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# Irreversibility, discontinuities in phase space and information flow

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**Abstract.** The kinetic theory formulation stemming from the Liouville equation which gives constant entropy for Hamiltonian systems is reviewed. This derivation is found to be inconsistent for configurations which include discontinuous changes in  $f_N$ , the  $N$ -body distribution function. A reformulated theory is presented for such systems whose entropy may not be stationary. The formalism is applied to two cases. In the first of these, in a gedanken-like process, a gas confined to an isolated cylindrical box undergoes an infinitesimal free expansion away from a discontinuity in  $f_N$ . A self-consistent estimate of the variation of the integral of the Gibbs microentropy over the expansion is found to give an increase in entropy. In a closely allied example a new description of entropy change of an enclosed fluid is presented according to which the flux of the Gibbs microentropy through an impenetrable confining wall is interpreted as a flux of information from the system. Such information loss increases the missing information on the system which, according to Shannon's interpretation, is equivalent to an increase in entropy.

## 1. Introduction

Significant advances have recently been made in the theory of the irreversibility of deterministic classical systems (Biel and Rae 1972, Hellerman and Ioos 1983, Schuster 1984, Zaslavsky 1983, Prigogine 1980). For the most part such studies are concerned with the relation between a loss of integrals of the motion and the ensuing chaotic behaviour. Related numerical studies chiefly consider systems with small numbers of degrees of freedom. Analytic theories examine these problems through perturbation of idealised completely integrable systems.

In this paper the problem of irreversibility of macroscopic systems is revisited from the viewpoint of the Liouville equation (Kubo 1957, Uhlenbeck and Ford 1963, Koga 1970, Kac 1958, Liboff and Heffernan 1980, Liboff 1979). For Hamiltonian systems this equation yields reversible macroscopic equations and constant entropy (Grad 1961, Ferziger and Kaper 1972, Cercignani 1969, Wehrl 1978).

For distribution functions which suffer discontinuous changes in phase space this derivation is inconsistent and must be reformulated. It is argued that the reformulated theory allows for a change in entropy.

Two problems are considered within this formalism. The first of these addresses the infinitesimal free expansion of a gas over a time interval which is short compared to the mean free collision time of its molecules. The expanding gas and its cylindrical

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container are taken to comprise an isolated system. An exact solution is obtained for the distribution function in the expanded domain of the gas. Variation of the integral expression for the Gibbs entropy over the expansion interval reveals that the process involves an increase in entropy. This result is attributed to the initial discontinuity of the distribution function for the system. In a closely allied problem it was established by Sinai (1967) that a confined gas of rigid spherical molecules exhibits mixing flow (Reichl 1980).

The second example addresses the change in entropy stemming from surface integrals which emerge from the integration of the entropy equation of motion over the accessible domain in phase space. The problem addressed is that of a gas enclosed at constant volume by a confining wall. If the wall is at higher temperature than the gas, particle-wall collisions cause information to flow from the system with an accompanying increase in entropy. This interpretation of information loss stems from the Shannon-Brillouin entropy-information formulation according to which an entropy increase corresponds to an increase in missing information on the system (Shannon 1949, Brillouin 1956, Liboff 1974, Katz 1967, Janes 1957, Goldstein and Penrose 1981, Lindblad 1983).

## 2. Entropic equation of motion

### 2.1. Stationary entropy for Hamiltonian systems

Stemming from the Liouville equation, it is readily shown that the entropy of a Hamiltonian system is constant in time. The argument is as follows. First we recall the Gibbs expression for entropy:

$$S = -k_B \int d\Gamma f_N \ln f_N. \quad (1)$$

In this relation  $k_B$  is Boltzmann's constant,  $d\Gamma$  is the volume element in coordinate-momentum phase space and  $f_N$  is the joint probability  $N$ -body distribution function normalised to unity

$$\int f_N d\Gamma = 1. \quad (2)$$

The distribution  $f_N$  satisfies the Liouville equation

$$df_N/dt = \partial f_N/\partial t + [f_N, H] = 0 \quad (3)$$

where  $H$  is the Hamiltonian of the system and  $[ , ]$  denotes Poisson brackets. To obtain constancy of  $S$ , one multiplies (3) through by  $(1 + \ln f_N)$ , obtaining

$$\partial h_N/\partial t + [h_N, H] = 0 \quad (4a)$$

where

$$h_N \equiv f_N \ln f_N. \quad (4b)$$

Substituting (4a) into (1) gives

$$dS/dt = 0 \quad (4c)$$

which establishes that  $S$  is stationary for a Hamiltonian system. We will call  $h_N$  the Gibbs microentropy.

