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Hamiltonian model of heat conductivity and Fourier law

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We investigate the stationary nonequilibrium states of a quasi one-dimensional system of heavy particles whose interaction is mediated by purely elastic collisions with light particles, in contact at the boundary with two heat baths with fixed temperatures T^+ and T^- . It is shown that Fourier law is satisfied with a thermal conductivity proportional to $\sqrt{T(x)}$ where T(x) is the local temperature. Entropy flux and entropy production are also investigated.

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I. INTRODUCTION

Although the Fourier's law $j_Q = -\kappa$ grad T, relating the macroscopic heat flux j_Q to the temperature gradient grad T, has been introduced almost two centuries ago [1], its microscopic basis is still an open issue. Actually, its status has long been purely phenomenological and its only justification was then its accurate and faithful agreement with observations in numerous experimental instances. Following the advances of nonequilibrium statistical mechanics, several microscopic models have been recently introduced aiming at *deducing* the Fourier's law from microscopic principles and relating the conductivity to the microscopic parameters of the system. In particular, the main issue is to determine what are the minimal requirements to get Fourier's law [2] [3] [4] [5] [6] [7].

The present study belongs to this line of research. It exploits recent results [9] [10] about the so-called "adiabatic piston problem" to devise a spatially extended, quasi-one-dimensional system, in contact at its ends with two heat baths at different temperatures $(T^- \text{ on the left and } T^+ \text{ on the right})$. In [10] two semi-infinite fluids separated by a movable piston were considered. Initially the fluids were in thermal equilibrium with temperature T_0^- on the left of the piston, T_0^+ on the right, and density n_0^- on the left. The initial density n_0^+ on the right was chosen such that the piston (which moves stochastically under the collisions with the fluid particles) remains on the average at its initial position. It was shown that there exists a stationary state of this system with temperature and density (T^-, n^-) on the left, (T^+, n^+) on the right, and distribution functions $\rho^{\pm}(v)$ for the velocities of fluid particles given by the sum of two Maxwellians. A key point discussed in [8] and [10] is that as soon as the temperatures on both sides of the piston are different, its stochastic motion induces a heat current. Conversely given a stationary state of the fluid on the left of the piston, specified by its temperature T^- , density n^- and the heat current j_0^- , given by the sum of two Maxwellians, one can

find the temperature T^+ , the density n^+ and the heat current $j_Q^+ = j_Q^-$ of the fluid on the right such that the piston remains on the average at the origin. It is again given by the sum of two Maxwellians. Moreover the fluctuations around the average position of the piston will be small if the mass m of each of the N fluid particles is much smaller than the mass M of the piston. This state of the fluid on the right of the first piston can then be considered as the state of a fluid on the left of a second piston and we can repeat the argument. It should be stressed that no thermodynamic limit is taken in the sense that M is strictly finite. Indeed in the thermodynamic limit when M tends to infinity with M/M_{fluid} fixed (where $M_{fluid} = Nm$ is the total mass of fluid particles) the piston becomes adiabatic and there is no heat current.

In this paper we consider a system composed of an array of K "pistons" (heavy point particles) separated by compartments filled with ΔN non-interacting light particles of mass m. The actual interactions are limited to elastic collisions between light particles and adjacent pistons: successive pistons are thus coupled through their interactions with the same fluid, while at the same time successive fluid compartments are coupled through their interactions with the same intermediary piston. The differing boundary temperatures force the system out of equilibrium, and one of the issues tackled in this paper is to determine the temperature profile in the system. Our model is simple enough to determine a consistent stationary state (with no drift) for any given heat flux; it thus sheds light on the controversial issue of heat conductivity in 1-dimension [11]. The derivation is performed analytically, in the frame of a perturbation approach developed in [9] with small parameter $m/\Delta M$ where m is the mass of fluid particles and ΔM the mass of one piston. If the ratio $m/\Delta M$ is small enough the fluctuations will be small and the pistons will not collide one another. Such an array is somehow reminiscent of chains of masses linked by springs, much studied since the pioneering work of Fermi, Pasta and Ulam [12] [13]. The masses correspond here to the pistons and the springs to the fluid compartments. But rather than being the nonlinearities, the key ingredient at the origin of transport in our setting will appear to be nonequilibrium fluctuations. Our model can also be related to the general class of models introduced by Eckmann and Young [7] with the pistons playing the role of the "Energy Storing Devices", and the fluid particles the role of the "Conducting Agents".

