Analytic calculation of energy transfer and heat flux in a one-dimensional system

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Abstract

In the context of the problem of heat conduction in one-dimensional systems, we present an analytical calculation of the instantaneous energy transfer across a tagged particle in a one-dimensional gas of equal-mass, hard-point particles. From this, we obtain a formula for the steady-state energy flux, and identify and separate the mechanical work and heat conduction contributions to it. The nature of the Fourier law for the model, and the nonlinear dependence of the rate of mechanical work on the stationary drift velocity of the tagged particle, are analyzed and elucidated.

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I. INTRODUCTION

Heat conduction in one-dimensional systems has evoked a considerable amount of interest in recent years. In particular, the validity or otherwise of the Fourier law of heat conduction in such systems is a non-trivial question, and hence one that has been the subject of lively discussion[1]. A comprehensive account of the current status of the problem is provided in Ref. [2].

Most of the results known in this regard are based on numerical studies of lattice models. An alternative and useful line of development is the analytical study of a model system, albeit a simplified one, which we call the Jepsen gas: a system of N identical classical point-particles of mass m moving on a line and undergoing perfectly elastic collisions when neighboring particles meet[3]. This system is a special case of the more general model investigated in the context of the so-called adiabatic piston problem[4], in which a central heavy particle of mass M is in a gas of particles of mass m on its left and right. The problem then is to analyze the dynamics of the central particle in the thermodynamic limit in which the one-dimensional gases to its left and right are in thermal equilibrium at specified temperatures and densities. The Jepsen gas is a *singular* limiting case of the unequal mass situation. The latter is not integrable, in marked contrast to the case $M = m$, which is integrable. Notwithstanding this simplification, non-trivial irreversible behavior is observed in the Jepsen gas in the limit $N \to \infty$ when appropriate averages over initial conditions are performed. In the initial studies of this system[3, 5], several quantities of interest such as the statistics of the displacement and velocity of one of the particles, which we shall refer to as the central or tagged particle (or "piston", as it is the counterpart of the adiabatic piston in the model at hand), have been calculated exactly by performing an average over equilibrium initial conditions for the rest of the particles. In particular, it can be shown that the motion of this tagged particle becomes diffusive asymptotically, i.e., converges to Brownian motion.

Recently, the model has been revisited and studied in greater detail[6, 7], one of the motivating factors being its relationship to the adiabatic piston problem. The non-equilibrium situation implied by different velocity distributions for the gases to the left and right of the tagged particle has been analyzed. In general, this particle acquires, in the thermodynamic limit, a systematic drift velocity over and above its diffusive motion. A notable feature is that this drift velocity is exclusively fluctuation-induced[6]. In the special case when the velocity distributions of the gases on the two sides are Maxwellian, so that the pressure of each gas can be identified with k_B times the product of its (linear) number density and temperature, an interesting feature emerges: even when the pressures of the two gases are equal, the drift velocity of the tagged particle does not vanish. Rather, it is directed from the lower temperature (higher density) side to the higher temperature (lower density) side. The drift velocity vanishes when the product of the number density and the *square root* of the temperature is the same on the two sides of the tagged particle, a condition already recognized in Ref. [3].

In the context of heat conduction in one dimension, the question that arises naturally is whether the heat flux can be calculated for the Jepsen gas. We show in this paper that this problem can be solved analytically: it is possible to calculate exactly the amount of energy that is transfered through the tagged particle or piston. At first, it would appear that the issue is a trivial one in the same way as it is in a linear chain of harmonic oscillators. In the latter system, the energy just travels ballistically, being carried by phonon modes which do not interact with each other. In a similar fashion, the kinetic energy carried by any particle in the Jepsen gas is just transfered upon collision to the next particle, and hence moves ballistically along the line. As a result, a Fourier law, which predicts the diffusive spreading of thermal energy, does not appear to be valid. We will show by an exact and explicit calculation that this "hand-waving" argument, while formally correct, is nevertheless misleading in the sense that a non-trivial energy flux obtains in the model. A closed expression can be derived for this quantity, comprising two components. One of these involves the asymptotic drift velocity of the tagged particle, while the other is present even when the drift velocity vanishes. This permits the identification, and hence a natural separation, of the "mechanical work" and "heat" contributions, respectively, to the energy transfer. In particular, for initial conditions corresponding to thermal equilibrium of the gases to the left and right of the tagged particle (with densities n^- and n^+ and temperatures T^- and T^+, respectively) such that $n^-\sqrt{T^-} = n^+\sqrt{T^+}$, so that the drift velocity is zero, the asymptotic steady-state energy flux through the tagged particle is shown to converge to a constant value. For small values of $(T^+ - T^-)$, this quantity is linearly proportional to the temperature difference itself, which can be interpreted as a manifestation of the Fourier law. Moreover, the "mechanical work" contribution itself is shown to have a part that is linear in the drift velocity, as might be expected, as well as a *nonlinear* part that starts (for small drift velocities) with the fourth power of the drift velocity.

We reiterate the following point. The Jepsen gas is admittedly a simplified special case of the more "realistic" models of one-dimensional transport that have been the subject of much attention. Nevertheless, it is the fact that analytical (and hence unambiguous) results can be obtained for this model that makes it worth studying, because these results help shed light on several of the essential issues involved in energy transport in one dimension.