It is important to our subsequent analysis to study briefly the relation between rates of change of  $h_N$  and  $f_N$ . Since  $f_N$  is the probability density it follows that

$$f_N \geq 0. \tag{5}$$

Consider that  $f_N$  is bounded so that

$$0 \leq f_N \leq M \tag{5a}$$

where  $M$  is some finite value. Introducing the scale change

$$\bar{f}_N = (1/M)f_N \tag{6a}$$

$$d\bar{\Gamma} = M d\Gamma \tag{6b}$$

and substituting into (2) gives

$$\int f_N d\Gamma = \int \bar{f}_N d\bar{\Gamma} = 1. \tag{7}$$

Furthermore, (5a) gives

$$0 \leq \bar{f}_N \leq 1. \tag{8}$$

As no loss in generality is introduced in the scale transformation (6), it is adopted in the subsequent discussion.

Dropping bars and letting  $z$  denote any phase variable, we find

$$\frac{\partial h_N}{\partial z} = (1 + \ln f_N) \frac{\partial f_N}{\partial z}. \tag{9}$$

In the interval given by (8),  $h_N = -|h_N|$  and we obtain

$$\begin{aligned} \frac{\partial h_N}{\partial z} &= -\frac{\partial |h_N|}{\partial z} \propto \frac{\partial f_N}{\partial z} & f_N > \exp(-1) \\ \frac{\partial h_N}{\partial z} &= -\frac{\partial |h_N|}{\partial z} \propto \frac{-\partial f_N}{\partial z} & f_N < \exp(-1). \end{aligned} \tag{10}$$

These relations indicate that in the more probable domain of phase space, derivatives of  $|h_N|$  and  $f_N$  are antialigned.

### 2.2. Discontinuous configurations

Consider that  $f_N$  or the first derivative in any of its variables is discontinuous across a surface in the accessible domain of phase space. As differentiation is not well defined on such surfaces, arguments leading to (4c) are inconsistent. To examine these situations we assume that  $h_N$  is a dynamical variable and consequently satisfies the equation of motion (3), namely

$$\frac{dh_N}{dt} = \frac{\partial h_N}{\partial t} + [h_N, H]. \tag{11}$$

This equation is appropriate to domains where  $h_N$  is continuous. If  $f_N$  is continuous over all accessible phase space then the entropy is stationary for the system and (11) reverts to (4a). If there are surfaces of discontinuity of  $f_N$  in phase space, then it is

conjectured that the entropy is not necessarily stationary. In this event we return to (1) and in the first example below apply it to calculate the change in  $S$  due to an infinitesimal variation about a discontinuity in  $f_N$ . In the second example we employ the integral relation obtained from (1) and (11):

$$\frac{1}{k_B} \frac{dS}{dt} = - \int d\Gamma \left( \frac{\partial h_N}{\partial t} + [h_N, H] \right) \tag{12}$$

in discussing the notion of entropy change due to information flux through a confining wall.

2.3. Infinitesimal expansion and accompanying entropy change

A simple gedanken-like procedure to effect a discontinuous configuration is by instantaneous removal of a workless constraint. Specifically we consider the example of an infinitesimal free expansion of a gas of  $N$  molecules away from a homogeneous equilibrium state at a given volume  $V$  at time  $t=0$  to an infinitesimally extended volume at time  $t=\tau$ . The initial volume  $V$  occupies a section of length  $L$  of a right circular cylinder with perfectly reflecting walls of finite thickness and of unit cross section so that we may write  $V=L$ . (We refer to this section of the cylinder as the ‘reservoir.’) The whole cylinder is of length  $L+l$ , (where  $L \gg l$ ) and is of mass greatly in excess of the confined gas. This entire system is isolated and initially in thermal equilibrium at a given temperature  $T$ . It is further assumed that the system suffers vanishingly small change in temperature during the expansion interval and that any such temperature change may be neglected in the ensuing study. It is evident that at  $t=0_+$ , the spatial component of  $f_N$  is discontinuous at the site of the initial constraining wall,  $\bar{x}=L$  (see figure 1). At the time  $\tau$  the coordinate space accessible to the system is the extended cylindrical volume  $L+l$ .

