the left in the volume element $(x, x+dx), (v, v+dv)$, with $0 < x < X(t)$. In the same way is $f_2(x,v,t)\,dx\,dv$ the fraction of all molecules on the right in the volume element $(x, x+dx), (v, v+dv)$, with $X(t) < x < L$. These functions are, therefore, normalised as

$$\int\limits_0^{X(t)} dx \int\limits_{-\infty}^{\infty} f_1(x,v,t)\,dv = 1 \quad \text{and} \quad \int\limits_{X(t)}^{L} dx \int\limits_{-\infty}^{\infty} f_2(x,v,t)\,dv = 1\,.$$

The fact that they do not change because of collisions, but only because of the free streaming of the gas, implies that they satisfy the continuity equations

$$\frac{\partial f_1(x,v,t)}{\partial t} + v\frac{\partial f_1(x,v,t)}{\partial x} = 0 \quad \text{for} \quad 0 < x < X(t) \quad \text{and all } v \text{ and } t \quad (2)$$

and

$$\frac{\partial f_2(x,v,t)}{\partial t} + v\frac{\partial f_2(x,v,t)}{\partial x} = 0 \quad \text{for} \quad X(t) < x < L \quad \text{and all } v \text{ and } t\,. \quad (3)$$

In a collision with one of the walls the particle velocity will be reversed: $v \to -v$, whereas in a collision with the piston the velocity of the (massless) particle will be transformed like $v \to 2V(t) - v$. The boundary values of $f_1(x,v,t)$ and $f_2(x,v,t)$, therefore, have to satisfy the following conditions

$$\begin{aligned} \text{for } x &= 0: \qquad f_1(0,-v,t) = f_1(0,v,t) \quad \text{for all } v \text{ and } t\,, \\ \text{for } x &= L: \qquad f_2(L,-v,t) = f_2(L,v,t) \quad \text{for all } v \text{ and } t \end{aligned} \qquad (4)$$

and

$$\begin{aligned} &\text{for} \quad x = X(t): \quad f_i(X(t), 2V(t) - v, t) = f_i(X(t), v, t)\,, \\ &\text{for} \quad \text{all } v \text{ and } t \text{ and } i = 1,2\,. \end{aligned}$$

The latter condition can also be written as

$$\begin{aligned} &\text{for} \quad x = X(t): \quad f_i(X(t), V(t) - v, t) = f_i(X(t), V(t) + v, t) \\ &\text{for} \quad \text{all } v \text{ and } t \text{ and } i = 1,2\,. \end{aligned} \qquad (5)$$

For given initial distributions $f_1(x,v,0)$ and $f_2(x,v,0)$ on the intervals $0 < x < X(0)$ and $X(0) < x < L$ and for all v, and assuming that $X(t)$ is a known function of t, equations (2) and (3), together with the boundary conditions (4) and (5), should be sufficient to calculate the distributions at later times. It will turn out that the solution of these equations is far from trivial, and the main part of this paper is, therefore, devoted to the study of this problem.

First of all we want to convince ourselves that the number of particles in each of the two compartments is conserved, or in terms of the continuum limit, that the total amount of fluid on each side does not vary in time. For that purpose we calculate the integral

$$\begin{aligned}
&\frac{d}{dt}\int\limits_0^{X(t)} dx \int\limits_{-\infty}^{\infty} f_1(x,v,t)\,dv\\
&= V\int\limits_{-\infty}^{\infty} f_1(X(t),v,t)\,dv + \int\limits_0^{X(t)} dx \int\limits_{-\infty}^{\infty} \frac{\partial f_1(x,v,t)}{\partial t} dv\\
&= V\int\limits_{-\infty}^{\infty} f_1(X(t),v,t)\,dv + \int\limits_0^{X(t)} dx \int\limits_{-\infty}^{\infty} (-v\,\frac{\partial f_1(x,v,t)}{\partial x}) dv\\
&= V\int\limits_{-\infty}^{\infty} f_1(X(t),v,t)\,dv - \int\limits_{-\infty}^{\infty} v f_1(X(t),v,t)\,dv + \int\limits_{-\infty}^{\infty} v f_1(0,v,t)\,dv\,. \qquad (6)
\end{aligned}$$

The third integral on the right hand side vanishes because of Eq. (4). The second integral can be written as

$$\begin{aligned}
&\int\limits_{-\infty}^{\infty} v f_1(X(t),v,t)\,dv\\
&= \int\limits_{-\infty}^{\infty} (V+v)\, f_1(X(t),V+v,t)\,dv\\
&= \int\limits_{-\infty}^{\infty} (V-v)\, f_1(X(t),V+v,t)\,dv\,, \qquad (7)
\end{aligned}$$

in which Eq. (5) was invoked. Taking half the sum of the last two integrals in Eq. (7) gives

$$\begin{aligned}
\int\limits_{-\infty}^{\infty} v f_1(X(t),v,t)\,dv &= V\int\limits_{-\infty}^{\infty} f_1(X(t),V+v,t)\,dv\\
&= V\int\limits_{-\infty}^{\infty} f_1(X(t),v,t)\,dv\,.
\end{aligned}$$

Substitution into Eq. (6) then shows that the sum of the integrals in the right-hand side of this equation is equal to zero, so that the conservation law has indeed been established. The same proof holds for $f_2(x,v,t)$.

With similar manipulations we can show that for an arbitrary function H, *e.g.* $H = f_1 \log f_1$, the integral $\int_0^{X(t)} dx \int_{-\infty}^{\infty} H[f_1(x,v,t)]\, dv$ is constant in time.

The total momentum of the system is not conserved, because the walls at $x = 0$ and $x = L$ exert a force on the gas. However, for collisions with the piston momentum conservation does hold. From this we can determine the force on the piston, by calculating the momentum transfer per unit time from the gas to the piston. Since for each collision this loss of momentum is equal to $m_i(v - v') = 2m_i(v - V(t))$ — for $m_i \ll M$ — the momentum transfer in the time dt from the gas on the left to the piston is equal to

$$(\text{momentum transfer in } dt) = N_1 \int\limits_{V(t)}^{\infty} dv \int\limits_{X(t)-(v-V(t))dt}^{X(t)} 2m_1(v-V(t)) f_1(x,v,t)\, dx\,.$$

From this follows the force on the piston due to the first gas

$$F_1(t) = 2N_1 m_1 \int\limits_{V(t)}^{\infty} (v - V(t))^2 f_1(X(t),v,t)\, dv\,. \tag{8}$$

The force due to the second gas becomes

$$F_2(t) = 2N_2 m_2 \int\limits_{-\infty}^{V(t)} (V(t) - v)^2 f_2(X(t),v,t)\, dv\,. \tag{9}$$

Using Eq. (5) these integrals can be written as integrals over the whole v-axis, so the equation of motion for the piston becomes

$$\begin{aligned} M\,\frac{d^2X(t)}{dt^2} &= F_1(t) - F_2(t) \\ &= \int\limits_{-\infty}^{\infty} (v - V(t))^2 \left[N_1 m_1 f_1(X(t),v,t) - N_2 m_2 f_2(X(t),v,t)\right] dv\,. \end{aligned} \tag{10}$$

Together with (2)–(5) we now have a closed set of equations for the description of the system in the continuum limit. (Remember that $\mu_1 = \frac{N_1 m_1}{M}$ and $\mu_2 = \frac{N_2 m_2}{M}$ are finite dimensionless numbers, which remain constant when $N_1, N_2 \to \infty$.)

Also the total energy

$$E = \frac{1}{2}M V^2(t) + \frac{1}{2}N_1 m_1 \int_0^{X(t)} dx \int_{-\infty}^{\infty} v^2 f_1(x,v,t)\, dv$$
$$+\frac{1}{2}N_2 m_2 \int_{X(t)}^{L} dx \int_{-\infty}^{\infty} v^2 f_2(x,v,t)\, dv$$

is conserved. This can be proved with the same method as above. If in addition we use the equation of motion of the piston and the fact that

$$\int_{-\infty}^{\infty} (v - V(t))^n\, f_i(X(t),v,t)\, dv = 0 \quad \text{for odd } n\,, \tag{11}$$

it is easy to show that indeed $\frac{dE}{dt} = 0$.