The paper is organized as follows. In Section II, we describe the stationary state and heat flux for a single piston surrounded with two fluids at different temperatures. In Section III, we investigate the fluid separating two pistons and the indirect coupling of the pistons that it achieves. In Section IV, we then bridge these two sets of results to get the behavior and heat conductivity of the abovementioned array. In Section V, the Fourier's law is recovered and discussed. In Section VI, we give explicit relations for entropy production and dissipation, before ending the paper with a final Section VII devoted to a discussion of the scope of our results.

II. SINGLE PISTON STATIONARY STATE WITH HEAT FLUX (AND NO DRIFT)

In [10] we investigated the quasi 1-dimensional problem of non-interacting point particles of mass m colliding elastically with a single heavy "piston" of mass $M \gg m$. Initially the piston is fixed at X = 0 and the particles on the left (resp. right) of the piston are in thermal equilibrium described by a Maxwellian distribution of velocities (parallel to the axis of the cylinder^{*}) with temperature T_0^- and uniform density n_0^- , i.e. pressure $p_0^- = n_0^- k_B T_0^-$ (resp. T_0^+, n_0^+, p_0^+). At time t_0 the piston is let free to move without any friction. The initial conditions (p_0^\pm, T_0^\pm) were chosen such that the piston, which moves stochastically under the collisions with the particles, remains on the average at X = 0. It was then shown that the system evolves to a nonequilibrium stationary state (Fig. 1) where the piston has a temperature T_P (average kinetic energy) and the fluids on the left/right of the piston are characterized by temperatures $T^- \neq T^+$, pressure $p^- = p^+ = p$, heat current $j_Q^- = j_Q^+ = j_Q$, and no drift ($w^- = w^+ = 0$).

^{*}The other velocity components, playing no role in this problem, can be initially set to zero and then remain zero at all times.

A. Stationary state of the fluid with prescribed (p, T, j_Q) and no drift

It was furthermore shown in [10] that the nonequilibrium stationary state of the fluid parametrized by

$$(p, T, j_Q, w = 0) \tag{1}$$

is characterized by the bimodal distribution function (θ being the Heaviside function)

$$\rho(x,v,t) = \rho(v) = \frac{2\beta p}{m} \left\{ \theta[v] \frac{2y}{1+y} \sqrt{\frac{\beta y}{\pi}} e^{-\beta y v^2} + \theta[-v] \frac{2}{1+y} \sqrt{\frac{\beta}{\pi y}} e^{-\beta v^2/y} \right\}$$
(2)

where

$$\beta = \frac{m}{2k_B T} \tag{3}$$

(not to be confused with the inverse temperature $1/k_BT$: here $\beta^{-1/2}$ is a velocity) and

$$y = 1 + \frac{C^2}{2} - \frac{C}{2}\sqrt{4 + C^2} \tag{4}$$

with C the dimensionless parameter

$$C = \sqrt{\pi} \beta^{1/2} \frac{j_Q}{p} \tag{5}$$

Let us note that the parameter y is strictly positive. Moreover since

$$C = \frac{1-y}{\sqrt{y}} \tag{6}$$

then $j'_Q = -j_Q$ implies y' = 1/y. It is straightforward to check the consistency between the above result (2) for the velocity distribution and the physical meaning of the associated thermodynamic parameters:

$$\int dv \,\rho(v) = n = \frac{p}{k_B T} \qquad \text{(number density } n \text{ of the ideal fluid)} \tag{7}$$

$$\int dv \,\rho(v)v = 0 \qquad \text{(no drift)} \tag{8}$$

$$\int dv \,\rho(v)v^2 = \frac{nk_BT}{m} \qquad \text{(kinetic temperature } T \text{ of the fluid)} \tag{9}$$

$$\int dv \,\rho(v)v^3 = \frac{2}{m} \,j_Q \qquad (\text{heat flux } j_Q) \tag{10}$$