The time  $\tau$  is such that  $C\tau \ll l_{MFP}$ , where  $C$  is the thermal speed and  $l_{MFP}$  is the collisional mean free path of molecules in the starting configuration. This latter inequality ensures that a vanishingly small number of particles collide in the interval  $\tau$ . If further we choose  $l$  so that  $l \gg C\tau$  then there is virtually no reflection of particles

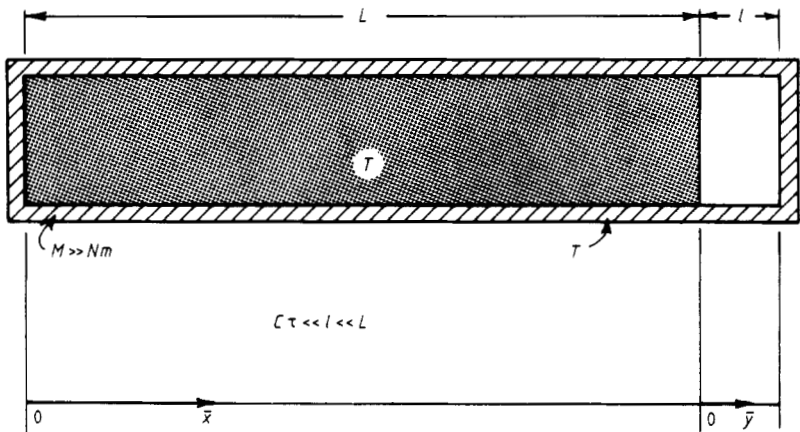


Figure 1. The isolated system at  $t=0$  is in thermal equilibrium at temperature  $T$ . The cylindrical enclosure has unit cross sectional area. Coordinates  $\bar{x}$  and  $\bar{y}$  are also shown.

from the newly positioned confining wall. Thus we write

$$L \gg l \gg C\tau \tag{13a}$$

$$C\tau \ll l_{\text{MFP}} \tag{13b}$$

$$mC^2 = k_B T \tag{13c}$$

where  $m$  is the molecular mass. As we are discussing expansion of the gas at  $t=0$  it is important to note that this expansion is guaranteed due to the isotropic quality of the velocity component of the distribution at  $t=0$ .

Further assumptions concerning this expansion are as follows.

(i) The gas is comprised of rigid-sphere molecules and is sufficiently rare so that at equilibrium the molecules are not correlated (Reichl 1980, McQuarrie 1973). Using (13b) this property may be extended over the expansion interval.

(ii) Variations in the transverse momentum component of  $f_N$  and in the transverse coordinate components are vanishingly small over the expansion and may be neglected in the ensuing analysis. Transverse components are those normal to the direction of expansion.

We wish to calculate the change in entropy in this expansion from the starting equation (1). Effecting a variation of (1) over the interval  $\tau$  gives (working with velocity  $v$  in place of momentum):

$$\delta S/k_B = - \int dx^N dv^N h_N(\tau, x^N, v^N) + \int dx^N dv^N h_N(0, x^N, v^N). \tag{14}$$

Given that molecules in the gas are uncorrelated we may write

$$f_N(1, 2, \dots, N) = \prod_{i=1}^N f_1(i). \tag{15}$$

It follows that

$$\int dx^N dp^N h_N = N \int h_1 dx_1 dp_1 \tag{15a}$$

where

$$h_1 = f_1 \ln f_1 \tag{15b}$$

is the one-particle Gibbs microentropy function. With these relations, (14) reduces to the simpler form

$$\delta S/Nk_B = - \int d\bar{x} d\bar{v} h_1(\tau) + \int d\bar{x} d\bar{v} h_1(0) \tag{16}$$

where  $\bar{x}$  and  $\bar{v}$  denote (dimensional) displacement and velocity parallel to the direction of expansion.