The plan of the rest of this paper is as follows. In the next section, we introduce the notation and summarize the salient results pertaining to the Jepsen gas for the purpose at hand. In Sec. III (and the Appendix), an exact formula is derived for the energy transfer across the piston at any instant of time. This leads to a formula for the total energy flux in the stationary state, which is obtained and analyzed in Sec. IV. In Sec. V, the contribution to the energy flux coming from the stationary heat flux is identified, and the nature of the Fourier law for the model is clarified. The rate of mechanical work is also deduced, and its nonlinear dependence on the stationary drift velocity elucidated. Section VI contains a few concluding remarks.

II. NOTATION AND RECAPITULATION

It is helpful to recapitulate in brief the relevant features of the model, in the notation used in earlier work[6, 7]. The tagged particle, located at $X = 0$ at $t = 0$ with an initial velocity V_0, separates a gas of N^- particles in the interval $[-L, 0)$ on its left from a gas of N^+ particles to its right, in $(0, L]$. Their initial positions X_j (where $-N^- \leq j \leq -1$ for the gas on the left, and $1 \leq j \leq N^+$ for the gas on the right) are independently and uniformly distributed in the corresponding intervals. Their initial velocities V_j are drawn from normalized distributions $\phi^-(V)$ and $\phi^+(V)$, respectively. To avoid unnecessary complications, we shall assume that these are symmetric distributions, i.e., $\phi^\pm(V) = \phi^\pm(-V)$. It can be shown that the system has a thermodynamic limit in which $N^+ \to \infty$, $L \to \infty$ with finite densities $\lim N^\pm/L = n^\pm$, provided only that the mean speeds $\langle |V| \rangle^\pm = \int_{-\infty}^{\infty} dV\, V\, \phi^\pm(V)$ are finite. Note that $\phi^\pm$ need not be Maxwellian distributions, although this is the case of direct interest in the present context of heat conduction. As all the particles (including the tagged particle) have equal masses, they merely exchange their identities on their original linear trajectories $X_j(t) \equiv$

$X_j + V_j\, t$ in each collision. This is what enables one to derive exact results for the system. Among other quantities, the exact one-particle distribution function of the tagged particle, $P(X, V, t|0, V_0)$, can be found. The complicated stochastic motion of the tagged particle (henceforth termed the "piston") can be interpreted[7] as being driven by two independent Poisson processes (corresponding to collisions from its left and right, respectively) with *state-* and *time-dependent* intensities $n^- \alpha(X/t)$ and $n^+ \beta(X/t)$, where

$$\alpha(W) = \int_W^\infty dV\,(V - W)\,\phi^-(V)\,,\;\; \beta(W) = \int_{-\infty}^W dV\,(W - V)\,\phi^+(V)\,. \tag{1}$$

The system does not equilibrate in the conventional sense of the term: the initial set of trajectories persists for all t. The piston acquires an asymptotic mean drift velocity $\overline{W}$ given by the unique solution of the implicit equation [6]

$$n^- \alpha(\overline{W}) = n^+ \beta(\overline{W})\,. \tag{2}$$

The asymptotic velocity distribution of the piston is a superposition of $\phi^+(V)$ and $\phi^-(V)$, and is given by

$$P_{\rm st}(V) = \left[n^- \phi^-(V)\theta(V - \overline{W}) + n^+ \phi^+(V)\theta(\overline{W} - V)\right] / \,\Xi(\overline{W})\,, \tag{3}$$

where

$$\Xi(\overline{W}) = n^-\,|\alpha'(\overline{W})| + n^+\,\beta'(\overline{W}) = n^- \int_{\overline{W}}^\infty dV\,\phi^-(V) + n^+ \int_{-\infty}^{\overline{W}} dV\,\phi^+(V) \tag{4}$$

is the normalization factor. Only in the special case of the *homogeneous system*, defined by $n^- = n^+ = n$ and $\phi^+(V) = \phi^-(V) = \phi(V)$, can one have stationarity and an approach to equilibrium, in the sense that $\overline{W} = 0$ and $P_{\rm st}(V) \equiv \phi(V)$. Note that $\overline{W}$ may vanish even in the *inhomogeneous* system, if the condition $n^- \int_0^\infty dV\,V\,\phi^-(V) = n^+ \int_0^\infty dV\,V\,\phi^+(V)$ (or $n^- \langle|V|\rangle^- = n^+ \langle|V|\rangle^+$) happens to be satisfied: that is, the *mean rates* at which the piston suffers collisions from its left and right, respectively, are equal.

We point out at this juncture that the stationary distribution $P_{\rm st}(V)$ in Eq. (3) may in fact be anticipated on physical grounds, as follows. In the equal-mass case under consideration, we may regard the particles as simply "passing through" each other in each collision, because they are identical particles. In the stationary state, after the memory of the initial velocity of the piston has been lost, it will only encounter such particles via collisions from its left, as have velocities *greater* than its asymptotic mean drift velocity W^*, whatever that be (trajectories corresponding to $V < W^*$ from the gas on the left will never again intersect the piston's trajectory). Similarly, the piston will encounter only those particles from the gas on its right as have velocities *less* than W^*. Moreover, after each collision, the piston simply acquires the velocity of the particle it collided with. Hence the stationary velocity distribution must necessarily be a superposition of the form

$$P_{\rm st}(V) \propto n^- \phi^-(V)\, \theta(V - W^*) + n^+ \phi^+(V)\, \theta(W^* - V) \tag{5}$$

apart from a normalization factor. The latter is easily seen to be just $1/\Xi(W^*)$ where the function Ξ is as given by Eq. (4). Taking the first moment of this equation, we find that consistency demands that W^* satisfy precisely the same implicit equation (Eq. (2)) as that written down above for the drift velocity $\overline{W}$. In other words, not only is the form in Eq. (3) for $P_{\rm st}(V)$ deducible on direct physical grounds, but also the existence of an asymptotic drift velocity $\overline{W}$ and the implicit equation satisfied by it.