3. An *Ansatz*

As an approximate solution of Eqs (2)–(5) we propose Maxwell distributions, shifted in velocity and with time dependent parameters $f_1(x,v,t) \simeq f_1^M(x,v,t)$ and $f_2(x,v,t) \simeq f_2^M(x,v,t)$ with

$$f_1^M(x,v,t) = \frac{1}{X(t)}\sqrt{\frac{m_1\beta_1(t)}{2\pi}}\exp -\frac{1}{2}m_1\beta_1(t)\left(v - \frac{x}{X(t)}V(t)\right)^2$$

for $0 \leq x \leq X(t)$

and

$$f_2^M(x,v,t) = \frac{1}{L - X(t)}\sqrt{\frac{m_2\,\beta_2(t)}{2\pi}}\exp -\frac{1}{2}m_2\,\beta_2(t)\left(v - \frac{L-x}{L-X(t)}V(t)\right)^2$$

for $X(t) \leq x \leq L$.

These same functions were used by Huang [17] as an approximate solution of Boltzmann's transport equation. They are properly normalised and satisfy the boundary conditions (4) and (5). Furthermore, these distributions give rise to uniform normalised spatial densities and linear spatial profiles for the local macroscopic gas velocities:

$$\rho_1^M(x,t) \equiv \int_{-\infty}^{\infty} f_1^M(x,v,t)\,dv = \frac{1}{X(t)}\,,$$

$$w_1^M(x,t) \equiv \frac{1}{\rho_1^M(x,t)} \int_{-\infty}^{\infty} v\, f_1^M(x,v,t)\,dv = \frac{x}{X(t)} V(t)\,.$$

Likewise for the other compartment:

$$\rho_2^M(x,t) = \frac{1}{L - X(t)} \quad \text{and} \quad w_2^M(x,t) = \frac{L-x}{L-X(t)} V(t)\,.$$

In order to determine the time dependence of the reciprocal temperatures $\beta_1(t)$ and $\beta_2(t)$ we first calculate the energy content of both gases:

$$E_1(t) = \frac{1}{2} N_1 m_1 \int_0^{X(t)} dx \int_{-\infty}^{\infty} v^2 f_1^M(x,v,t)\,dv = \frac{N_1}{2\beta_1(t)} + \frac{1}{6} N_1 m_1 V^2(t)\,,$$

$$E_2(t) = \frac{1}{2} N_2 m_2 \int_{X(t)}^{L} dx \int_{-\infty}^{\infty} v^2 f_2^M(x,v,t)\,dv = \frac{N_2}{2\beta_2(t)} + \frac{1}{6} N_2 m_2 V^2(t)\,.$$

Both expressions contain a contribution from the local macroscopic velocity, which for the first gas is

$$\frac{1}{2} N_1 m_1 \int_0^{X(t)} \rho_1^M(x,t)\,(w_1^M(x,t))^2\,dx = \frac{1}{6} N_1 m_1 V^2(t)\,,$$

and one from the internal energy. The equation of motion (10) for the piston takes the form

$$M\,\frac{d^2X(t)}{dt^2} = \frac{N_1}{\beta_1(t)\,X(t)} - \frac{N_2}{\beta_2(t)\,(L - X(t))}\,, \tag{12}$$

from which the time evolution of the total energy follows:

$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt}\left[\frac{1}{2} M\,V^2(t) + E_1(t) + E_2(t)\right] \\ &= \frac{1}{3} N_1 m_1 V(t) \frac{dV}{dt} + \frac{N_1 V(t)}{\beta_1(t)\,X(t)} - \frac{N_1}{2\beta_1^2(t)} \frac{d\beta_1}{dt} \\ &\quad + \frac{1}{3} N_2 m_2 V(t) \frac{dV}{dt} - \frac{N_2 V(t)}{\beta_2(t)\,(L - X(t))} - \frac{N_2}{2\beta_2^2(t)} \frac{d\beta_2}{dt}\,. \end{aligned}$$

Since we insist on energy conservation, also for the approximate solutions, we choose the time dependence of the temperatures such that they obey the equations

$$\frac{dT_1}{dt}+2\frac{V(t)}{X(t)}T_1(t)+\frac{m_1}{3\,k}\frac{dV^2(t)}{dt}=0 \tag{13}$$

and

$$\frac{dT_2}{dt}-2\frac{V(t)}{L-X(t)}T_2(t)+\frac{m_2}{3\,k}\frac{dV^2(t)}{dt}=0\,. \tag{14}$$

Notice that Boltzmann's constant only appears in the combinations $\frac{m_i}{k}$, which attain definite values in the continuum limit. Using these equations we can derive the equations which should be satisfied by the distributions $f_1^M(x,v,t)$ and $f_2^M(x,v,t)$:

$$\left(\frac{\partial}{\partial t}+v\frac{\partial}{\partial x}\right)f_1^M(x,v,t)=C_1(x,v,t)\,f_1^M(x,v,t)\quad\text{for}\quad 0<x<X(t)$$

and

$$\left(\frac{\partial}{\partial t}+v\frac{\partial}{\partial x}\right)f_2^M(x,v,t)=C_2(x,v,t)\,f_2^M(x,v,t)\quad\text{for}\quad X(t)<x<L\,,$$

with $C_1(x,v,t)$ and $C_2(x,v,t)$ defined by

$$\begin{aligned}C_1(x,v,t)&=m_1\beta_1(t)\frac{dV(t)}{dt}\\&\times\left[\frac{1}{3}V(t)+\left(v-w_1^M(x,t)\right)\frac{x}{X(t)}-\frac{1}{3}m_1\beta_1(t)\left(v-w_1^M(x,t)\right)^2V(t)\right]\end{aligned}$$

and

$$\begin{aligned}C_2(x,v,t)&=m_2\beta_2(t)\frac{dV(t)}{dt}\\&\times\left[\frac{1}{3}V(t)+\left(v-w_2^M(x,t)\right)\frac{L-x}{L-X(t)}-\frac{1}{3}m_2\beta_2(t)\left(v-w_2^M(x,t)\right)^2V(t)\right].\end{aligned}$$

Clearly, the shifted Maxwell distributions in general only give an approximate solution of equations (2) and (3). They become exact when the molecular masses or the piston's acceleration become small. In order to elucidate this point we rewrite the equations in dimensionless variables, which will also be used in the sections on hydrodynamics and on simulations.

As units of length, velocity, time and temperature we take

$$L, V_0\equiv\sqrt{2\frac{E}{M}},\ t_0\equiv\frac{L}{V_0}\ \text{ and }\ T_0\equiv 2\frac{E}{Nk}\,,\ \text{ respectively, where }\ N=N_1+N_2$$

is the total number of gas molecules (this number tends to infinity in the continuum limit, but the product Nk stays finite). The unit of velocity is equal to the velocity of the piston if it would carry all energy of the system and the molecules were at rest. In terms of these units we define

$$\begin{aligned}&x = yL, \quad v = \widetilde{v}\,V_0, \quad N_i = n_i N, \quad N_i m_i = \mu_i M, \quad L\,V_0 f_i^M \equiv h_i^M(y,\widetilde{v},\tau)\,,\\ &t = \tau t_0, \quad X(t) = x(\tau)L, \quad V(t) = \widetilde{V}(\tau)V_0, \quad T_i(t) = u_i(\tau)T_0\,,\\ &t_0 C_i = D_i(y,\widetilde{v},\tau)\,.\end{aligned}$$