It is to be underlined that Eq. (2) reflects the fact that three different temperatures are involved in the nonequilibrium stationary state of the fluid (see Fig. 1): the temperature $T_0^- = T/y$ of particles going to the right (v > 0), the temperature $T_0^+ = Ty$ of particles going to the left (v < 0) and the average kinetic temperature T defined by (9). These three temperatures coincide only at thermal equilibrium, when y = 1, $j_Q = 0$ and $\rho(v)$ coincide with the usual Maxwellian distribution. They differ as soon as a heat current $j_Q \neq 0$ is forced into the system and shifts the velocity distribution away from the equilibrium Maxwellian distribution. Note that y < 1 iff j_Q is positive, and y > 1 iff j_Q is negative. The parameters of the fluid in the nonequilibrium state can thus be reformulated as

$$(p, \beta, y = y(p, \beta, j_Q), w = 0)$$
 (11)

B. Stationary state of the piston

In the situation sketched in Fig. 1, we denote by T^- (resp. T^+) the temperature of the fluid in the stationary state on the left (resp. right) side of the piston, and by T_P the temperature of the piston. In a stationary state, Eq. (2) is to be written on each side of the piston with respectively $\beta = \beta^- = m/2k_BT^-$ and $y^- = y(p, \beta^-, j_Q)$ in the left compartment, and $\beta = \beta^+ = m/2k_BT^+$ and $y^+ = y(p, \beta^+, j_Q)$ in the right compartment. X_P being the position of the piston, it was shown in [10] that in the stationary state for the piston

$$T(X_P - 0) = T_0^- \sqrt{1 + \delta^-} \qquad \text{(left of the piston)} \tag{12}$$

$$T(X_P + 0) = T_0^+ \sqrt{1 + \delta^+} \qquad \text{(right of the piston)} \tag{13}$$

where

$$\delta_{\pm} = \alpha (2 - \alpha) \left(\frac{T_P}{T_0^{\pm}} - 1 \right) \tag{14}$$

with T_P being the temperature of the piston (average kinetic energy of its stochastic motion) and

$$\alpha = \frac{2m}{M+m} \tag{15}$$

C. Stationarity state of the piston and surrounding fluids

Stationarity for the whole system (piston, fluid on the left and fluid on the right) finally yields the consistency conditions

$$T(X_P - 0) = T^- = T_0^- y$$
 and $T(X_P + 0) = T^+ = \frac{T_0^+}{y}$ (16)

From (4) we have

$$y - \frac{1}{y} = -C \sqrt{4 + C^2} \tag{17}$$

and thus from (13) and (14)

$$T_P = T^+ \left[y^+ + \frac{1}{\alpha(2-\alpha)} \left(\frac{1}{y^+} - y^+ \right) \right]$$

= $T^+ \left[1 + \frac{1}{2} (C^+)^2 + C^+ \sqrt{1 + \frac{(C^+)^2}{4}} \left(\frac{2}{\alpha(2-\alpha)} - 1 \right) \right]$ (18)

Similarly, from (14)

$$T_P = T^{-} \left[\frac{1}{y^{-}} + \frac{1}{\alpha(2-\alpha)} \left(y^{-} - \frac{1}{y^{-}} \right) \right]$$
$$= T^{-} \left[1 + \frac{1}{2} (C^{-})^2 - C^{-} \sqrt{1 + \frac{(C^{-})^2}{4}} \left(\frac{2}{\alpha(2-\alpha)} - 1 \right) \right]$$
(19)