III. EXACT EXPRESSION FOR ENERGY TRANSFER

To derive of an exact formula for the rate of transport of energy across the piston, we first calculate the difference $\Delta E(t)$ between the mean energy $E(t)$ of the gas on the left of the piston at time t and its initial value $E(0)$.

We have

$$E(0) = \tfrac{1}{2} m \,\textstyle\sum_{j=-N^-}^{-1} \langle V_j^2 \rangle = \tfrac{1}{2} m \,\textstyle\sum_{j=-N^-}^{N^+} \big\langle V_j^2\, \theta(-X_j) \big\rangle \,, \tag{6}$$

while

$$E(t) = \tfrac{1}{2} m \,\textstyle\sum_a \sum_{j\neq a} \Big\langle V_j^2\, \theta(X_a(t) - X_j(t))\, \delta^{\rm Kr}[N^-, \textstyle\sum_{\ell\neq a} \theta(X_a(t) - X_\ell(t))] \Big\rangle \,. \tag{7}$$

Here each sum runs over the entire set of particle labels $\{-N^-, \ldots, -1, 0, 1, \ldots, N^+\}$; the subscript a is used to distinguish the instantaneous variables of the piston from those of the other particles; $\delta^{\rm Kr}[n, m]$ is the Kronecker delta δ_{nm}; and $\langle \ldots \rangle$ denotes an average over the already-specified distributions of the initial conditions comprising the set $\{X_j\,, V_j\}$. Using the crucial fact that

$$\sum_{\ell\neq a} \theta\big(X_a(t) - X_\ell(t)\big) = N^- \tag{8}$$

for all $t \geq 0$, the gain in energy of the gas on the left at time t can be written as

$$\Delta E(t) = \sum_{a} \sum_{j\neq a} \Big\langle V_j^2 \big[\theta\big(X_a(t) - X_j(t)\big) - \theta(-X_j)\big]\, \delta^{\rm Kr}\big[N^-, \sum_{\ell\neq a} \theta\big(X_a(t) - X_\ell(t)\big)\big] \Big\rangle. \quad (9)$$

The representation $\delta_{nm} = (2\pi i)^{-1} \oint z^{n-m-1}\, dz$ enables us write this as

$$\begin{aligned}\Delta E(t) \;=\; & \tfrac{1}{2} m \oint \frac{dz}{2\pi i z} \sum_{a} \sum_{j\neq a} \Big\langle V_j^2 \left[\theta(X_a + V_a\, t - X_j - V_j\, t) - \theta(-X_j)\right] \\ & \times z^{N^-} \prod_{\ell\neq a} \left[1 + (z^{-1} - 1)\, \theta(X_a + V_a\, t - X_\ell - V_\ell\, t)\right] \Big\rangle\,, \end{aligned} \quad (10)$$

where the contour encloses the origin. We break up $\Delta E(t)$ as

$$\Delta E(t) = \Delta E^0(t) + \Delta E^-(t) + \Delta E^+(t)\,, \quad (11)$$

corresponding to the three distinct contributions to $\Delta E(t)$ coming, respectively, from the cases $a = 0$, $-N^- \leq a \leq -1$ and $1 \leq a \leq N^+$. The calculation of these quantities is broadly similar to, but a little more intricate than, that involved [5, 7] in evaluating quantities like the one-particle distribution function $P(X, V, t|X_0, V_0)$ of the piston. An outline of the main steps leading to the expression for $\Delta E(t)$ is given in the Appendix. The exact result for $\Delta E(t)$ is given by Eqs. (A.8)-(A.10).

IV. FORMULA FOR THE STATIONARY ENERGY FLUX

To find the asymptotic or steady-state rate of transport of energy across the piston, we pass to the long-time limit of the expression for $\Delta E(t)$. Using the asymptotic behavior $I_r(z) \sim e^z/(2\pi z)^{1/2}$ as $|z| \to \infty$, it is evident from Eq. (A.8) that $\Delta E^0(t)$ decays exponentially to zero as $t \to \infty$, unless it so happens that $n^-\,\alpha(0) = n^+\,\beta(0)$, i.e., the asymptotic drift velocity of the piston is zero. In that case $\Delta E^0(t) \sim t^{1/2}$ at long times; but this again implies a rate of transport that vanishes (like $t^{-1/2}$) as $t \to \infty$. Therefore $\Delta E^0(t)$ may be dropped from further consideration.

Turning to Eqs. (A.9) and (A.10) for $\Delta E^-(t)$ and $\Delta E^+(t)$, we observe that the asymptotic behavior of the modified Bessel functions leads to the occurrence of a factor $\exp\left\{-t\left[\big(n^-\alpha(w)\big)^{1/2} - \big(n^+\beta(w)\big)^{1/2}\right]^2\right\}$ in the integration over w (which runs from $-\infty$ to $+\infty$). Since the exponent has a unique zero at precisely the asymptotic drift velocity $\overline{W}$ as defined in Eq. (2), the long-time behavior of $\Delta E^{\pm}(t)$ can be deduced by a standard