Inserting these quantities into the shifted Maxwell distributions we find

$$\begin{aligned} h_1^M(y,\widetilde{v},\tau) &= \frac{1}{x(\tau)}\sqrt{\frac{\mu_1}{2\pi n_1 u_1(\tau)}}\exp -\frac{\mu_1}{2n_1u_1(\tau)}\left(\widetilde{v}-\frac{y}{x(\tau)}\widetilde{V}(\tau)\right)^2 \\ &\text{for } 0\le y\le x(\tau) \end{aligned} \tag{15}$$

and

$$\begin{aligned} h_2^M(y,\widetilde{v},\tau) &= \frac{1}{1-x(\tau)}\sqrt{\frac{\mu_2}{2\pi n_2 u_2(\tau)}}\exp -\frac{\mu_2}{2n_2u_2(\tau)}\left(\widetilde{v}-\frac{1-y}{1-x(\tau)}\widetilde{V}(\tau)\right)^2 \\ &\text{for } x(\tau)\le y\le 1\,. \end{aligned} \tag{16}$$

The distributions $h_1^M(y,\widetilde{v},\tau)$ and $h_2^M(y,\widetilde{v},\tau)$ are normalised to unity and satisfy the equations

$$\frac{\partial h_1^M(y,\widetilde{v},\tau)}{\partial\tau}+\widetilde{v}\frac{\partial h_1^M(y,\widetilde{v},\tau)}{\partial y} = D_1(y,\widetilde{v},\tau)\,h_1^M(y,\widetilde{v},\tau) \quad \text{for } 0\le y\le x(\tau)$$

and

$$\frac{\partial h_2^M(y,\widetilde{v},\tau)}{\partial\tau}+\widetilde{v}\frac{\partial h_2^M(y,\widetilde{v},\tau)}{\partial y} = D_2(y,\widetilde{v},\tau)\,h_2^M(y,\widetilde{v},\tau) \quad \text{for } x(\tau)\le y\le 1\,,$$

in which

$$\begin{aligned} D_1(y,\widetilde{v},\tau) &= \frac{\mu_1}{n_1u_1(\tau)}\frac{d\widetilde{V}(\tau)}{d\tau} \\ &\times\left[\frac{1}{3}\widetilde{V}(\tau)+\left(\widetilde{v}-\frac{y}{x(\tau)}\widetilde{V}(\tau)\right)\frac{y}{x(\tau)}-\frac{1}{3}\frac{\mu_1}{n_1u_1(\tau)}\left(\widetilde{v}-\frac{y}{x(\tau)}\widetilde{V}(\tau)\right)^2\widetilde{V}(\tau)\right] \end{aligned}$$

and

$$\begin{aligned} D_2(y,\widetilde{v},\tau) &= \frac{\mu_2}{n_2u_2(\tau)}\frac{d\widetilde{V}(\tau)}{d\tau}\left[\frac{1}{3}\widetilde{V}(\tau)+\left(\widetilde{v}-\frac{1-y}{1-x(\tau)}\widetilde{V}(\tau)\right)\frac{1-y}{1-x(\tau)}\right. \\ &\left.-\frac{1}{3}\frac{\mu_2}{n_2u_2(\tau)}\left(\widetilde{v}-\frac{1-y}{1-x(\tau)}\widetilde{V}(\tau)\right)^2\widetilde{V}(\tau)\right]. \end{aligned}$$

Since in most discussions of this problem $n_1 \equiv 1 - n_2 \simeq \frac{1}{2}$, we see that $h_1^M(y, \widetilde{v}, \tau)$ and $h_2^M(y, \widetilde{v}, \tau)$ describe free streaming fluids when the temperatures $u_1(\tau)$ and $u_2(\tau)$ are not too low and the relative fluid masses μ_1 and μ_2 or the acceleration of the piston are small.

Let us now turn to the solutions of Eqs (12), (13) and (14), which we first write in dimensionless form. In order to make contact with the thermodynamic description in Section 1.2, we will use the dimensionless pressures $P_1(\tau)$ and $P_2(\tau)$ instead of the temperatures $u_1(\tau)$ and $u_2(\tau)$:

$$\widetilde{P}_1(\tau) = \frac{n_1 u_1(\tau)}{x(\tau)} \quad \text{and} \quad \widetilde{P}_2(\tau) = \frac{n_2 u_2(\tau)}{1 - x(\tau)} \,. \tag{17}$$

Eqs (12)–(14) then read

$$\begin{aligned}
\frac{d^2 x(\tau)}{d\tau^2} &= \widetilde{P}_1(\tau) - \widetilde{P}_2(\tau) \,, \\
\frac{d\widetilde{P}_1(\tau)}{d\tau} &= -\frac{1}{x(\tau)} \left[\gamma_1 \widetilde{P}_1(\tau) - \alpha_1 \widetilde{P}_2(\tau)\right] \frac{dx(\tau)}{d\tau} \,, \\
\frac{d\widetilde{P}_2(\tau)}{d\tau} &= \frac{1}{1 - x(\tau)} \left[\gamma_2 \widetilde{P}_2(\tau) - \alpha_2 \widetilde{P}_1(\tau)\right] \frac{dx(\tau)}{d\tau} \,,
\end{aligned} \tag{18}$$

in which $\alpha_i = \frac{2}{3}\mu_i$ and $\gamma_i = 3 + \alpha_i$, $i = 1, 2$.

Eliminating τ by the substitution $d\tau = dx/\widetilde{V}$ we finally get for the pressure equations

$$\frac{d\widetilde{P}_1(x)}{dx} = -\frac{1}{x} \left[\gamma_1 \widetilde{P}_1(x) - \alpha_1 \widetilde{P}_2(x)\right]$$

and

$$\frac{d\widetilde{P}_2(x)}{dx} = \frac{1}{1 - x} \left[\gamma_2 \widetilde{P}_2(x) - \alpha_2 \widetilde{P}_1(x)\right] \,.$$

The exact solution in terms of hypergeometric functions can be given, but is rather uninformative and will not be exhibited here. Since the velocity $\widetilde{V}$ does not appear in this solution the piston will perform a periodic motion without damping. One integration constant is the energy, which in dimensionless units is equal to

$$\frac{E}{\frac{1}{2} M V_0^2} = 1 = \left(1 + \frac{1}{2}\alpha_1 + \frac{1}{2}\alpha_2\right) \left(\frac{dx(\tau)}{d\tau}\right)^2 + x\widetilde{P}_1(x) + (1 - x)\widetilde{P}_2(x) \,.$$

From this an expression for the period of the piston's motion can easily be derived

$$\mathcal{T} = \sqrt{2(2+\alpha_1+\alpha_2)} \int_{x_-}^{x_+} \frac{dx}{\sqrt{1 - x\widetilde{P}_1(x) - (1-x)\widetilde{P}_2(x)}}\,,$$

in which x_- and x_+ are the turning points.

For the special case of massless gases, *i.e.* $\mu_1 = \mu_2 = 0$, the solution can be given in terms of elementary functions. If, moreover, we consider only oscillations of small amplitudes the frequency becomes equal to the frequency calculated by the thermodynamic method and given by Eq. (1), which reads in scaled variables

$$\widetilde{\omega}^2 \equiv \omega^2 t_0^2 = \frac{3\,n_1 u_1(\overline{x})}{\overline{x}^2(1-\overline{x})}\,,$$

$\overline{x}$ now being the scaled equilibrium point.

The conclusion of this section is that for small values of μ_1 and μ_2 the shifted Maxwell distributions probably give a good approximation to the exact distributions. It is, however, still not clear whether and how these functions, when started from arbitrary values, will be approached for large times. The perpetual oscillatory behaviour of the pressures and temperatures is in conflict with the predictions of ensemble theory. It remains to be seen whether this conflict is due to the approximations and will disappear in an exact solution, or whether it is a property of the special system we are considering here.