The system we address exists in the half-open time interval

$$0 < t \leq \tau.$$

Note that the system so defined is isolated and evolves according to Hamiltonian dynamics. Note also that the state of the system at  $t=\tau$  is *not* in thermodynamic equilibrium.

We now wish to assign, more carefully, coordinates for the expansion. Let  $\bar{x} = 0$  denote the origin of the cylinder so that the constraint removed at time  $t = 0$  is at the point  $\bar{x} = L$ . It is convenient to label points in the extended volume with  $\bar{y}$  so that in this domain

$$\bar{x} = L + \bar{y}$$

(see figure 1). We further introduce the non-dimensionalised  $x$  component of velocity

$$v = \bar{v}/\sqrt{2} C$$

where  $\bar{v}$  is the actual speed and, as noted previously,  $C$  is the thermal speed. The distribution at  $t = 0$  is given by the Maxwellian

$$f(0) = \frac{1}{\sqrt{2\pi} LC} \exp(-v^2) \equiv \frac{1}{LC\sqrt{2}} f_M(v) \quad (17)$$

$$\int_0^L d\bar{x} \int_{-\infty}^{\infty} d\bar{v} f(0) = \int_{-\infty}^{\infty} dv f_M(v) = 1$$

$$f_M(v) = \frac{1}{\sqrt{\pi}} \exp(-v^2). \quad (17a)$$

To construct the distribution at time  $\tau$  we divide the problem into two parts. First we consider  $f(\tau)$  in the expansion domain  $0 \leq \bar{y} \leq l$ . As particles do not collide in the interval  $\tau$ , the  $\bar{x}$  coordinate of a particle moves with constant velocity. Consider an arbitrary point in the expansion  $\bar{y}$ . At this point, at the time  $\tau$ , only velocities in the interval

$$I(\bar{v}) \equiv [\bar{y}/\tau \leq \bar{v} \leq (\bar{y} + L)/\tau] \quad (18)$$

contribute to the distribution. Such particles carry their Maxwell distribution. This property follows from the following observation. First consider slow particles arriving at a given value of  $\bar{y}$  which originate in the reservoir near the value  $\bar{x} = L$ . Next consider faster particles which originate closer to  $\bar{x} = 0$ . As the ratio of such particles is in a Boltzmann distribution we may conclude that the distribution is Maxwellian. Thus we write

$$\begin{aligned} f(\tau) &= \frac{1}{LC\sqrt{2}} f_M(v) & v \in I(v) \\ f(\tau) &= 0 & v \notin I(v). \end{aligned} \quad (18a)$$

The distribution (18a) is a half-Maxwellian ( $v \geq 0$ ) with the section of velocities  $v \notin I(v)$  omitted (see figure 2).

Concerning the reflection of molecules from the wall at  $\bar{x} = 0$  of the reservoir, we observe the following. To account for such reflections we would replace  $L$  by  $2L$  in (18). Note, however, that  $\exp[-\frac{1}{2}(L/C\tau)^2]$  is vanishingly small in the present study (recall (13a)) and such reflections may be neglected.

The remaining component of  $f(\tau)$  in the reservoir is constructed on the basis that the perturbation to the initial configuration due to the expansion is infinitesimal and the fact that molecules from the entire reservoir contribute to the expansion. Namely, it is assumed that this component of the distribution remains Maxwellian in velocity space and is diminished infinitesimally in amplitude. Accordingly we write

$$f(\tau) = \frac{a}{LC\sqrt{2}} f_M(v) \quad 0 \leq \bar{x} \leq L \quad (18b)$$

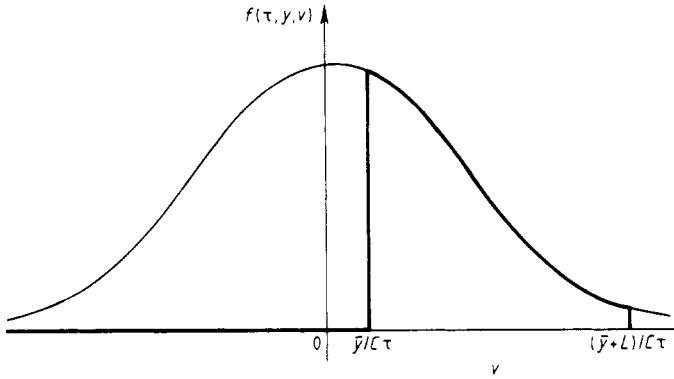


Figure 2. The attenuated half-Maxwellian in velocity space at a given value of  $\bar{y}$  at time  $\tau$ .