Gaussian approximation about $w = \overline{W}$. The leading asymptotic behavior of each of these two contributions is then seen to be $\sim t$, implying the existence of a finite, non-vanishing stationary rate of energy transfer $\lim_{t\to\infty} d\Delta E(t)/dt$, that we denote by $\Delta\dot{E}_{\rm st}$. Carrying out the algebra required, our final result for this quantity is remarkably simple (for reasons to be explained shortly). We find

$$\Delta\dot{E}_{\rm st} = \tfrac{1}{2}m\Big\{n^+ \textstyle\int_{-\infty}^{\overline{W}} dU\, U^2(\overline{W}-U)\,\phi^+(U) - n^- \int_{\overline{W}}^{\infty} dU\, U^2(U-\overline{W})\,\phi^-(U)\Big\}. \tag{12}$$

For ready reference, we recall that the asymptotic drift velocity $\overline{W}$ of the piston is given by the implicit equation (2), which may be written in the alternative form

$$\overline{W} = \frac{n^- \int_{\overline{W}}^{\infty} dU\, U\,\phi^-(U) + n^+ \int_{-\infty}^{\overline{W}} dU\, U\,\phi^+(U)}{n^- \int_{\overline{W}}^{\infty} dU\, \phi^-(U) + n^+ \int_{-\infty}^{\overline{W}} dU\, \phi^+(U)}\,. \tag{13}$$

We remark that the result in Eq. (12) is valid for arbitrary initial velocity distributions $\phi^\pm(V)$, and not just for Maxwellian $\phi^\pm$ (see below). It must also be noted that the existence of the *third* moment of the speed, $\langle |V|^3\rangle^\pm$, is necessary in order that $\Delta\dot{E}_{\rm st}$ be finite. The exact result in Eq. (12) has several other noteworthy features, that we take up in turn.

(i) *Physical interpretation*: The formula in Eq. (12) can be given a direct physical interpretation, extending the heuristic argument described in Sec. II for $P_{\rm st}(V)$ and $\overline{W}$: once again, the fact that the particles merely exchange velocities upon colliding implies that the mean stationary rate of energy transfer across the piston can be constructed by an energy balance argument. If the piston has a stationary drift velocity $\overline{W}$, the trajectories belonging originally to the gas on its right that collide with it are those corresponding to velocities from $-\infty$ to $\overline{W}$. The energy carried by (a particle on) each such trajectory is $\frac{1}{2}mU^2$. The rate of collisions of such trajectories with that of the piston is $n^+\,(\overline{W}-U)$, the second factor being the relative velocity between the two. Therefore

$$\frac{mn^+}{2}\int_{-\infty}^{\overline{W}} dU\, U^2\,(\overline{W}-U)\,\phi^+(U) \tag{14}$$

is the mean rate at which energy is transferred to the piston by the gas on its right, in the stationary state. Exactly the same argument shows that

$$\frac{mn^-}{2}\int_{\overline{W}}^{\infty} dU\, U^2\,(U-\overline{W})\,\phi^-(U) \tag{15}$$

is the mean rate at which the gas on the left transfers energy to the piston. The difference between the two is precisely the formula of Eq. (12) for the mean stationary rate of transfer of energy from the right to the left across the piston. Our rigorous derivation serves to corroborate this physical argument, in addition to providing an exact result for the time-dependent transients as well.

(ii) Dichotomous and three-valued velocity distributions: The dichotomous velocity distribution

$$\phi^+(V) = \phi^-(V) = \phi(V) = \tfrac{1}{2}\left[\delta(V+c) + \delta(V-c)\right] \tag{16}$$

yields, as always, a simple and tractable special case that serves as a useful check on the calculations. We have, in this case, $\overline{W} = c\,(n^- - n^+)/(n^- + n^+)$. Evaluating the various quantities appearing in Eq. (12), we find that $\Delta\dot{E}_{\text{st}}$ vanishes identically for the dichotomous distribution above. However, valuable insight into the structure of the result for $\Delta\dot{E}_{\text{st}}$ is provided by a slight generalization of the dichotomous distribution of Eq. (16) to the distribution

$$\phi^+(V) = \phi^-(V) = \phi(V) = \mu\,\delta(V) + \tfrac{1}{2}(1-\mu)\,\left[\delta(V+c) + \delta(V-c)\right]\,, \tag{17}$$

where $0 < \mu < 1$. It has been shown in Ref. [7] that the introduction of a non-vanishing probability mass μ at $V = 0$ significantly alters the long-time properties of the homogeneous system. For instance, the velocity autocorrelation function acquires a $t^{-3/2}$ tail, in contrast to its exponential decay in the case of a dichotomous $\phi(V)$. In the present context, too, a non-vanishing value of μ leads to a strikingly different result for $\Delta\dot{E}_{\text{st}}$. We have in this instance

$$\overline{W} = \frac{c(1-\mu)(n^- - n^+)}{(1-\mu)n_> + (1+\mu)n_<}\,, \tag{18}$$

where $n_> = \max\,(n^-, n^+)$ and $n_< = \min\,(n^-, n^+)$. Computing the various quantities occurring in Eq. (12), we arrive at the result

$$\Delta\dot{E}_{\text{st}} = \frac{mc^3}{2}\,\frac{\mu\,(1-\mu)\,n^-\,(n^+ - n^-)}{(1-\mu)\,n_> + (1+\mu)\,n_<}\,. \tag{19}$$

Thus $\Delta\dot{E}_{\text{st}}$ vanishes identically if $n^+ = n^- = n$ (which, together with $\phi^+ = \phi^-$ as already imposed by Eq. (17), implies a homogeneous system), as it must in the homogeneous system. Similarly, $\Delta\dot{E}_{\text{st}}$ vanishes when $\mu = 0$ (the case of a dichotomous $\phi^{\pm}(V)$), or when $\mu = 1$ (the trivial case of no motion at all). Comparing the expressions in Eqs. (18) and (19), we observe that $\Delta\dot{E}_{\rm st}$ can be written in this case in the revealing form

$$\Delta\dot{E}_{\rm st} = \tfrac{1}{2}\, mc^2\, \mu\, n^-(-\overline{W}). \tag{20}$$

(Recall that we have defined $\Delta\dot{E}$ as the rate of transfer of energy to the gas on the *left* of the piston, and that $\overline{W}$ is negative if $n^+ > n^-$, i.e., if the piston drifts to the left.)