4. The hydrodynamic description

4.1. The general equations

Despite their simple appearance equations (2) and (3), together with the boundary conditions (4) and (5), are hard to solve exactly. A less ambitious task, in which we abandon the idea to calculate the full distribution functions, is to try and find solutions for the hydrodynamic equations. As shown *e.g.* by Huang [17], these can be derived from Eqs (2)–(5). To this end we define

the normalised spatial densities ($i = 1, 2$) :

$$\rho_i(x,t) = \int_{-\infty}^{\infty} f_i(x,v,t)\,dv, \qquad \int_0^{X(t)} \rho_1(x,t)\,dx = 1, \qquad \int_{X(t)}^{L} \rho_2(x,t)\,dx = 1\,,$$

the local velocities:

$$w_i(x,t) = \frac{1}{\rho_i(x,t)} \int_{-\infty}^{\infty} v\, f_i(x,v,t)\, dv\,,$$

the local temperatures:

$$T_i(x,t) = \frac{m_i}{k} \frac{1}{\rho_i(x,t)} \int_{-\infty}^{\infty} (v - w_i(x,t))^2\; f_i(x,v,t)\, dv\,,$$

and the local heat fluxes:

$$q_i(x,t) = \frac{1}{2} m_i N_i \int_{-\infty}^{\infty} (v - w_i(x,t))^3\; f_i(x,v,t)\, dv\,.$$

The local pressures are related to the local spatial densities and temperatures by the ideal gas law

$$\widetilde{P}_i(x,t) = N_i\, \rho_i(x,t)\, kT_i(x,t)\,.$$

The boundary conditions (4) and (5) impose boundary conditions on some of these quantities:

$$w_1(0,t) = w_2(L,t) = 0 \quad \text{and} \quad w_1(X(t),t) = w_2(X(t),t) = V(t)$$

and

$$q_1(0,t) = q_2(L,t) = 0 \quad \text{and} \quad q_1(X(t),t) = q_2(X(t),t) = 0\,, \tag{19}$$

the latter equality following from Eq. (11).

The equation of motion for the piston (10) then takes the form

$$M\, \frac{d^2 X(t)}{dt^2} = P_1(X(t),t) - P_2(X(t),t)\,. \tag{20}$$

From Eqs (2)–(5) one easily derives the standard conservation laws:

the continuity equation:

$$\frac{\partial \rho_i(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\rho_i(x,t)\, w_i(x,t)\right) = 0\,,$$

momentum conservation:

$$\rho_i(x,t)\left[\frac{\partial}{\partial t}+w_i(x,t)\frac{\partial}{\partial x}\right]w_i(x,t)=-\frac{1}{N_i m_i}\frac{\partial P_i(x,t)}{\partial x}\,,$$

energy conservation:

$$\rho_i(x,t)\left[\frac{\partial}{\partial t}+w_i(x,t)\frac{\partial}{\partial x}\right]T_i(x,t)=-\frac{2}{N_i\,k}\left[\frac{\partial q_i(x,t)}{\partial x}+P_i(x,t)\frac{\partial w_i(x,t)}{\partial x}\right].$$

In order to assess the relative importance of the various terms in these expressions we write them in dimensionless form, using the units of Section 3. The distribution functions are replaced by $h_i(y,\widetilde{v},\tau)=L\,V_0\,f_i(x,v,t)$, which are normalised as

$$\int\limits_0^{x(\tau)} dy \int\limits_{-\infty}^{\infty} h_1(y,\widetilde{v},\tau)\,d\widetilde{v}=1 \quad \text{and} \quad \int\limits_{x(\tau)}^{1} dy \int\limits_{-\infty}^{\infty} h_2(y,\widetilde{v},\tau)\,d\widetilde{v}=1\,.$$

In addition we introduce

the scaled local densities:

$$\rho_i(x,t)=\frac{1}{L}\widetilde{\rho}_i(y,\tau), \quad \text{so that} \quad \widetilde{\rho}_i(y,\tau)=\int\limits_{-\infty}^{\infty} h_i(y,\widetilde{v},\tau)\,d\widetilde{v}\,,$$

the scaled local velocities:

$$w_i(x,t)=V_0\widetilde{w}_i(y,\tau) \quad \text{so that} \quad \widetilde{w}_i(y,\tau)=\frac{1}{\widetilde{\rho}_i(y,\tau)}\int\limits_{-\infty}^{\infty}\widetilde{v}\,h_i(y,\widetilde{v},\tau)\,d\widetilde{v}\,,$$

the scaled local temperatures: $T_i(x,t)=T_0\,u_i(y,\tau)$ so that

$$u_i(y,\tau)=\frac{\mu_i}{n_i\,\widetilde{\rho}_i(y,\tau)}\int\limits_{-\infty}^{\infty}(\widetilde{v}-\widetilde{w}_i(y,\tau))^2\,h_i(y,\widetilde{v},\tau)\,d\widetilde{v}\,,$$

the scaled local pressures:

$$P_i(x,t)=\frac{M\,V_0^2}{L}\widetilde{P}_i(y,\tau) \quad \text{so that} \quad \widetilde{P}_i(y,\tau)=n_i\widetilde{\rho}_i(y,\tau)\,u_i(y,\tau)\,,$$

and the scaled local heat fluxes: $q_i(x,t)=\frac{MV_0^3}{L}\widetilde{q}_i(y,\tau)$ so that

$$\widetilde{q}_i(y,\tau)=\frac{\mu_i}{2}\int_{-\infty}^{\infty}(\widetilde{v}-\widetilde{w}_i(y,\tau))^3 h_i(y,\widetilde{v},\tau)\,d\widetilde{v}\,.$$

In these units the equations expressing the conservation laws read:

$$\frac{\partial\widetilde{\rho}_i(y,\tau)}{\partial\tau}+\frac{\partial}{\partial y}\left(\widetilde{\rho}_i(y,\tau)\,\widetilde{w}_i(y,\tau)\right) = 0\,. \tag{21}$$

$$\begin{aligned}\widetilde{\rho}_i(y,\tau)\left[\frac{\partial}{\partial\tau}+\widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]\widetilde{w}_i(y,\tau) &= -\frac{1}{\mu_i}\frac{\partial\widetilde{P}_i(y,\tau)}{\partial y}\\ &= -\frac{n_i}{\mu_i}\frac{\partial}{\partial y}\left(\widetilde{\rho}_i(y,\tau)\,u_i(y,\tau)\right)\,. \end{aligned}\tag{22}$$

$$\begin{aligned}\widetilde{\rho}_i(y,\tau)\left[\frac{\partial}{\partial\tau}+\widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]u_i(y,\tau) &= -\frac{2}{n_i}\left[\frac{\partial\widetilde{q}_i(y,\tau)}{\partial y}+\widetilde{P}_i(y,\tau)\frac{\partial\widetilde{w}_i(y,\tau)}{\partial y}\right]\end{aligned}$$

$$= -\frac{\mu_i}{n_i}\frac{\partial}{\partial y}\int_{-\infty}^{\infty}(\widetilde{v}-\widetilde{w}_i(y,\tau))^3 h_i(y,\widetilde{v},\tau)\,d\widetilde{v}-2\,\widetilde{\rho}_i(y,\tau)\,u_i(y,\tau)\frac{\partial\widetilde{w}_i(y,\tau)}{\partial y}\,. \tag{23}$$

In the new units the total energy is equal to unity. With the scaled variables it can be expressed in terms of the scaled local functions as $K+Q=1$,

in which K is the total kinetic energy of the piston and of the local motions of the fluid

$$K=\left(\frac{dx(\tau)}{d\tau}\right)^2+\mu_1\int_0^{x(\tau)}\widetilde{\rho}_1(y,\tau)\widetilde{w}_1(y,\tau)^2dy+\mu_2\int_{x(\tau)}^{1}\widetilde{\rho}_2(y,\tau)\widetilde{w}_2(y,\tau)^2dy \tag{24}$$

and Q is the total internal energy. This is the kinetic energy as measured relative to the local velocities

$$Q=n_1\int_0^{x(\tau)}\widetilde{\rho}_1(y,\tau)\,u_1(y,\tau)\,dy+n_2\int_{x(\tau)}^{1}\widetilde{\rho}_2(y,\tau)\,u_2(y,\tau)\,dy\,. \tag{25}$$