where  $a$  is a modification parameter. For self-consistency we must find that  $a - 1$  is infinitesimal or, equivalently, that a vanishingly small number of particles take part in the expansion. The parameter  $a$  is determined by normalisation. Namely, with the preceding two expressions we write

$$\int_{-\infty}^{\infty} d\bar{v} \int_0^{L+l} d\bar{x} f(\tau) = \int_{-\infty}^{\infty} dv \int_0^L d\bar{x} \frac{a}{L} f_M(v) + \frac{1}{L} \int_0^l d\bar{y} \int_{v_1}^{v_2} dv f_M(v) = 1 \tag{19}$$

where  $v_1$  and  $v_2$  are given by

$$v_1 = \frac{\bar{y}}{\sqrt{2}C\tau} = y \left( \frac{l}{\sqrt{2}C\tau} \right) \equiv y/\varepsilon_1 \tag{20a}$$

$$v_2 = \frac{\bar{y} + L}{\sqrt{2}C\tau} = v_1 + \frac{L}{\sqrt{2}C\tau} \equiv v_1 + \frac{1}{\varepsilon_2} \gg v_1.$$

Using (13a) we write

$$1 \gg \varepsilon_1 \gg \varepsilon_2 = (l/L)\varepsilon_1. \tag{20b}$$

Thus (19) may be written

$$1 - a = \pi^{-1/2} \frac{l}{L} \int_0^l dy \int_{v_1}^{v_2} dv \exp(-v^2). \tag{21}$$

2.3.1. Evaluation of  $1 - a$ . The integral on the RHS of (21) may be rewritten

$$I \equiv \pi^{-1/2} \int_0^l dy \int_{v_1}^{v_2} dv \exp(-v^2) = \frac{1}{2} \int_0^l dy (\text{erf } v_2 - \text{erf } v_1) \tag{21a}$$

where  $\text{erf } v$  represents the error function of  $v$ . Carrying out the preceding integrations we find (Gradsteyn and Ryzhik 1965)

$$2I = -\varepsilon_1 [w \text{ erf } w + \pi^{-1/2} \exp(-w^2)]_0^u + \varepsilon_1 [w \text{ erf } w + \pi^{-1/2} \exp(-w^2)]_z^{z+u} \tag{21b}$$

where  $w$  is a dummy variable and

$$u \equiv 1/\varepsilon_1 \quad z \equiv 1/\varepsilon_2.$$

Using (20b) we recall

$$z \gg u \gg 1. \tag{21c}$$



Isolating the  $w = 0$  term in (21b) gives

$$2I = \pi^{-1/2} \varepsilon_1 - \varepsilon_1 [u \operatorname{erf} u + \pi^{-1/2} \exp(-u^2)] \\ + \varepsilon_1 [(z+u) \operatorname{erf}(z+u) + \pi^{-1/2} \exp[-(z+u)^2]] - z \operatorname{erf} z - \pi^{-1/2} \exp(-z^2). \quad (21d)$$

For large  $z$  we may write (Abramowitz and Stegun 1970)

$$z \operatorname{erf} z + \pi^{-1/2} \exp(-z^2) = z + \pi^{-1/2} \exp(-z^2) \left( \frac{1}{2z^2} - \dots \right).$$

Substituting this expression into (21d) gives

$$2I = \pi^{-1/2} \varepsilon_1 \left( 1 - \frac{\exp(-u^2)}{2u^2} + \frac{\exp[-(z+u)^2]}{2(z+u)^2} - \frac{\exp(-z^2)}{2z^2} \right) \\ 2I \approx \pi^{-1/2} \varepsilon_1 \left( 1 - \frac{\exp(-u^2)}{2u^2} \right).$$

In the limit of large  $u$  we neglect the exponential term and obtain, finally,

$$I = \frac{1}{2} \pi^{-1/2} \varepsilon_1. \quad (21e)$$

Substituting this result in (21) and recalling (20b), we obtain

$$1 - a = \frac{1}{2} \pi^{-1/2} \varepsilon_1 l / L = \frac{1}{2} \pi^{-1/2} \varepsilon_2 \ll 1. \quad (22)$$

Returning to the normalisation statement (19) and multiplying through by  $N$  yields (22) similarly augmented. We may conclude that

$$\delta N / N = 1 - a \ll 1 \quad (22a)$$

is the fractional incremental number of molecules which contribute to the expansion. As stated previously, the property (22a) is necessary for self-consistency of the analysis.