(*iii*) *The case of Maxwellian distributions*: The situation that is of direct physical interest is of course that of Maxwellian velocity distributions $\phi^{\pm}(V)$ characterized by temperatures $T^{\pm}$. For arbitrary densities n^+ and n^-, the asymptotic drift velocity $\overline{W}$ is still given by the solution of a transcendental equation, which reads in this case

$$\overline{W} = \frac{n^-\,(2k_BT^-/m\pi)^{1/2}\, e^{-m\overline{W}^2/2k_BT^-} - n^+\,(2k_BT^+/m\pi)^{1/2}\, e^{-m\overline{W}^2/2k_BT^+}}{n^-\left[1-\mathrm{erf}\,(m\overline{W}^2/2k_BT^-)^{1/2}\right] + n^+\left[1+\mathrm{erf}\,(m\overline{W}^2/2k_BT^+)^{1/2}\right]}\,. \tag{21}$$

In terms of $n^{\pm}$, $T^{\pm}$ and $\overline{W}$ as given above, we get

$$\begin{aligned}\Delta\dot{E}_{\rm st} \;=\; & (2\pi m)^{-1/2}\left\{n^+(k_BT^+)^{3/2}e^{-m\overline{W}^2/2k_BT^+} - n^-(k_BT^-)^{3/2}e^{-m\overline{W}^2/2k_BT^-}\right\}\\ & +\tfrac{1}{4}\overline{W}\left\{n^+(m\overline{W}^2 + k_BT^+)\big[1+\mathrm{erf}\,(m\overline{W}^2/2k_BT^+)^{1/2}\big]\right.\\ & \left. + \,n^-(m\overline{W}^2 + k_BT^-)\big[1-\mathrm{erf}\,(m\overline{W}^2/2k_BT^-)^{1/2}\big]\right\}\,. \end{aligned} \tag{22}$$

The nonlinear dependence of $\Delta\dot{E}_{\rm st}$ on $\overline{W}$ is explicit in this formula. We shall comment further on this subsequently. It is also clear that $\Delta\dot{E}_{\rm st}$ is *not* proportional to the temperature difference $(T^+ - T^-)$, though one might perhaps naively expect such a proportionality based on an incorrect identification of $\Delta\dot{E}_{\rm st}$ with the heat flux, together with an application of the Fourier law to the system under discussion.

(*iv*) *Mechanical work and heat contributions*: This brings us, finally, to a very important point. The general expression obtained in Eq. (12) for $\Delta\dot{E}_{\rm st}$ incorporates the effects (on the energy transfer rate) of both the *drift* of the piston and its *diffusive* motion (or fluctuations about its mean position, namely, about $\overline{W}t$). In broad terms, one might regard the respective contributions as the rate of mechanical work done upon the gas on the left of the piston ($\overline{W}$ being the rate of compression or expansion, depending on whether $\overline{W} < 0$ or $\overline{W} > 0$), and the rate at which its entropy changes. However, these contributions are intricately mixed up in the formula for $\Delta\dot{E}_{\rm st}$. Moreover, the dependence of $\Delta\dot{E}_{\rm st}$ upon $\overline{W}$ is in general highly nonlinear. Disentangling these contributions will enable us, in principle, to isolate the parts of $\Delta\dot{E}_{\rm st}$ that may be identified with the "heat flux" $\Delta\dot{Q}_{\rm st}$ and the "rate of mechanical work", respectively. In some cases, the former may vanish altogether — as in the example of the distribution considered in Eq. (17), for which Eq. (20) shows clearly that $\Delta\dot{E}_{\rm st}$ arises entirely from the drift of the piston. In general, however, such a clear separation does not occur in the system under study. It is also important to bear in mind the fact that a non-vanishing drift velocity $\overline{W}$ is itself a consequence of the statistics of collisions in the system under consideration [6].

V. STATIONARY HEAT FLUX

A direct way to isolate and examine the "heat flux" is to impose the condition of zero drift ($\overline{W} = 0$) by adjusting, for instance, the value of the ratio n^-/n^+ of the densities of the two gases. As we shall now see, this leads to considerable simplification in the formula for $\Delta\dot{E}_{\rm st}$, which we are now justified in re-labeling as $\Delta\dot{Q}_{\rm st}$.

As emphasized more than once, the asymptotic drift velocity $\overline{W}$ of the piston vanishes if the densities $n^\pm$ and initial velocity distributions $\phi^\pm$ are related by the condition $n^-\alpha(0) = n^+\beta(0)$, or $n^-\langle|V|\rangle^- = n^+\langle|V|\rangle^+$, i.e., the mean rates at which the piston suffers collisions from the gases on either side of it are equal. The motion of the piston is then purely diffusive in the long-time limit, with a variance $\langle X^2(t)\rangle$ that tends asymptotically to $2Dt$, where the diffusion coefficient is given by [7, 8]

$$D = 2n^-\langle|V|\rangle^-/(n^- + n^+)^2\,. \tag{23}$$

We note that the homogeneous system (defined by $n^- = n^+, \phi^- = \phi^+$) automatically has $\overline{W} = 0$. The converse is not necessarily true, of course: $\overline{W} = 0$ does not necessarily imply a homogeneous system. Recall also that we have already considered situations in which $\phi^+(V) = \phi^-(V) = \phi(V)$, but $n^+ \neq n^-$; we then have an inhomogeneous system in which, moreover, $\overline{W} \neq 0$.

