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Abstract

Previous work has shown that if f_F minimizes Fisher information $I_F[\tilde{f}]$ associated with distribution $\tilde{f}$, then $-I_F[f_F]$ obeys a Gibbs equation and agrees with Jaynesian entropy in equilibrium in a classical fluid. When $\partial \tilde{f}/\partial t$ obeys a Fokker–Planck equation, $I_F[\tilde{f}]$ and also the Tsallis information measure with Tsallis parameter $q = 2$ satisfy H-type theorems for some processes. $-I_F$ has some properties of a statistical entropy model. An exact equation is obtained here for $\partial f_F/\partial t$ and shows that $-\{\partial I_F[f_F]/\partial t\}_{\text{irrev}}$ is not always $\geqslant 0$ in heat conduction or viscous relaxation, so that $I_F[f_F]$ does not satisfy a condition imposed by non-equilibrium thermodynamics. By contrast, similar arguments do not invalidate Jaynesian entropy as a thermodynamic model.

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1. Introduction

In a previous paper [1] a comparison has been made of the Shannon [2] and Fisher [3] measures of information contained in the distribution $\tilde{f}(x)$ for a classical fluid in the space of phase coordinates x. We shall designate these measures by $I_J[f]$ and $I_F[f]$ respectively. If f_J minimizes I_J and f_F minimizes I_F subject to specification of the values of a set of measurable variables, then $-I_J[f_J]$ in the first instance and $-I_F[f_F]$ in the second are functions having at least many of the properties of thermodynamic entropy [4]. The first of these statistical entropy models comes from the work of Jaynes [5] and will be called S_J while the second will be called S_F. f_F has been shown for a gas [6, 7] and for a fluid of interacting particles [1] to agree with the Boltzmann distribution in equilibrium, and S_F agrees in equilibrium with the Jaynesian model. f_F was shown in [4, 6] to agree in non-equilibrium with classical results of Rumer and Rivkin [8]. In the present paper, we examine S_F in non-equilibrium to see whether it satisfies the principle of positive definiteness of irreversible entropy production. Significant cases are found where it does not. If $-I_F[f_F]$ is not a thermodynamic entropy model, this fact has no bearing on the use of $I_F[\tilde{f}]$ as an information measure or on statistical inference based on this measure. The property ascribed to thermodynamic entropy, namely that it increases throughout

an irreversible process occurring at a finite rate in an isolated system (entropy principle), is a requirement in addition to information minimization on which statistical inference is based. In what follows the term *entropy* will always refer to $-I_w[f_w]$ ($w =$ J, F), and the corresponding $I_w[\tilde{f}]$ will be called *information*.

To calculate $S_F[f_F]$, we find the Euler equation for f_F which minimizes $I_F[f_F]$ subject to the available experimental information. This information consists in measured values of a set of variables $\{A_i\}$ where

$$A_i = \int f_F(x)\hat{A}_i(x)\,\mathrm{d}x = \int f(x)\hat{A}_i(x)\,\mathrm{d}x \qquad (1 \leqslant i \leqslant \nu). \tag{1}$$

The operators $\{\hat{A}_i(x)\}$ are functions such as $\hat{H}(x)$, the Hamiltonian, or $\hat{\vec{Q}}(x)$, the heat flux, at point x in phase space. f is the solution of the Liouville equation. The variational problem in the notation used here is

$$\delta I_F[f_F] - \int \mathrm{d}x\, \delta f_F \left[\alpha + \sum_{i=0}^{\nu} \lambda_i \hat{A}_i(x) \right] = 0 \tag{2}$$

where α and $\{\lambda_i(\{A_i\})\}$ are Lagrange multipliers. These are chosen to make the solution of (2) satisfy (1) identically. α assures that f_F is normalized to unity. This variational calculation is described in chapter 3 of [6] and also in [1, 4].