For an ideal one-dimensional gas the relation between pressure, density and entropy is given by

$$P=\kappa\,\rho^3\mathrm{e}^{S/c_v}\,,$$

in which κ is some constant. Therefore, if instead of using the local temperature, we want to use a quantity which can be interpreted as (a function of) the local entropy, the above relation suggests to define the following dependent variables

$$s_i^2 = \frac{\kappa \mathrm{e}^{S_i/c_v}}{MV_0^2L^2}\,.$$

With these functions the dimensionless pressures can be written as

$$\widetilde{P}_i(y,\tau) = n_i\widetilde{\rho}_i(y,\tau)\,u_i(y,\tau) = \widetilde{\rho}_i^3(y,\tau)\,s_i^2(y,\tau)\,.$$

Eqs (21)–(23) can now be written as

$$\frac{\partial\widetilde{\rho}_i(y,\tau)}{\partial\tau} + \frac{\partial}{\partial y}\left(\widetilde{\rho}_i(y,\tau)\,\widetilde{w}_i(y,\tau)\right) \;=\; 0\,, \tag{26}$$

$$\left[\frac{\partial}{\partial\tau} + \widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]\widetilde{w}_i(y,\tau) \;=\; -\frac{1}{\mu_i\,\widetilde{\rho}_i}\frac{\partial}{\partial y}\left(\widetilde{\rho}_i^3(y,\tau)s_i^2(y,\tau)\right)\,, \tag{27}$$

$$\left[\frac{\partial}{\partial\tau} + \widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]s_i^2(y,\tau) \;=\; -\frac{2}{\widetilde{\rho}_i^3}\frac{\partial\widetilde{q}_i}{\partial y}\,. \tag{28}$$

Eqs (26)–(28) form a set of conservation laws, which put constraints on the unknown functions $\widetilde{\rho}_i(y,\tau), \widetilde{w}_i(y,\tau)$, $s_i(y,\tau)$ and $\widetilde{q}_i(y,\tau)$, but which are not sufficient to fix them completely.

This situation is changed when we assume that the spatial derivative of the heat flux, which according to Eq. (28) is the source of entropy production, can be neglected. In view of the boundary conditions (19) this is equivalent to assuming that $\widetilde{q}_i(y,\tau)\equiv 0$ for all y and τ. For the *Ansatz* we made in Eqs (15) and (16) for the distribution funtions $h_i^M(y,\widetilde{v},\tau)$ this assumption is satisfied, because the heat fluxes $\widetilde{q}_i^M(y,\tau)$ are identically zero. If in the general case we also assume that the heat flux is the same in all points (this is called an ideal fluid), Eq. (28) becomes

$$\left[\frac{\partial}{\partial\tau} + \widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]s_i(y,\tau) = 0\,.$$

This equation shows that $s_i(y,\tau)$ is constant along each stream line defined as the solution $y(\tau;y_0)$ of $\frac{dy(\tau;y_0)}{d\tau} = \widetilde{w}_i(y,\tau)$, with $y(0;y_0)=y_0$.

Together with Eqs (26) and (27) we now have a set of hydrodynamic equations for the initial value problem, from which for a prescribed motion of the piston, the functions $\widetilde{\rho}_i(y,\tau), \widetilde{w}_i(y,\tau)$ and $s_i(y,\tau)$ can in principle be solved.

The only boundary conditions are

$$\widetilde{w}_1(0,\tau) = \widetilde{w}_2(1,\tau) = 0 \quad\text{and}\quad \widetilde{w}_1(x(\tau),\tau) = \widetilde{w}_2(x(\tau),\tau) = \frac{dx(\tau)}{d\tau}\,.$$

4.2. Special cases

We now have a complete set of equations for the functions $\widetilde{\rho}_i(y,\tau)$, $\widetilde{w}_i(y,\tau)$ and $s_i(y,\tau)$, to which we add Eq. (20) in scaled form for the piston's motion:

$$\begin{aligned}\frac{\partial\widetilde{\rho}_i(y,\tau)}{\partial\tau}+\frac{\partial}{\partial y}\left(\widetilde{\rho}_i(y,\tau)\,\widetilde{w}_i(y,\tau)\right) &= 0\,, &(29)\\ \left[\frac{\partial}{\partial\tau}+\widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]\widetilde{w}_i(y,\tau) &= -\frac{1}{\mu_i\,\widetilde{\rho}_i}\frac{\partial}{\partial y}\left(\widetilde{\rho}_i^3(y,\tau)s_i^2(y,\tau)\right)\,, &(30)\\ \left[\frac{\partial}{\partial\tau}+\widetilde{w}_i(y,\tau)\frac{\partial}{\partial y}\right]s_i(y,\tau) &= 0\,, &(31)\end{aligned}$$

$$\frac{d^2x(\tau)}{d\tau^2}=\widetilde{\rho}_1^3(x(\tau),\tau)s_1^2(x(\tau),\tau)-\widetilde{\rho}_2^3(x(\tau),\tau)\,s_2^2(x(\tau),\tau)\,, \qquad (32)$$

together with the boundary conditions

$$\widetilde{w}_1(0,\tau)=\widetilde{w}_2(1,\tau)=0 \quad\text{and}\quad \widetilde{w}_1(x(\tau),\tau)=\widetilde{w}_2(x(\tau),\tau)=\frac{dx(\tau)}{d\tau}\,. \qquad (33)$$

They are nonlinear partial differential equations, which cannot be solved in closed form. Apart from applying numerical methods, we therefore can only get some insight into the content of these equations, by using physically motivated approximations. Some of these will be discussed in this subsection.

The energy conservation law (24)–(25) can be expressed as

$$\begin{aligned}\left(\frac{dx(\tau)}{d\tau}\right)^2 &+ \mu_1\int\limits_0^{x(\tau)}\widetilde{\rho}_1(y,\tau)\,\widetilde{w}_1(y,\tau)^2dy+\mu_2\int\limits_{x(\tau)}^{1}\widetilde{\rho}_2(y,\tau)\,\widetilde{w}_2(y,\tau)^2dy\\ &+\int\limits_0^{x(\tau)}\widetilde{\rho}_1^3(y,\tau)s_1^2(y,\tau)\,dy+\int\limits_{x(\tau)}^{1}\widetilde{\rho}_2^3(y,\tau)s_2^2(y,\tau)\,dy=1\,.\end{aligned}$$

This relation can of course also be derived directly from Eqs (29)–(33).

We will now consider a number of special cases of these equations.

4.2.1. Case 1

As a preparation for obtaining a special solution to these equations we assume that the distribution functions $h_i(y,\widetilde{v},\tau)$, which are needed to calculate $\widetilde{\rho}_i(y,\tau),\widetilde{w}_i(y,\tau)$ and $u_i(y,\tau)$, are given by the shifted distributions

$h_i^M(y,\widetilde{v},\tau)$ of the *Ansatz* (15) and (16). Using these distributions we obtain

$$\begin{aligned}
\widetilde{\rho}_1^M(y,\tau) &= \frac{1}{x(\tau)}\,, & \widetilde{\rho}_2^M(y,\tau) &= \frac{1}{1-x(\tau)}\,,\\
\widetilde{w}_1(y,\tau) &= \frac{y}{x(\tau)}\frac{dx(\tau)}{d\tau}\,, & \widetilde{w}_2(y,\tau) &= \frac{1-y}{1-x(\tau)}\frac{dx(\tau)}{d\tau}\,,\\
u_1(y,\tau) &= u_1(\tau)\,, & u_2(y,\tau) &= u_2(\tau)\,,
\end{aligned}$$

while the heat fluxes $\widetilde{q}_i(y,\tau)$ vanish identically, in compliance with the assumption made in the derivation of equations (29)–(33). On substitution of the above results in the equation of motion for the piston (32), this equation attains the same form as in (17), (18):

$$\frac{d^2x(\tau)}{d\tau^2} = \frac{n_1u_1(\tau)}{x(\tau)} - \frac{n_2u_2(\tau)}{1-x(\tau)}\,. \tag{34}$$

At this point we observe that the spatial uniformity of the densities $\widetilde{\rho}_i$ and of the temperatures u_i and the linear interpolation between the walls and the piston of the local velocities $\widetilde{w}_i$, valid for all times, is a consequence of the special form of the distribution functions $h_i^M(y,\widetilde{v},\tau)$; these functions only constitute exact solutions to the free flow equations (2) and (3) when $\mu_i = 0$ (*cf.* the discussion in Section 3). However, for $\mu_i = 0$, the same behaviour also follows from the solutions of Eqs (29) and (31), with Eq. (30) replaced by

$$n_i\frac{\partial}{\partial y}\left(\widetilde{\rho}_i(y,\tau)\,u_i(y,\tau)\right) = \frac{\partial \widetilde{P}_i(y,\tau)}{\partial y} = 0$$

and the assumption of uniform initial conditions, without using the special form of the underlying distribution functions.