Setting $\overline{W} = 0$ in Eq. (12), we find that the stationary energy flux in the absence of drift is simply

$$\Delta\dot{Q}_{\rm st} = \tfrac{1}{4}\,m\big[n^+\langle|V|^3\rangle^+ - n^-\langle|V|^3\rangle^-\big]\,, \tag{24}$$

in terms of the third moments

$$\langle|V|^3\rangle^\pm = 2\int_0^\infty dU\,U^3\,\phi^\pm(U) \tag{25}$$

of the particle speed in the two gases. For the homogeneous system, of course, $\Delta\dot{Q}_{\rm st}$ vanishes identically, as it must.

Turning again to the case of Maxwellian distributions $\phi^{\pm}(V)$ at temperatures $T^{\pm}$, the drift velocity $\overline{W}$ vanishes, as is well known, if $n^{-}\sqrt{T^{-}} = n^{+}\sqrt{T^{+}}$. Equation (22) then reduces to

$$\Delta\dot{Q}_{\rm st} = n^{+}\left(\frac{k_B T^{+}}{2\pi m}\right)^{1/2} k_B\,(T^{+} - T^{-}). \tag{26}$$

We see that the heat flux is indeed given by the Fourier law in this case, with a "coefficient of thermal conductivity" that is proportional to the square root of the temperature.

It is revealing and instructive to pause at this stage to compare the result in Eq. (26) with that for the heat flux between two reservoirs held at different temperatures and densities, coupled by virtue of their sharing a common piston [9]. When the mass of the latter is equal to that of the gas particles, the Boltzmann equation can be solved exactly for the stationary distribution; concomitantly, the heat flux conveyed via the shared piston from one reservoir to the other can also be calculated. While the exact expression for this quantity (see [9]) is slightly more complicated than that of Eq. (26) above, it reduces to the latter result to leading order in the temperature difference $(T^{+} - T^{-})$, apart from an extra numerical factor $\pi/\sqrt{2}$. This lends additional support to our identification of the portion of the energy flux that corresponds to the heat flux. The fact that the heat flux is about twice as large in the case of the shared piston is readily understood by recalling that the piston now suffers collisions with the gas particles belonging to both reservoirs, so that the effective rate of collisions is roughly twice as large. For a detailed discussion of the relevance of the problem of the shared piston to the general questions addressed here, we refer to [9].

Finally, let us return to the full expression for the stationary energy flux $\Delta\dot{E}_{\rm st}$ in Eq. (12), and analyze its dependence on the drift velocity $\overline{W}$. For sufficiently small $\overline{W}$, we may expand $\Delta\dot{E}_{\rm st}$ in powers of $\overline{W}$, taking care to incorporate the fact that $\overline{W} = 0$ imposes the condition $n^{-}\langle|V|\rangle^{-} = n^{+}\langle|V|\rangle^{+}$ on the parameters occurring in the coefficients of the expansion. (This has been done in the Maxwellian case, Eq. (26) above, to reduce $n^{+}(T^{+})^{3/2} - n^{-}(T^{-})^{3/2}$ to $n^{+}(T^{+})^{1/2}(T^{+} - T^{-})$.) For distributions $\phi^{\pm}(V)$ that have derivatives of all orders at $V = 0$, the formal expansion in powers of $\overline{W}$ is given by

$$\Delta\dot{E}_{\rm st} = \Delta\dot{Q}_{\rm st} + \frac{m\overline{W}}{4}\left[n^{+}\langle V^2\rangle^{+} + n^{-}\langle V^2\rangle^{-}\right] + \frac{m\overline{W}^{\,4}}{2}\sum_{k=0}^{\infty}\frac{\overline{W}^{\,k}\,\psi^{(k)}(0)}{(k+3)(k+4)k!}\,, \tag{27}$$

where

$$\psi(V) = n^+\phi^+(V) - n^-\phi^-(V)\,, \tag{28}$$

$\psi^{(k)}$ denotes its k^{th} derivative, and $\Delta\dot{Q}_{\text{st}}$ is given by Eq. (24). This representation isolates the contribution to $\Delta\dot{E}_{\text{st}}$ owing to the systematic drift of the piston from that arising from the fluctuations about its mean position. We observe that the part that is nonlinear in $\overline{W}$ is $\mathcal{O}(\overline{W}^4)$. Considering the Maxwellian case once again, we find

$$\Delta\dot{E}_{\text{st}} \approx \left(\frac{k_B T^+}{2\pi m}\right)^{1/2} n^+\, k_B\,(T^+ - T^-) + \left(\frac{k_B T^+ T^-}{8\pi m}\right)^{1/2} k_B\,\left(n^-\sqrt{T^-} - n^+\sqrt{T^+}\right) \tag{29}$$

correct to first order in the difference $\left(n^-\sqrt{T^-} - n^+\sqrt{T^+}\right)$, the next term being of fourth order in this quantity. In contrast to the relatively simple expression to which $\Delta\dot{E}_{\text{st}}$ reduces when $n^-\sqrt{T^-} = n^+\sqrt{T^+}$ (Eq. (26)), no significant simplification of the general expression in Eq. (22) occurs when $n^-T^- = n^+T^+$ (equal *pressures* on either side of the piston). Some simplification does occur, however, when the *temperatures* on the two sides are equal, $T^+ = T^- = T$ (but $n^+ \neq n^-$). We find that the drift velocity is now given by the implicit equation

$$\overline{W} = \left(\frac{n^- - n^+}{n^- + n^+}\right)\left[\left(\frac{2k_BT}{m\pi}\right)^{1/2} e^{-m\overline{W}^2/2k_BT} + \overline{W}\,\text{erf}\,(m\overline{W}^2/2k_BT)^{1/2}\right]. \tag{30}$$