If we set $f_F \equiv \psi^2$, the Euler equation for (2) has the simplified form in the case of an interacting fluid [1, 4]:

$$(4\Gamma_p/\psi)\partial^2\psi/\partial\vec{P}^2 + (4\Gamma_c/\psi)\partial^2\psi/\partial\vec{R}^2 + \alpha + \sum_{i=0}^{\nu} \lambda_i \hat{A}_i(x) = 0 \tag{3a}$$

$$\beta\Gamma_p = \tfrac{1}{2}\mathrm{m} \tag{3b}$$

$$4\Gamma_c = \hbar^2\beta/2m. \tag{3c}$$

The structure of (3a) is discussed in section 2. $\partial\psi/\partial\vec{P}$ and $\partial\psi/\partial\vec{R}$ are $3N$ dimensional gradients, respectively, in the spaces of particle momenta $\{\vec{p}_i\}$ and configuration coordinates $\{\vec{r}_i\}$. (3b) and (3c) with $\beta = (\kappa T)^{-1}$ are values chosen to assure that f_F is the usual canonical distribution in equilibrium if the system interacts weakly with a heat bath at temperature T. κ is the Boltzmann constant.

From (2) we can readily obtain [4] with $S_F = -\kappa I_F[f_F]$, $\lambda_0 = -\beta$, $\hat{A}_0 = \hat{H}(x)$:

$$(1/\kappa\beta)\,\mathrm{d}S_F = -\sum_{i\geqslant 0}(\lambda_i/\beta)\,\mathrm{d}A_i. \tag{4}$$

If we identify S_F with thermodynamic entropy S, $(\kappa\beta)^{-1}$ with thermodynamic temperature T and λ_i/β ($i > 0$) with the thermodynamic force Φ_i associated with A_i, then (4) has the form of the Gibbs equation which is one of the fundamental postulates of non-equilibrium thermodynamics [9]. This identification of $\{\lambda_i\}$ permits us to ascribe thermodynamic significance to the statistical Lagrange multipliers. The thermodynamic forces are defined in such a way that their values are measurable, and so we have a way of measuring $\{\lambda_i\}$. T in thermodynamics is operationally defined. Here $\beta = (\kappa T)^{-1}$ where T is the temperature of the heat bath which is constant and can be measured with a thermometer. Identification of Lagrange multipliers with quantities in the thermodynamic Gibbs equation is common in texts on equilibrium statistical mechanics and has been used in calculating S_J. For $\mathrm{d}S_J$, one has an equation closely resembling (4) which can be compared with the Gibbs equation in the

same way. Interaction with the bath is weak and there is negligible exchange of heat and work with the surroundings; thus there is no work term in the Gibbs equation. The $\{\lambda_i\}$ $(i > 0)$ vanish in equilibrium where S_F is the usual canonical entropy [1], as is also demonstrated by Frieden [6] for a gas. The fact that the model S_F has the property (4) and can generate Legendre transformations of thermodynamic potentials in equilibrium and non-equilibrium has been observed by Frieden [10].

Equation (4) can be used to derive an expression for the rate $\dot{S}_F$ of Fisher entropy production in terms of the rates $\{\dot{A}_i\}$. Exact equations for the time derivatives $\{\dot{A}_i\}$ can be derived from the Liouville equation via a projection operator technique of Robertson [11]. We can use these results to check whether the irreversible part of $\dot{S}_F$ satisfies $\dot{S}_{F,irrev} \geqslant 0$ [9].

It has been shown [12] that if $\tilde{f}(x, t)$ obeys a Fokker–Planck equation, as it does for some systems and processes, then $I_F[\tilde{f}]$ satisfies an H-type theorem [13]. Thus, for the processes in question, $dI_F/dt \leqslant 0$. This is not the same as the entropy principle, because $S_F = -\kappa\, I_F[f_F]$ is not the same as $-\kappa\, I_F[\tilde{f}]$ when we measure only a finite number of variables. However, in a dilute gas, where $\tilde{f}$ obeys the kinetic theory Boltzmann equation and $dI_J[\tilde{f}]/dt \leqslant 0$ [13], the existence of an H-type theorem appears to be a concomitant of the appearance of irreversible behaviour. As we shall find in what follows, by considering a classical fluid for which $\tilde{f}$ obeys the Liouville equation, S_F does not, in general, obey the entropy principle. There may, however, exist an H-type theorem for an information measure dependent on $g(a_1, \ldots, a_\nu)$, a distribution in a-space, the space of numerical values of the $\{\hat{A}_i\}$. Existence of a Fokker–Planck equation or an H-type theorem is not an argument for using $-\kappa\, I_F[f_F]$ as a statistical entropy model in non-equilibrium.