From the definition of C, Eq. (5), and the fact that $p^+ = p^- = p$ and $j_Q^+ = j_Q^- = j_Q$, we have the equality $T^+(C^+)^2 = T^-(C^-)^2$ relating the fluid nonequilibrium parameters on each side of the piston in the stationary state; this relation gives, using (18) and (19)

$$\sqrt{T^{+}} - \sqrt{T^{-}} = -\left[\frac{2}{\alpha(2-\alpha)} - 1\right] \sqrt{\frac{\pi m}{2k_B}} \frac{j_Q}{p} \left(1 + \mathcal{O}\left(\frac{j_Q}{p}\right)^2\right)$$
(20)

with

$$\frac{2}{\alpha(2-\alpha)} - 1 = \frac{M}{2m} \left(1 + \frac{m^2}{M^2}\right) \tag{21}$$

which shows that $j_Q = \mathcal{O}(m/M)$, as discussed in [10]. Let us remark that (18) and (19) imply also

$$2T_P = T^+ + T^- + \frac{\pi m}{2k_B} \left(\frac{j_Q}{p}\right)^2 + \left[\frac{1}{\alpha(2-\alpha)} - \frac{1}{2}\right] \sqrt{\frac{\pi m}{2k_B}} \frac{j_Q}{p} \left[\sqrt{T^+} \sqrt{4 + \frac{\pi m}{2k_B T^+}} \left(\frac{j_Q}{p}\right)^2 - \sqrt{T^-} \sqrt{4 + \frac{\pi m}{2k_B T^-}} \left(\frac{j_Q}{p}\right)^2\right]$$
(22)

Using Eq. (20) and the fact that $j_Q = \mathcal{O}(m/M)$, we conclude that the temperature of the piston separating the two fluids is given by

$$T_P = \sqrt{T^+ T^-} + \mathcal{O}\left[\left(\frac{m}{M}\right)^2\right]$$
(23)

III. STATIONARY STATE OF TWO OR MORE PISTONS

Let us now consider the stationary state defined by $(p, T, j_Q, w = 0)$ where the fluid is bounded by two identical stochastic pistons, each of mass $M \gg m$, which remain on the average at the same position under collisions from both sides (no drift). We shall use the same notations as in [10] where T_0^- (respectively T_0^+) denotes the temperature of the particles incident on the right piston from the left, i.e. with v > 0 (respectively on the left piston from the right, i.e. with v < 0), and T is the (average kinetic) temperature of the fluid, Eq. (9), in the intermediary compartment in the stationary state, see Fig. 2.

A. Temperature T_P^R of right piston

From Eqs. (12) and (16), we have on the left side of the right piston

$$T_0^{-} = \frac{T}{y} = \frac{T}{\sqrt{1+\delta^{-}}}$$
(24)

(joint stationarity of the fluid and the right piston) i.e.

$$y^2 = 1 + \delta^- \tag{25}$$

Denoting T_P^R the temperature of the right piston (see Fig. 2), plugging Eqs. (24-25) in Eq. (14) for δ^- yields

$$y^2 - 1 = \alpha(2 - \alpha) \left[\frac{T_P^R}{T} y - 1 \right]$$
(26)

i.e.

$$T_P^R = T\left[\frac{1}{y} + \frac{1}{\alpha(2-\alpha)}\left(y - \frac{1}{y}\right)\right]$$
(27)

B. Temperature T_P^L of left piston

Similarly denoting T_P^L the temperature of the left piston (see Fig. 2), Eqs. (13) and (16) give for the right side of the left piston

$$T_0^+ = Ty = \frac{T}{\sqrt{1+\delta^+}}$$
(28)

i.e.

$$(\delta^+)^2 = \frac{1}{y} - 1 \tag{29}$$

and thus from Eqs.(14) and (28-29) we obtain

$$T_P^L = T\left[y + \frac{1}{\alpha(2-\alpha)}\left(\frac{1}{y} - y\right)\right] \tag{30}$$

Let us note that

$$T_P^R + T_P^L = T\left(\frac{1}{y} + y\right) = T(2 + C^2)$$
 (31)

Therefore the temperature T of the fluid is related to the temperature of the surrounding pistons by

$$T = \frac{1}{2}(T_P^R + T_P^L) - \frac{\pi m}{4k_B} \left(\frac{j_Q}{p}\right)^2$$
(32)

Results of Section II can then be applied to each piston to obtain the temperature T^- on the left of the left piston and temperature T^+ on the right of the right piston. Bridging the ensuing relations allows to determine heat conductivity of this composite system, as follows in the next section.