**2.3.2. Entropy calculation.** With the distributions (18a, b) at hand we return to (16) and write for the total entropy change in the time  $\tau$

$$\frac{\delta S}{Nk_B} = \frac{2}{\sqrt{\pi}} \int_0^\infty \exp(-v^2) \ln \left( \frac{\exp(-v^2)}{K} \right) dv - \frac{2a}{\sqrt{\pi}} \int_0^\infty \exp(-v^2) \ln \left( \frac{a \exp(-v^2)}{K} \right) dv \\ - \frac{1}{\sqrt{\pi}} \frac{l}{L} \int_0^1 dy \int_{v_1}^{v_2} \exp(-v^2) \ln \left( \frac{\exp(-v^2)}{K} \right) dv \quad (23)$$

where

$$K \equiv \frac{1}{LC\sqrt{2\pi}}.$$

The relation (23) may be more concisely written

$$\frac{\delta S}{Nk_B} = \frac{2}{\sqrt{\pi}} (1-a) \int_0^\infty dv \exp(-v^2) \ln \left( \frac{\exp(-v^2)}{K} \right) - a \ln a \\ - \frac{1}{\sqrt{\pi}} \frac{l}{L} \int_0^1 dy \int_{v_1}^{v_2} \exp(-v^2) \ln \left( \frac{\exp(-v^2)}{K} \right). \quad (23a)$$

Further expanding the logarithmic terms gives

$$\frac{\delta S}{Nk_B} = -\frac{1}{2}(1-a) - a \ln a + \frac{1}{\sqrt{\pi}} \frac{l}{L} \int_0^1 dy \int_{v_1}^{v_2} \exp(-v^2) v^2 dv. \tag{23b}$$

Integrating the last term by parts we find

$$\frac{1}{\sqrt{\pi}} \frac{l}{L} \int_0^1 dy \int_{v_1}^{v_2} \exp(-v^2) v^2 dv = \frac{1}{\sqrt{\pi}} \frac{l}{L} \int_0^1 dy \left( \int_{v_1}^{v_2} \frac{1}{2} \exp(-v^2) dv - \frac{1}{2} [v \exp(-v^2)]_{v_1}^{v_2} \right).$$

Inserting this result into (23b) gives

$$\frac{\delta S}{Nk_B} = -a \ln a - \frac{1}{2\sqrt{\pi}} \frac{l}{L} \int_0^1 dy [v \exp(-v^2)]_{v_1}^{v_2}. \tag{23c}$$

Integrating over  $y$  and passing to the small  $\epsilon_1, \epsilon_2$  limit, with  $v_2 \gg v_1$ , gives

$$\int_0^1 dy [v \exp(-v^2)]_{v_1}^{v_2} \approx \frac{1}{2} \epsilon_1. \tag{23d}$$

Inserting this result into (23c) we obtain

$$\frac{\delta S}{Nk_B} = -a \ln a - \frac{1}{4\sqrt{\pi}} \epsilon_2. \tag{23e}$$

Recalling (22),

$$1-a = \frac{1}{2\sqrt{\pi}} \epsilon_2$$

we find that the leading order of all terms in (23e) are  $O(\epsilon_2)$ . There results

$$\frac{\delta S}{Nk_B} = \frac{1}{4\sqrt{\pi}} \epsilon_2 > 0. \tag{24}$$

As stated previously, we attribute this change in entropy to the discontinuity in the starting value of the distribution function. To within the stated approximations, (24) represents an entropy change of an isolated system and stems from the entropy integral (1).

It is possible to interpret the result (24) on the basis of the information interpretation of entropy change as described below.

**2.3.3. Information interpretation of entropy change.** The Shannon-Brillouin information interpretation of entropy change states that

$$k_B^{-1} \Delta S = \Delta I. \tag{25}$$

In this relation  $\Delta I$  is the change in missing information accompanying the given process.