Equations (31) turn into equations for $u_1(\tau)$ and $u_2(\tau)$, now both independent of y:

$$\frac{du_1(\tau)}{d\tau} = -2\frac{u_1(\tau)}{x(\tau)}\frac{dx(\tau)}{d\tau} \quad \text{and} \quad \frac{du_2(\tau)}{d\tau} = 2\frac{u_2(\tau)}{1-x(\tau)}\frac{dx(\tau)}{d\tau}\,.$$

The solutions, written as functions of the position of the piston, are

$$u_1(\tau) = \left(\frac{x(0)}{x(\tau)}\right)^2 u_1(0) \quad \text{and} \quad u_2(\tau) = \left(\frac{1-x(0)}{1-x(\tau)}\right)^2 u_2(0)\,.$$

The corresponding pressures are also uniform and are given by

$$\widetilde{P}_1(\tau) = \left(\frac{x(0)}{x(\tau)}\right)^3 \widetilde{P}_1(0) \quad \text{and} \quad \widetilde{P}_2(\tau) = \left(\frac{1-x(0)}{1-x(\tau)}\right)^3 \widetilde{P}_2(0)\,.$$

The "entropies" s_i turn out to be independent of y and τ.

Eq. (34) is the same as Eq. (18) when $\mu_i = 0$ and also as the equation of motion obtained in Section 1.2.2, on the basis of purely thermodynamic considerations. Therefore, they lead to the same oscillatory behaviour without damping of the piston.

We might add that the same results are also obtained in a much more complicated calculation, in which the hydrodynamic equations are linearised with respect to small excursions around the stationary solutions.

4.2.2. Case 2

We now consider the case where in Eqs (29)–(31) it is assumed that the "entropy" $s_i(y,\tau)$ is a constant s_0 throughout. The remaining equations (29), (30) become (omitting the tilde and index)

$$\frac{\partial\rho}{\partial\tau} + w\frac{\partial\rho}{\partial y} + \rho\frac{\partial w}{\partial y} = 0$$

and

$$\frac{\partial w}{\partial\tau} + \alpha\rho\frac{\partial\rho}{\partial y} + w\frac{\partial w}{\partial y} = 0 \quad \text{with} \quad \alpha = \frac{3s_0^2}{\mu}\,.$$

By incorporating a factor $\sqrt{\alpha}$ into ρ it is seen that there is no loss of generality when we put $\alpha = 1$. Taking the sum and the difference of these two equations and defining $u_\pm = \rho \pm w$, we obtain the equations

$$\frac{\partial u_+}{\partial\tau} + u_+\frac{\partial u_+}{\partial y} = 0 \quad \text{and} \quad \frac{\partial u_-}{\partial\tau} - u_-\frac{\partial u_-}{\partial y} = 0\,.$$

They can be written as

$$\frac{du_+}{d\tau} = 0 \quad \text{on characteristics} \quad y(\tau;\xi) \quad \text{through} \quad y(0;\xi) = \xi \quad \text{given by}$$
$$\frac{dy(\tau;\xi)}{d\tau} = u_+(y,\tau)$$

and

$$\frac{du_-}{d\tau} = 0 \quad \text{on characteristics} \quad y(\tau;\xi) \quad \text{through} \quad y(0;\xi) = \xi \quad \text{given by}$$
$$\frac{dy(\tau;\xi)}{d\tau} = -u_-(y,\tau)\,.$$

On each of these characteristics the values of $u_+(y,\tau)$ and $u_-(y,\tau)$ are constant in time and are, therefore, given by their values at $\tau = 0$ and $y = \xi$. The characteristics themselves are straight lines with slopes $u_+(\xi,0)$ and $-u_-(\xi,0)$.

For the case where $w(\xi,0) = 0$ for all ξ between $\xi = 0$ and $\xi = x$ (fixed), we have chosen, as an example, the initial density

$$\rho(\xi,0) = 1 + f\cos\frac{\pi\xi}{2x} \equiv \rho_0(\xi)\,.$$

This also fixes the values of $u_+(\xi,0) = u_-(\xi,0) = \rho_0(\xi)$. The standard procedure for calculating $\rho(y,\tau)$ and $w(y,\tau)$ is as follows:

1. Solve $\xi_\pm(y,\tau)$ from $y = \xi_\pm \pm \rho_0(\xi_\pm)\tau$.
2. Then $\rho(y,\tau)$ and $w(y,\tau)$ are given by

$$\rho(y,\tau) = \tfrac{1}{2}\left[\rho_0(\xi_+(y,\tau)) + \rho_0(\xi_-(y,\tau))\right]$$

and

$$w(y,\tau) = \tfrac{1}{2}\left[\rho_0(\xi_+(y,\tau)) - \rho_0(\xi_-(y,\tau))\right]\,.$$

At a boundary point $y = 0$ or $y = x$ only one characteristic passes through this point. This is, however, sufficient to determine the value of ρ at that point, since $w = 0$ on the boundary, when x is fixed.

A more difficult problem arises when the equation $y = \xi_+ + \rho_0(\xi_+)\tau$ has two solutions for ξ_+. In figure 3, where in the y-τ plane we have drawn the two families of characteristics, the dark region indicates where these multiple solutions occur for our choice of $\rho_0(\xi)$ with $f = 0.9$. The tip of this region

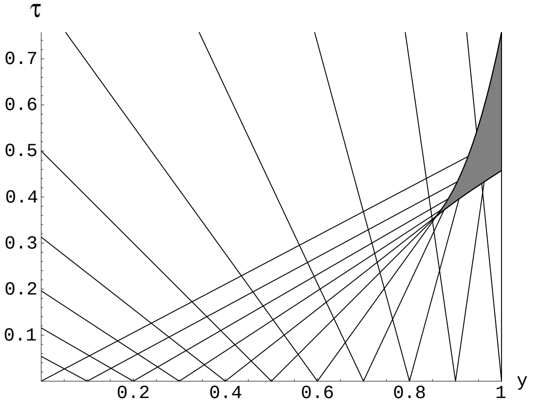

Fig. 3. Two families of characteristics.

is the point where for the first time the slope of $\rho(y,\tau)$ becomes infinite. Beyond this time the density would become multiple valued, which is clearly unacceptable. One way to handle this problem is to allow discontinuous, but single valued solutions, which describe shock fronts. Whitham [18], in chapters 2 and 6, discusses methods to find the shock velocity. However, they involve assumptions about a functional relation between ρ and w, which we are not allowed to make for the system we are considering. This is not to say that shock waves do not appear, as will become clear in the next section, where the results of some simulations will be discussed.

Applying this technique to the situation of a moving piston with uniform initial conditions and zero gas velocities leads to inconsistencies. These are probably due to the assumption of constant and uniform "entropy", an assumption which will be abandoned in the case considered next.