IV. EXPRESSION OF HEAT CONDUCTIVITY

A. Elementary case of a single fluid compartment bounded by two pistons

We first derive auxiliary relations for an elementary unit, by considering again the stationary state for two pistons of area A separated (on the average) by a distance ΔL , with ΔN points particles between them (see Fig. 2). From (27) and (30), we have

$$T_P^R - T_P^L = T \left(\frac{1}{y} - y\right) \left(1 - \frac{2}{\alpha(2 - \alpha)}\right)$$
(33)

Introducing Eq.(17) and the expression (5) of C, together with (21) and $p \ A \ \Delta L = \Delta N \ k_B \ T$, we obtain

$$\frac{1}{\Delta L} \left(T_P^R - T_P^L \right) = -\frac{M}{m} \left(1 + \frac{m^2}{M^2} \right) \sqrt{\frac{\pi m}{2k_B^3}} j_Q \left(\frac{A}{\Delta N} \right) \frac{1}{\sqrt{T}} \sqrt{1 + \frac{\pi m}{8k_B T} \left(\frac{j_Q}{p} \right)^2} \tag{34}$$

where the temperature T of the fluid between the two pistons is given by (32), i.e.

$$T = \frac{1}{2} \left(T_P^R + T_P^L \right) - \frac{\pi m}{4k_B} \left(\frac{j_Q}{p} \right)^2$$
(35)

For the fluids on the left and on the right, Eq. (23) gives at lower order in m/M

$$T^{-} = \frac{(T_P^L)^2}{T} + \mathcal{O}\left[\left(\frac{m}{M}\right)^2\right] \qquad T^{+} = \frac{(T_P^R)^2}{T} + \mathcal{O}\left[\left(\frac{m}{M}\right)^2\right]$$
(36)

B. Heat transport through an array of K pistons

We are now in position to derive the law describing the fluctuation-driven heat transport equation for our model of spatially extended system and to investigate whether, and in which conditions, the usual Fourier's law can be recovered. We now consider the system of K identical (movable) pistons of mass ΔM , with ΔN point particles of mass m between them. In the stationary state defined by (T^-, p, j_Q) on the left, (T^+, p, j_Q) on the right, the pressure and the heat flux in each compartment (defined by successive pistons) will also be given by p and j_Q , and we denote respectively T_k and $T_{P,k}$ the temperatures of the successive compartments and successive pistons (see Fig. 4). The average distance ΔL_k between adjacent pistons will adapt to ensure that the pressure is actually homogeneous across the system (local mechanical equilibrium); it is thus given by

$$\langle X_{k+1} \rangle - \langle X_k \rangle = \Delta L_k = \left(\frac{\Delta N}{A}\right) \frac{k_B T_k}{p}$$
(37)

From Eqs. (34-35) applied to the k-th compartment

$$\frac{1}{\Delta L_k}(T_{P,k+1} - T_{P,k}) = -\frac{\Delta M}{m} \left[1 + \left(\frac{m}{\Delta M}\right)^2 \right] \sqrt{\frac{\pi m}{2k_B^3}} \left(\frac{A}{\Delta N}\right) \frac{j_Q}{\sqrt{T_k}} \sqrt{1 + \frac{\pi m}{8k_B T_k} \left(\frac{j_Q}{p}\right)^2}$$
(38)

with

$$T_k = \frac{1}{2} (T_{P,k} + T_{P,k+1}) - \frac{\pi m}{4k_B} \left(\frac{j_Q}{p}\right)^2$$
(39)

The system considered is defined by the total mass of pistons $M = K\Delta M$, the total number of point particles $N = (K - 1)\Delta N$, the uniform pressure p and the temperatures T^- and T^+ of the outer (semi-infinite) compartments. With K sufficiently large, but such that

$$\Delta M = \frac{M}{K} \gg m, \qquad \qquad 1 \ll \Delta N = \frac{N}{K-1} \ll N = \frac{ALp}{k_B T}$$
(40)