The corresponding stationary energy flux is found to be

$$\Delta\dot{E}_{\text{st}} = (n^- - n^+)\left(\frac{mk_BT}{8\pi}\right)^{1/2}\left(\overline{W}^2 - \frac{k_BT}{m}\right) e^{-m\overline{W}^2/2k_BT}\,. \tag{31}$$

Written in terms of the moments of the (Maxwellian) velocity distribution, this is just

$$\Delta\dot{E}_{\text{st}} = \tfrac{1}{4}\, m\,\left(\overline{W} - \langle V^2\rangle\right)\,(n^- - n^+)\,\langle\,|V|\,\rangle\, e^{-m\overline{W}^2/2k_BT}\,. \tag{32}$$

Finally, if the two *densities* are equal ($n^+ = n^- = n$, but $T^+ \neq T^-$), we find that $\overline{W}$ becomes independent of n, and $\Delta\dot{E}_{\text{st}}$ is directly proportional to n.

VI. CONCLUDING REMARKS

We have already commented at the appropriate junctures on the special and interesting features of the structure of our analytical result for the stationary rate of energy transfer, as given by Eqs. (12) and (27). We conclude with a comment on the question of the finiteness or otherwise of the heat conductivity of the system under study[1, 2]. It may be argued that the coefficient of heat conductivity of our system is essentially infinite: The contention is that in the expression for the heat flux, the conductivity is the coefficient of the gradient of the temperature, and the latter is $\propto (T^+ - T^-)/L$. This gradient tends to zero in the thermodynamic limit, although a finite energy flux persists in the long time limit. Hence the coefficient multiplying the gradient has to diverge.

While we agree with this argument, we point out that the system can be viewed in a different way: the gases on the left and right of the piston are heat reservoirs which have a single microscopic degree of contact, namely, the tagged particle we have termed the piston. There is no relevant length scale in the problem, so the "heat flux" is expected to appear solely as a result of this thermal contact. The fact that the Boltzmann calculation gives a comparable value for the conductivity supports the meaningfulness of our result. Furthermore, one can construct a physical system that will display exactly the behavior predicted by our model calculation. Consider a two- or three-dimensional cylinder of axial length $2L$ with a central piston that can move without friction along the axis of the cylinder. The compartments to its left and right are filled with gases in equilibrium, at respective densities and temperatures $n^{\pm}, T^{\pm}$. In the limit of low densities and $L \to \infty$, the dynamics of the piston will be exactly as described by the one-dimensional model: in the physical set-up, the particles only interact with the piston, while in our one-dimensional model, they exchange velocities upon collision, which is effectively tantamount to their passing through each other without interaction.

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APPENDIX: CALCULATION OF $\Delta E(t)$

As stated in the main text, we write Eq. (10) for $\Delta E(t)$ as the sum $\Delta E^0(t)+\Delta E^-(t)+\Delta E^+(t)$ of contributions coming, respectively, from the possibilities that at time t, the piston is (i) on its original trajectory, so that $a=0$, or (ii) on a trajectory belonging to the gas on its left, so that $-N^-\le a\le -1$, or (iii) on a trajectory belonging to the gas on its right, so that $1\le a\le N^+$. Consider ΔE^0 first. We have in this case $X_0=0$, $V_0=0$. We find

$$\begin{aligned}\Delta E^0(t) \;=\; & m\oint\frac{dz}{4\pi iz}\sum_{j\neq 0}\big\langle V_j^2\,[\theta(-X_j-V_j\,t)-\theta(-X_j)]\,\big\rangle\\ & \times\prod_{\ell-}\big[z+(1-z)\big\langle\theta(-X_\ell-V_\ell\,t)\big\rangle\big]\prod_{\ell'+}\big[1+(z^{-1}-1)\big\langle\theta(-X_{\ell'}-V_{\ell'}t)\big\rangle\big]\end{aligned}\tag{A.1}$$

where the symbols $\ell-$ and $\ell'+$ are used to denote the fact that ℓ and ℓ' run over $-N^-\le\ell\le -1$ and $1\le\ell'\le N^+$, respectively, in the products concerned. We shall use the convenient notation $\langle\ldots\rangle_j^{\pm}$ for the corresponding averages. The evaluation of the contributions $\Delta E^{\pm}(t)$ is somewhat more involved. We get

$$\begin{aligned}\Delta E^-(t) \;=\; & m\oint\frac{dz}{4\pi iz}N^-\,\Big\langle\Big\{(N^--1)\big\langle V_j^2\,[\theta(X_a+V_a\,t-X_j-V_j\,t)-\theta(-X_j)]\big\rangle_j^-\\ & +N^+\,\big\langle V_j^2\,[\theta(X_a+V_a\,t-X_j-V_j\,t)-\theta(-X_j)]\big\rangle_j^+\Big\}\\ & \times[z+(1-z)\big\langle\theta(X_a+V_a\,t-X_\ell-V_\ell t)\big\rangle_\ell^-]^{N^--1}\;[z+(1-z)\,\theta(X_a+V_a t)]\\ & \times[1+(z^{-1}-1)\big\langle\theta(X_a+V_a\,t-X_{\ell'}-V_{\ell'}t)\big\rangle_{\ell'}^+]^{N^+}\Big\rangle_a^-\,,\end{aligned}\tag{A.2}$$