Thus, for example, for the system at hand, the result (24) indicates that in the overall expansion the process is accompanied by a net increase of missing information in the system. In this context we note that the term  $-\epsilon_2/4\sqrt{\pi}$  in (23e) may be traced to the attenuated half-Maxwellian (18a), which describes particles moving in a given direction, and contributes to a decrease in missing information when compared to the original state of the system. In a similar vein we see that the positive contribution to (24) stems from the  $-a \ln a$  term in (23c) which may be identified with the canonical gain in missing information due to expansion. For the present example we find that the gain in missing information in coordinate space outweighs the decrease in missing information in velocity space.

### 3. Information transport through a confining wall

Let us return to the entropy equation (12). Expanding the Poisson bracket gives

$$-\frac{1}{k_B} \frac{dS}{dt} = \int d\Gamma \frac{\partial h_N}{\partial t} + \int d\Gamma \sum_{i=1}^N \left( \frac{\partial h_N}{\partial x_i} \cdot \frac{p_i}{m} + \frac{\partial h_N}{\partial p_i} \cdot G_i \right) \tag{26}$$

where  $G_i$  is the force

$$G_i = -\frac{\partial}{\partial x_i} \sum_{n \neq i}^N \Phi(x_i, x_n) \tag{26a}$$

and  $\Phi$  is a two-particle potential. Neglecting, for the moment, the partial time derivative term in (19) and converting the remaining terms to surface integrals gives

$$\frac{1}{k_B} \frac{dS}{dt} = \sum_{i=1}^N \left( \iint d\mathbf{p}^N d\boldsymbol{\sigma}_i \cdot \frac{p_i}{m} |h_N(\boldsymbol{\sigma}_i, \mathbf{p}^N)| + \iint d\mathbf{x}^N d\boldsymbol{\sigma}_i \cdot G_i |h_N(\boldsymbol{\sigma}_i, \mathbf{x}^N)| \right) \tag{27}$$

where  $d\boldsymbol{\sigma}$  is the differential of surface in phase space. The absolute magnitudes in (27) stem from the observation, that, with (8), we find

$$h_N \leq 0 \tag{28}$$

where the equality is satisfied at the endpoints,  $f_N = 0, 1$ .

Hamilton's equations

$$\dot{x}_i = p_i/m \quad \dot{p}_i = G_i$$

(dots denote time derivatives) permit us to interpret the surface integrals in (27) as a flux of  $h_N$  through the respective surfaces in phase space. We wish to apply this interpretation to the following example. We imagine a gas at temperature  $T_G$  confined to a fixed volume by a rigid impenetrable wall. Assuming that  $h_N$  is zero at the bounds of the momentum component of phase space, then only the first surface integral in (27) remains non-zero. Let  $T_w$  denote the temperature of the wall. Consider the case that  $T_w > T_G$ . We may then expect that, on average, the reflected normal velocity components of molecules will be greater than the incident normal velocity components. In this event,  $f_N(\mathbf{p}^N)$  is biased in the direction away from the wall into the gas. From (10) we may infer that  $|h_N|$  is biased in the direction from the gas to the wall. Thus the first integral in (27) will be positive and the entropy will grow. We may interpret this positive surface integral as a flux of information out of the system resulting in an increase in missing information and an accompanying increase in entropy.

For  $T_w < T_G$  a similar argument indicates that the first surface integral in (27) is negative and the entropy diminishes. We may interpret this effect as a positive flux of information into the system, thereby decreasing its missing information with a corresponding decrease in entropy.

These findings are in accord with the first two laws of thermodynamics (Pippard 1966), namely that, at constant volume one obtains

$$T\delta S = \delta E$$

where  $E$  is the internal energy. Thus an infinitesimal increase or decrease in internal energy at constant volume is accompanied by a corresponding increase or decrease in entropy.

#### 4. Conclusions

In this analysis the equation of motion for the Gibbs microentropy was revisited and it was concluded that the derivation which yields constant entropy for isolated systems is inconsistent for systems described by a discontinuous distribution function. It was conjectured that for such cases entropy may not be stationary. Two problems were discussed.