Eqs. (38-39) give

$$\left(\begin{array}{l}
\frac{dT_P(x)}{dx} = -\frac{M}{m} \frac{A}{N} \sqrt{\frac{\pi m}{2k_B^3}} \frac{j_Q}{\sqrt{T}} \sqrt{1 + \frac{\pi m}{8k_B T_k} \left(\frac{j_Q}{p}\right)^2} \\
T(x) = T_P(x) \left[1 - \frac{\pi m}{4k_B T_P} \left(\frac{j_Q}{p}\right)^2\right]$$
(41)

where the position of the piston and the location of nearby fluid can be identified, and the discrete set of temperature values interpolated by smooth functions $T_P(x)$ and T(x) at this spatial scale and perturbation order. With N/A given, then j_Q will be of the order m/M in order that grad T is uniformly bounded. Therefore to first order in m/M, we have

$$\begin{cases} \frac{dT_P(x)}{dx} = -\frac{1}{\kappa(x)} j_Q \\ \kappa(x) = \frac{m}{M} \frac{N}{A} \sqrt{\frac{2k_B^3}{\pi m}} \sqrt{T_P(x)} \end{cases}$$
(42)

which gives by integration the temperature profile in the system

$$T_P(x) = T(x) = \left[(T^-)^{3/2} + \frac{x}{L} \left((T^+)^{3/2} - (T^-)^{3/2} \right) \right]^{2/3}$$
(43)

This temperature profile fulfills, in a purely Hamiltonian setting, the expected general relation

$$T(x) = \left[(T^{-})^{\alpha} + \frac{x}{L} \left((T^{+})^{\alpha} - (T^{-})^{\alpha} \right) \right]^{1/\alpha}$$
(44)

given in [7], hence supports its universality. We here find an exponent $\alpha = 2/3$ as mentionned in [7], related to the fact that the fluids are confined to a limited region between pistons and the energy is purely kinetic. Our result moreover shows that local thermodynamic equilibrium is not required to get such a temperature profile provided there is a natural way to define local temperature, here through (2), see also [10]. We recover the currently observed linear profile if $|T^+ - T^-| \ll T^-$, or in boundary layers where $x \ll L$ or $(L - x) \ll L$ (there interchanging the role of T^+ and T^- in (43)). From Eq. (42), we finally get

$$j_Q = -\kappa \, \frac{dT}{dx} = -\frac{m}{M} \, \frac{N}{A} \, \sqrt{\frac{2k_B^3}{\pi m}} \, \frac{2}{3L} \left[(T^+)^{3/2} - (T^-)^{3/2} \right] \tag{45}$$

Moreover from the knowledge of the integrated number density profile N(x) of the fluid, such that N(0) = 0, N(L) = N and (37)

$$\frac{dN}{dx} = \frac{Ap}{k_B T(x)} = \frac{Ap}{k_B} \left[(T^-)^{3/2} + \frac{x}{L} \left((T^+)^{3/2} - (T^-)^{3/2} \right) \right]^{-2/3}$$
(46)

we obtain the length L of the system:

$$Nk_B = 3p A L \frac{\sqrt{T^+} - \sqrt{T^-}}{(T^+)^{3/2} - (T^-)^{3/2}}$$
(47)

i.e.

$$p A L = \frac{Nk_B}{3} \left[T^+ + T^- + \sqrt{T^+ T^-} \right]$$
(48)

Therefore

$$j_Q(x) = -\frac{m}{M} \sqrt{\frac{8k_B}{\pi m}} p \left[\sqrt{T^+} - \sqrt{T^-}\right]$$
(49)

which shows that the term we have neglected when passing from (41) to (42) is of the order $(m/M)^2$.