4.2.3. Case 3

For that purpose we try and bring Eqs (29)–(31) in the so called "characteristic form". Following Whitham [18] we first write them as

$$\left(\frac{\partial}{\partial\tau}+A\frac{\partial}{\partial y}\right)\begin{pmatrix}\rho\\ w\\ s\end{pmatrix}=0\,, \tag{35}$$

where

$$A(\rho,w,s)=\begin{pmatrix} w & \rho & 0\\ \frac{3}{\mu}\rho s^2 & w & \frac{2}{\mu}\rho^2 s\\ 0 & 0 & w\end{pmatrix}.$$

The left-eigenvectors $\vec{l}_+,\vec{l}_-,\vec{l}_0$ and eigenvalues c_+,c_-,c_0 of this matrix are equal to

$$\vec{l}_\pm = \left(\frac{3s}{2\rho},\pm\frac{1}{2\rho}\sqrt{3\mu},1\right) \quad \text{with} \quad c_\pm = w\pm\rho s\sqrt{\frac{3}{\mu}}$$

and

$$\vec{l}_0 = (0,0,1) \quad \text{with} \quad c_0 = w\,.$$

The characteristic form is obtained after left-multiplication of Eq. (35) by each of the eigenvectors. The result is

on the characteristics $\frac{dy}{d\tau}=c_+$:

$$s\frac{d\rho}{d\tau}+\sqrt{\frac{\mu}{3}}\frac{dw}{d\tau}+\frac{2}{3}\rho\frac{ds}{d\tau}=0 \quad \text{with} \quad \frac{d}{d\tau}=\frac{\partial}{\partial\tau}+c_+\frac{\partial}{\partial y}\,. \tag{36}$$

on the characteristics $\frac{dy}{d\tau} = c_-$:

$$s\frac{d\rho}{d\tau} - \sqrt{\frac{\mu}{3}}\frac{dw}{d\tau} + \frac{2}{3}\rho\frac{ds}{d\tau} = 0 \quad \text{with} \quad \frac{d}{d\tau} = \frac{\partial}{\partial\tau} + c_-\frac{\partial}{\partial y}\,. \tag{37}$$

on the characteristics $\frac{dy}{d\tau} = c_0$:

$$\frac{ds}{d\tau} = 0 \quad \text{with} \quad \frac{d}{d\tau} = \frac{\partial}{\partial\tau} + c_0\frac{\partial}{\partial y}\,. \tag{38}$$

Only the last of these equations can be directly integrated along the characteristic $\frac{dy}{d\tau} = c_0 = w$, and s is found to be constant on that line. An explicit form can of course be given only after $w(y,\tau)$ has been found. The other two equations have the form of Pfaff's problem for three variables

$$P\,d\rho + Q_\pm\,dw + R\,ds = 0 \quad \text{with} \quad P = s, \quad Q_\pm = \pm\sqrt{\frac{\mu}{3}}, \quad R = \frac{2}{3}\rho\,.$$

For the integrability of this equation, *i.e.*, for a relation $F(\rho,w,s) = 0$ to exist, it is necessary (and sufficient) that the vector $\vec{V}_\pm = (P, Q_\pm, R)$ satisfy the condition (see Sneddon [19], chapter 1, Section 5)

$$D_\pm = \vec{V}_\pm \cdot \mathrm{curl}\,\vec{V}_\pm = 0\,.$$

In the present case we find $D_\pm = \pm\frac{1}{3}\sqrt{\frac{\mu}{3}}$. Since this quantity is not equal to zero the Pfaffian problem is not integrable. This is not to say that equations (36)–(38) have no solution. It only means that the solution cannot be obtained by the method of Riemann invariants, as discussed by Whitham [18], Section 5.3.

5. Simulations

In this section we will show the results of a numerical simulation of Callen's piston with $N_1 = N_2 = 1000$ molecules to the left and to the right and for varying mass ratios $\mu_1 = N_1 m_1/M$ and $\mu_2 = N_2 m_2/M$. We will restrict ourselves to the cases where $\mu_1 = \mu_2 = \mu$.

Figures 4 and 5 show the velocity distribution of the molecules on the left after 4.000.000 and after 5.000.000 collisions, respectively. Actually these are accumulated distributions, meaning that for each bin on the horizontal velocity axis, the height gives the total time a molecule happened to have a velocity in this bin. Only for $v \simeq 0$ there is a persistent and varying difference with a Maxwellian velocity distribution with equal temperatures left and right.

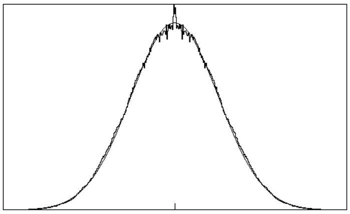

Fig. 4. Distribution for $\mu = 1.0$ and 4 million collisions.

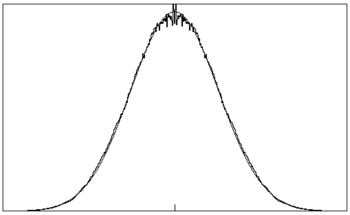

Fig. 5. Distribution for $\mu = 1.0$ and 5 million collisions.

All remaining figures describe properties of the piston. The number N_c of collisions varies from 1 million to 10 million, whereas μ takes values between 0.1 and 5.0. In figures with two pictures the one on the left, to be denoted by (a), refers to the first 20.000 collisions, while the right picture (b) is obtained from the last 20.000 collisions.

Figure 6 shows the orbits of the piston in its X-V phase-space with $N_c = 1$ million. In figure 7 we have plotted the position of the piston as a function of time for $N_c = 10$ million and $\mu = 1.0$, whereas figure 8 gives the phase-space orbit for this case. Especially in figure 8(b) for the last 20.000 collisions, the appearance of shorter sub-cycles can be clearly seen. We will call them epicycles. Notice that the horizontal scale in figure 8(b) is stretched by a factor of about 2.

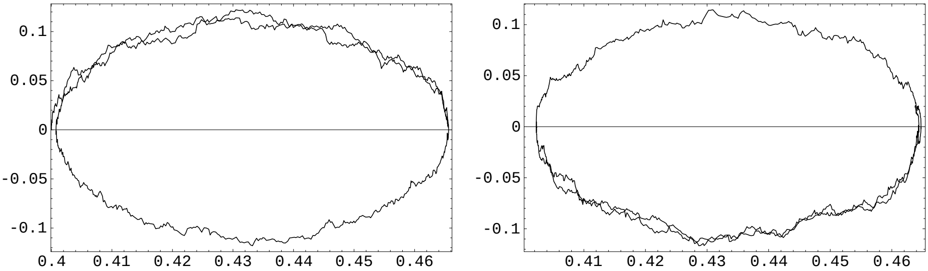

Fig. 6. X-V phase-space of piston for $\mu = 0.1$

Figure 9 gives the position of the piston, averaged over 20.000 collisions, as a function of time, for the whole period of 10 million collisions, again with $\mu = 1.0$.

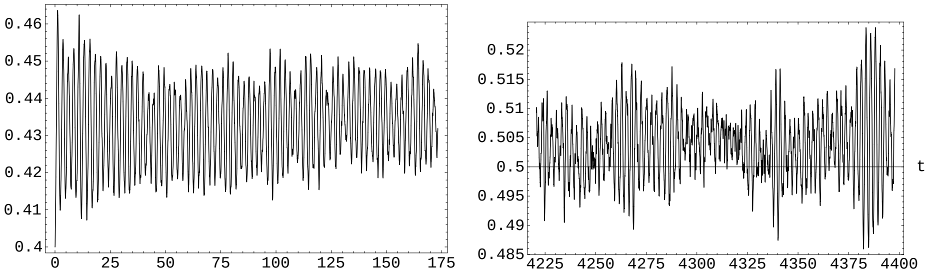

Fig. 7. X(t) for $N_c = 10$ million and $\mu = 1.0$.

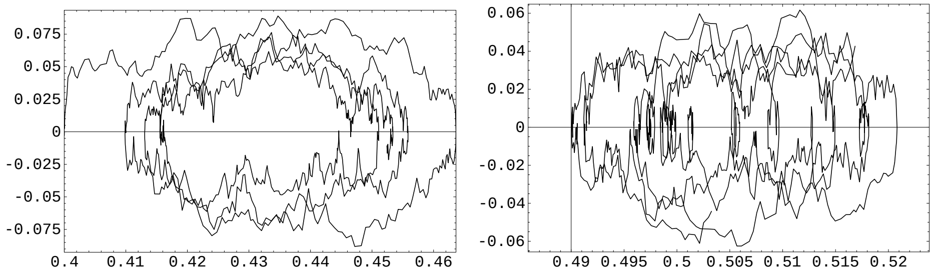

Fig. 8. X-V phase-space for $N_c = 10$ million and $\mu = 1.0$.