In the first of these, we returned to the *a posteriori* study of the irreversibility of macroscopic phenomena. Here we examined an infinitesimal expansion of a correlationless gas of rigid-sphere molecules encased in a cylindrical cavity which together were taken to comprise an isolated system. Choosing the interval of expansion to be very small compared to the mean free collision time permitted a reasonably consistent kinetic model to be drawn for the process. Variation of the integral expression for the Gibbs entropy yielded an increase in entropy. This result was analysed on the basis of the information theory interpretation of entropy change.

In the event that this decremental change in entropy is realised in a somewhat more realistic but closely allied configuration, one may conjecture that this increase would grow more sharply when collisions come into play at  $\tau \approx l_{\text{MFP}}/C$ . An estimate for the interval of entropy to maximise is given by the Bogoliubov time,  $\tau \approx L/C$  (Bogoliubov 1959, Liboff 1985).

In the second application, the entropic equation of motion (12) was applied to a new description of entropy change in which this change is associated with a flux of information through a confining wall. Thus, for example, a gas enclosed by a wall at a higher temperature than that of the gas was found to have positive information flux out of the system. This process in turn increased the missing information on the system with accompanying increase in entropy.

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#### References

- Abramowitz M and Stegun I A 1970 *Handbook of Mathematical Functions* (New York: Dover)
- Biel J and Rae J (ed) 1972 *Irreversibility in the Many-Body Problem* (New York: Plenum)
- Bogoliubov N N 1959 *Problems of a Dynamical Theory in Statistical Physics* (Providence, RI: Providence College)
- Brillouin L 1956 *Science and Information Theory* (New York: Academic)
- Cercignani C 1969 *Mathematical Methods in Kinetic Theory* (New York: Plenum)
- Ferziger J H and Kaper H G 1972 *Mathematical Theory of Transport Processes in Gases* (Amsterdam: North-Holland)
- Goldstein S and Penrose J 1981 *J. Stat. Phys.* **24** 325
- Grad H 1961 *Commun. Pure Appl. Math.* **14** 323
- Gradsteyn I S and Ryzhik I M 1965 *Tables of Integrals, Series and Products* (New York: Academic)

- Hellerman R G H and Ioos G (ed) 1983 *Chaotic Behaviour in Deterministic Systems* (Amsterdam: North-Holland)
- Janes E T 1957 *Phys. Rev.* **106** 620
- Kac M 1958 *Probability and Related Topics in Physical Sciences* (New York: Interscience)
- Katz A 1967 *Principles of Statistical Mechanics* (San Francisco: Freeman)
- Koga T 1970 *Introduction to Kinetic Theory: Stochastic Processes in Gaseous Systems* (Oxford: Pergamon)
- Kubo R J 1957 *J. Phys. Soc. Japan* **12** 570
- Liboff R L 1974 *J. Stat. Phys.* **11** 343
- 1979 *Introduction to the Theory of Kinetic Equations* (Melbourne, FL: Krieger)
- 1985 *Phys. Rev. A* **31** 1883
- Liboff R L and Heffernan D M 1980 *Phys. Lett.* **79A** 29
- Lindblad G 1983 *Non-Equilibrium Entropy and Irreversibility* (Dordrecht: Reidel)
- McQuarrie D A 1973 *Statistical Mechanics* (New York: Harper and Row)
- Pippard A B 1966 *Elements of Classical Thermodynamics* (Cambridge: Cambridge University Press)
- Prigogine I 1980 *From Being to Becoming* (San Francisco: Freeman)
- Reichl L 1980 *A Modern Course in Statistical Physics* (Austin: University of Texas Press)
- Schuster H G 1984 *Deterministic Chaos* (Weinheim: Physik-Verlag)
- Shannon C E 1949 *Proc. Inst. Radio Eng.* **37** 10
- Sinai Ya G 1967 *Statistical Mechanics* ed A Bak (New York: Benjamin) pp 559–73
- Uhlenbeck G E and Ford G W 1963 *Lectures in Statistical Mechanics* (Providence, RI: American Mathematical Society)
- Wehrl A 1978 *Rev. Mod. Phys.* **50** 221
- Zaslavsky G M 1983 *Chaos in Dynamic Systems* (New York: Harwood)