V. FOURIER'S LAW

We have thus established that for our model, the Fourier's law

$$j_Q = -\kappa \operatorname{grad} T \tag{50}$$

is valid at some mesoscopic scale allowing to consider the continuous limit of the discrete microscopic temperature profile, with the heat conductivity κ given by

$$\kappa = \frac{m}{M} \frac{N}{A} \sqrt{\frac{2k_B^3}{\pi m}} \sqrt{T}$$
(51)

We thus find that κ depends on the local temperature in agreement with the general statement made in [7] when communicating agents (here the light particles) remain confined (here between the adjacent pistons). As one could expect, this heat conductivity is proportional to the number N/Aof gas particles per unit area and also proportional to the ratio m/M, measuring the efficiency of interaction between the piston and gas particles. It is however independent of the length L of the system (except for L-dependent corrections to the continuous limit involved in the derivation of the gradient term). Let us note that for a strictly 1-dimensional system (for which the area A is zero), one should introduce the power of heat P_Q which is transmitted through the system. In this case, Fourier's law reads

$$P_Q = -\bar{\kappa} \ \text{grad} \ T \tag{52}$$

and we have

$$\bar{\kappa} = \frac{mN}{M} \sqrt{\frac{2k_B^3}{\pi m}} \sqrt{T}$$
(53)

Finally, let us recall that Clausius-Maxwell-Boltzman obtained a theoretical expression for κ for gases with $\kappa \sim \sqrt{T}$ independent of the gas density [6]. $\kappa \sim \sqrt{T}$ for the conductivity [6].

VI. ENTROPY PRODUCTION AND DISSIPATION

Since the system considered (defined by the (K - 1) elementary units and K pistons) is in a stationary state, its thermodynamic entropy S remains constant. Thus, in the framework of irreversible thermodynamics, we have

$$\frac{dS}{dt} = I + P_Q \left(\frac{1}{T^-} - \frac{1}{T^+}\right) = 0$$
(54)

which gives for the total entropy production per unit time of the system

$$I = P_Q \left(\frac{1}{T^+} - \frac{1}{T^-}\right) = \frac{Nm}{M} \sqrt{\frac{2k_B^3}{\pi m}} \frac{2}{3L} \left(T^+ - T^-\right)^2 \frac{T^+ + T^- + \sqrt{T^+ T^-}}{T^+ T^- \left[\sqrt{T^+} - \sqrt{T^-}\right]}$$
(55)

Therefore I > 0 as required by the Second Law of thermodynamics. The same argument remains valid locally where the entropy density s(x,t) satisfies

$$\frac{\partial}{\partial t}s(x,t) = i(x,t) - \frac{\partial}{\partial x}\left(\frac{j_Q}{T}\right)$$
(56)

(since there is no drift, hence no extra entropy current coming from transport of matter). For the stationary state, it implies [10] for the source term i(x) associated with irreversibility

$$i(x) = \frac{d}{dx} \left(\frac{j_Q}{T}\right) \tag{57}$$

i.e. (recall that j_Q is constant throughout the system)

$$i(x) = -j_Q \frac{1}{T^2} \operatorname{grad} T$$

= $\kappa \left(\frac{\operatorname{grad} T}{T}\right)^2$
= $\frac{Nm}{M} \frac{1}{A} \sqrt{\frac{2k_B^3}{m}} \left[\frac{2}{3L} ((T^+)^{3/2} - (T^-)^{3/2})\right]^2 \frac{1}{\sqrt{T(x)}}$ (58)

Let us note that I is also the total entropy production for the system plus the two "reservoirs". In conclusion, the irreversibility i(x) is proportional to the parameter R = Nm/M. Moreover, we see that if R is large, which corresponds to the strong damping case [9] [14], i.e. a high dissipation, the heat conductivity is large whereas for R small, which corresponds to the weak damping regime, i.e. a weak dissipation, the heat conductivity will be negligible.