For $N_c = 5$ million and $\mu = 5.0$ figure 10 gives again the position of the piston, while figure 11 shows the phase orbits. It is seen that the position approaches the value $\frac{1}{2}$, but oscillations remain appreciable.

The *average* position of the piston for this case is shown in figure 12. Also this average position still shows appreciably irregular behaviour.

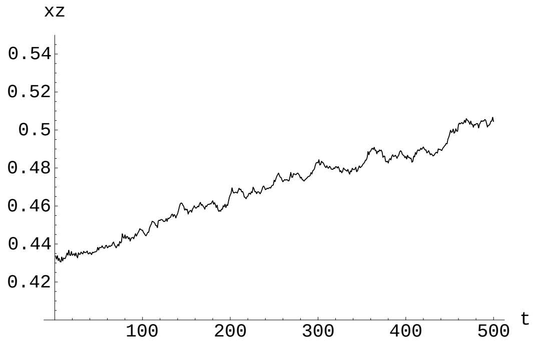

Fig. 9. Averaged position of the piston for $\mu = 1.0$.

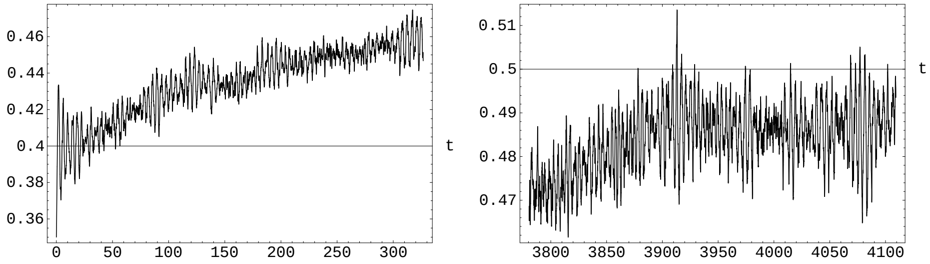

Fig. 10. $X(t)$ for $N_c = 5$ million and $\mu = 5.0$.

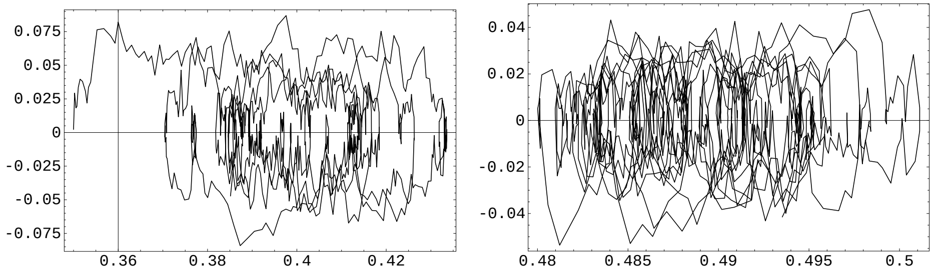

Fig. 11. X-V phase-space for $N_c = 5$ million and $\mu = 5.0$.

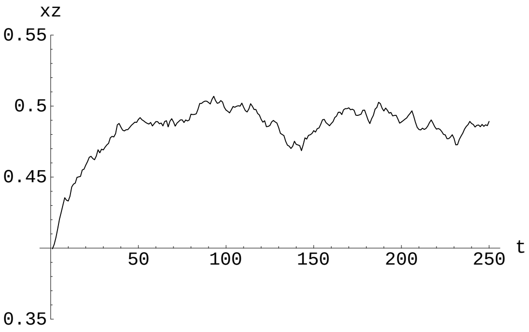

Fig. 12. Averaged position of the piston for $\mu = 5.0$.

6. Conclusions

In this paper we have presented a new approach to the problem of Callen's piston, as defined in Section 1.2.2. The question is whether the adiabatic piston, when it is moving, will allow heat to pass from one compartment to the other, thus allowing the temperatures on the left and right to become equal. It is generally believed that in a relatively short time the piston will pass through an oscillatory damped motion to a position which depends on its initial position. During this time the pressures will equalise, but the temperatures will still be different. In [8] this picture was supported by a theory in which the momentum exchange in a particle-piston collision was taken into account, as long as the mass ratio m/M is not exactly equal to zero. In addition, however, it was assumed that the particle densities are always uniform and that the instantaneous velocity distributions are always unshifted Maxwellian. These assumptions may be harmless, but they are certainly not exactly true. In a much later stage the piston is then supposed to move toward a final position under the influence of Brownian forces, while at the same time the temperatures become equal.

In two papers [9,14] on the same subject, Gruber and Frachebourg derive equations for the long time behaviour of the system. They show that with dissipation the piston damps out and the temperatures will become equal. Without damping they find that the oscillations will go on forever. In order to derive these results they had to assume that the correlation between the velocity of the piston and the velocities of the particles can be neglected. They also assumed that the particle densities left and right are uniform for all times. Our results, derived both from hydrodynamic equations and from numerical simulations, indicate that these assumptions are incorrect.

The same unjustified assumption about the absence of correlations between particle- and piston velocity is used in [10] and [11]: "In the absence of recollisions the piston always 'sees' the unperturbed Maxwell distributions of the arriving fluid particles, and no correlations can occur between its velocity and the precollisional velocity of the fluid particles."

In [12] the same problem is addressed, but now for the special case in which the mass of the piston and the mass of the molecules are equal. Some interesting results are derived about the motion of the piston, but it will be clear that an arbitrary initial velocity distribution will never tend to a Maxwellian distribution, because there is no momentum transfer in a collision.

The authors of [13] derive an interesting "nonlinear differential equation for the motion of the massive piston coupled to linear partial differential equations for the evolution of the one particle distribution of the light particles." In their concluding remarks they admit, however, that they cannot answer the question whether the piston converges to a stationary state.

A more realistic situation is described in [15] where the gas of Callen's piston consists of hard disks. Numerical calculations show that in this case "the insulating piston qualitatively behaves as expected — it moves and conducts heat". As a result the temperatures left and right become equal.

In the present paper we have again studied the one-dimensional ideal gas case. Instead, however, of considering the thermodynamic limit, we have taken the continuum limit, defined in Section 2. For this limiting case we used the equations for the single particle distributions to derive a closed set of hydrodynamic equations. This was possible by assuming that the gas behaved as an ideal fluid, meaning that the internal entropy production could be neglected. In addition we performed some simulations and compared the results with the conclusions that could be drawn from the hydrodynamic equations.

Our main conclusions can be summed up in the following points.

1. We find an approximate solution for the single particle distributions, which give Maxwellian velocity distributions. This is in agreement with numerical simulations, as is shown in figures 4 and 5. It is not clear, however, how this state is reached in the course of time.

2. This approximate solution also shows oscillatory behaviour of the position of the piston and of the temperatures to the left and to the right, in agreement with numerical simulations. It does not show a tendency of the piston to shift its oscillation centre towards the midpoint of the tube (for equal densities), although this behaviour is observed in numerical simulations.

3. The epicycles of the piston movement, which are noticeable in figures 8 and 11, may be caused by the impact of shock fronts in the gas. The existence of shock waves was established in the context of the hydrodynamic equations of Section 4, but it remains to be seen whether their effect on the piston can be really understood from a closer study of these equations coupled to the equation of motion of the piston.

4. If so, this will mean that the difference between the two temperatures will keep oscillating around zero and therefore that for this composite system, considered as one isolated unit, thermodynamic equilibrium will not be reached for $t \to \infty$.

One of the authors (M.J.R.) thanks the Institute of Theoretical Physics for its hospitality.

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