while

$$\begin{aligned}\Delta E^+(t) \;=\; & m\oint\frac{dz}{4\pi iz}N^+\,\Big\langle\Big\{N^-\big\langle V_j^2[\theta(X_a+V_a\,t-X_j-V_j\,t)-\theta(-X_j)]\big\rangle_j^-\\ & +(N^+-1)\big\langle V_j^2\,[\theta(X_a+V_a\,t-X_j-V_j\,t)-\theta(-X_j)]\big\rangle_j^+\Big\}\\ & \times[z+(1-z)\big\langle\theta(X_a+V_a\,t-X_\ell-V_\ell t)\big\rangle_\ell^-]^{N^-}\;[1+(z^{-1}-1)\,\theta(X_a+V_a\,t)]\\ & \times[1+(z^{-1}-1)\big\langle\theta(X_a+V_a\,t-X_{\ell'}-V_{\ell'}t)\big\rangle_{\ell'}^+]^{N^+-1}\Big\rangle_a^+\,.\end{aligned}\tag{A.3}$$

Evaluating the averages required, we get, for instance,

$$\begin{aligned}\big\langle V_j^2[\theta(-X_j-V_j\,t)-\theta(-X_j)]\big\rangle_j^- &= -\textstyle\int_{L/t}^{\infty}dU\,U^2\,\phi^-(U)-(t/L)\int_0^{L/t}dU\,U^3\,\phi^-(U)\,,\\ \big\langle V_j^2\,[\theta(-X_j-V_j\,t)-\theta(-X_j)]\big\rangle_j^+ &= \textstyle\int_{-\infty}^{-L/t}dU\,U^2\,\phi^+(U)-(t/L)\int_{-L/t}^{0}dU\,U^3\,\phi^+(U)\,,\\ \big\langle\theta(-X_\ell-V_\ell t)\big\rangle_\ell^- &= \textstyle\int_{-\infty}^{L/t}dU\,\phi^-(U)-(t/L)\int_0^{L/t}dU\,U\,\phi^-(U)\,,\\ \big\langle\theta(-X_{\ell'}-V_{\ell'}t)\big\rangle_{\ell'}^+ &= \textstyle\int_{-\infty}^{-L/t}dU\,\phi^+(U)-(t/L)\int_{-L/t}^{0}dU\,U\,\phi^+(U)\,.\end{aligned}\tag{A.4}$$

The other averages are similarly calculated. Inserting all these results in Eqs. (A.1) - (A.3), we pass to the thermodynamic limit $N^{\pm} \to \infty$, $L \to \infty$, such that $\lim N^{\pm}/L = n^{\pm}$. Using the well-known expression for the generating function of the modified Bessel function $I_r(z)$, the final expressions are as follows:

Recall the definitions of the rates $\alpha(w)$ and $\beta(w)$ in Eq. (1), and let

$$\lambda^-(w\,;\,n^-) = n^- \,\alpha(w)\,,\;\; \lambda^+(w\,;\,n^+) = n^+ \,\beta(w). \tag{A.5}$$

Define the effective rates

$$\lambda(w\,;\,n^-, n^+) = (\lambda^- \lambda^+)^{1/2}\,,\;\; \Lambda(w\,;\,n^-, n^+) = \lambda^- + \lambda^+\,. \tag{A.6}$$

Further, let

$$F(w\,;\,n^-, n^+) = n^- \int_w^\infty dU\, U^2 (w-U)\, \phi^-(U) + n^+ \int_{-\infty}^w dU\, U^2 (w-U)\, \phi^+(U)\,. \tag{A.7}$$

Then, suppressing the $n^{\pm}$ dependence in λ and Λ for notational simplicity, we find

$$\Delta E^0(t) = \tfrac{1}{2}\, m\, t\, e^{-\Lambda(0)t}\, I_0\big(2\lambda(0)t\big)\, F(0\,;\,n^-, n^+)\,, \tag{A.8}$$

$$\begin{aligned} \Delta E^-(t) \;&=\; \tfrac{1}{2}\, m n^- t^2 \textstyle\int_{-\infty}^{\infty} dw\, e^{-\Lambda(w)t}\, |\alpha'(w)|\, F(w\,;\,n^-, n^+) \\ &\quad \times \left\{\theta(w)\, I_0\big(2\lambda(w)t\big) + \theta(-w)\, [\lambda^+(w)/\lambda^-(w)]^{1/2}\, I_1\big(2\lambda(w)t\big)\right\}\,, \end{aligned} \tag{A.9}$$

$$\begin{aligned} \Delta E^+(t) \;&=\; \tfrac{1}{2}\, m n^+ t^2 \textstyle\int_{-\infty}^{\infty} dw\, e^{-\Lambda(w)t}\, \beta'(w)\, F(w\,;\,n^-, n^+) \\ &\quad \times \left\{\theta(-w)\, I_0\big(2\lambda(w)t\big) + \theta(w)\, [\lambda^-(w)/\lambda^+(w)]^{1/2}\, I_1\big(2\lambda(w)t\big)\right\}\,. \end{aligned} \tag{A.10}$$

$\Delta E(t)$ is the sum of the right-hand sides of Eqs. (A.8)-(A.10).

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