VII. CONCLUSIONS

We have considered a quasi-one-dimensional system composed of K-1 ($K \gg 1$) identical subsystems, in contact at the boundaries with two fluids with temperatures T^{\pm} and the same pressure p. We have shown that there exists a nonequilibrium stationary state with heat current $j_Q \neq 0$ given by (49) for which the Fourier's law $j_Q = -\kappa$ grad T is satisfied. For this model, the heat conductivity κ is proportional to \sqrt{T} , as could be expected from kinetic theory. It is also proportional to the factor R = Nm/M, with Nm the total mass of the light particles and M the total mass of the heavy particles (or pistons), as expected from previous work where it was shown that dissipation (i.e. friction) is proportional to R. It should be remarked that κ is of the order of the small parameter $\epsilon = m/M$ because the length unit introduced is microscopic. In this stationary state, the fluid in each subsystem is characterized by the thermodynamic parameters $(T(x), p, j_Q, w = 0)$ where T(x) is defined as the local average kinetic energy, see Eq. (9). However, it is not a state of local equilibrium since the velocity distribution function is given by the bimodal expression Eq. (2) and not by the Maxwell distribution with temperature T(x). Relaxation from an arbitrary initial condition towards this stationary state with no drift has not vet been investigated, but is expected to hold as was the case for one piston. The fluids are moreover characterized by the equation of state $p = nk_BT$, e = p/2. Furthermore, the total length L of the system will adjust to be given by $p A L = (Nk_B/3) (T^+ + T^- + \sqrt{T^+T^-})$. Therefore introducing an "average temperature" for the whole system $T_{Av} = (1/3) (T^+ + T^- + \sqrt{T^+ T^-})$, we have the equation of state for a single component general ideal gas [15] $pV = Nk_BT_{Av}, E = Nk_BT_{Av}/2$ (since the number of fluid particles is much large than the number of pistons). Finally we have shown that the total entropy production per unit time I of our system (i.e. K-1 subsystems) as well as the total irreversibility i(x) are strictly positive in agreement with the Second Law of thermodynamics. As mentioned in [10], the entropy of the "heat baths" will change only due to the heat flow and there is no internal entropy production. Therefore the entropy production for the total system (i.e. system + heat baths) is simply the quantity I computed above.

We have assumed that the pistons are much heavier than the fluid particles. One may wonder whether our results are more general and remain valid if this assumption is dropped. It is an open problem, but clearly the mass of the "piston" must be different from the mass of the fluid particles, otherwise we would loose the stochasticity necessary for dissipation. It is to note that the respective roles of fluid compartments and pistons are more symmetric than it might seem: two successive fluid compartments are coupled through the fluctuations of the intermediate piston, and two successive pistons are coupled through their interaction (during collisions) with the same intermediate fluid compartment (also fluctuating and out of equilibrium). We have here considered ideal fluids, i.e. noninteracting light particles. In the case of a single piston, simulations with non-interacting particles or with hard-core particles gave (surprinsingly) similar results [14] [9], allowing us to conjecture that the results given in this paper would remain valid in the case of hard-core fluid particles. Behavior for particles interacting through a binary finite-range potential, for which energy no longer reduces to kinetic energy, is still unknown [7].

We should stress that we have not limited our discussion to states which are close to equilibrium $(T^+ - T^-)$ is arbitrary). No assumption of linear response has thus been involved in the derivation of Fourier's law. In agreement with a caveat first underlined by Van Kampen [16], macroscopic linearity of the response is not the reflection of a linearity of the microscopic response, but rather an emerging feature following from averaging and cancellation of nonlinear microscopic contributions. In the present case, it is the perturbation approach and the underlying scale separation $m/M \ll 1$ which leads to cancellation of nonlinear terms at lowest order.

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VIII. FIGURE CAPTIONS

Figure 1: Stationary state of the piston problem (with no drift). If $T_0^+ \neq T_0^-$, it is a nonequilibrium state with $j_Q \neq 0$ and $T^+ \neq T^-$.

Figure 2: Stationary state with two pistons with prescribed current j_Q , prescribed boundary temperatures T^{\pm} , and no drift (uniform pressure p). T_0^- and T_0^+ are auxiliary temperatures, associated with subpopulations of fluid particles, going respectively to the right (v > 0) and to the left (v < 0) inside the middle fluid compartment.

Figure 3: Temperature profile for the stationary state of two identical pistons. T_P^L and T_P^R are the temperatures (average kinetic energy) of the pistons, whereas T^- , T and T^+ are temperatures within the fluids as defined in (9).

Figure 4: Stationary state with K pistons. The pressure p and the heat flux j_Q are identical in each subsystem, the drift velocity is zero and the pistons remain on the average at fixed positions $\langle X_k \rangle$.



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