Section 2 summarizes the arguments from [1] to the effect that in many cases, $f_J = f_F + O(\lambda^2)$, for a gas interacting weakly with a heat bath. This shows that f_J and f_F obey the same kinetic equation neglecting non-linear terms which, in a fluid, are negligibly small. In section 3 the exact general kinetic equation for $\partial f_F/\partial t$ is derived, following the method of Robertson [11]. By taking a moment of this equation, we obtain an equation for $\dot{\vec{Q}}$, the rate of change of heat flux $\vec{Q}$. Coefficients of this rate equation do not satisfy a necessary condition for compatibility with the entropy principle. Therefore, in the significant case of heat conduction, S_F is not a model for non-equilibrium thermodynamic entropy.

In section 5, it is shown that, for certain processes in a classical fluid, there are information measures which satisfy an H-type theorem while the distribution corresponding to $\tilde{f}$ obeys a Fokker–Planck equation to a good approximation. The sample space over which the system is distributed is the space of possible values $\{a_i\}$ of the set $\{\hat{A}_i\}$ (fluctuation space). The information measure is not necessarily Fisher entropy. Such an H-type theorem can be proved for an entropy model appropriate to Tsallis statistics [14] even if not for $I_F[\tilde{f}]$. As has been observed, the existence of an H-type theorem does not imply that the entropy principle is satisfied. Where it is not, I_F and f_F may be useful in statistical inference, but not in calculation of thermodynamic potentials.

2. Arguments that f_F can approximate f_J for many processes in gases

In an N-particle fluid in phase space, the Fisher information takes the form [1]

$$I[\tilde{f}] = \Gamma_p \int dx\, \tilde{f}^{-1}[\partial \tilde{f}/\partial \vec{P}]^2 + \Gamma_c \int dx\, \tilde{f}^{-1}[\partial \tilde{f}/\partial \vec{R}]^2. \tag{5}$$

$I[\tilde{f}]$ given here specializes the form given by Frieden [7] for multivariate distributions to the present problem. Γ_p and Γ_c given by (3b) and (3c) assure commensurability of the two terms in (5) and agreement of f_F with the canonical distribution in equilibrium. It should be possible

to make Γ_p and Γ_c equal if $\vec{P}, \vec{R}$ are expressed in terms of dimensionless variables. (5) has been used in (2) to yield the Euler equation (3a) for f_F. Consider, for simplicity, the case where there is one variable A_1 which is a tensor of some arbitrary specified order. Then $\lambda_1 \hat{A}_1$ in (3a) can be written as a contracted tensor product $\lambda_1 \odot \hat{A}_1$. The solution to (3a), to terms linear in λ_1, can be put in the form

$$\psi = \psi_0[1 + \lambda_1 \odot \phi_1] + O(\lambda_1^2) \tag{6}$$

where ψ_0 is the equilibrium solution to (3a) which, in a system in equilibrium with a heat bath, is proportional to a Maxwell–Boltzmann distribution in $\vec{P}$ space. When there are several variables, $\lambda_1 \odot \phi_1$ is replaced by

$$\sum_{k \geqslant 1} \lambda_k \odot \phi_k.$$

In a dilute gas, $\hat{A}_1 = \hat{A}_1(\vec{P})$ and $\phi_1 = \phi_1(\vec{P})$. Putting (6) into (3a), we get for ϕ_1 the equation

$$\hat{O}(\vec{P})\phi_1 \equiv 2[m\kappa T \partial^2 \phi_1/\partial \vec{P}^2 - \vec{P} \cdot \partial \phi_1/\partial \vec{P}] = -\hat{A}_1. \tag{7}$$

This equation is readily solved when $\hat{A}_1$ is an eigenfunction of $\hat{O}(\vec{P})$. If we define $\bar{\vec{p}}_k \equiv \vec{p}_k/(m\kappa T)^{\frac{1}{2}}$, the dimensionless momentum of particle k, and if $H^{(n)}(\bar{\vec{p}}_i)$ is a tensor Hermite function of tensorial order n [15], then

$$\hat{O}(\vec{P})H^{(n)}(\bar{\vec{p}}_i) = -2nH^{(n)}(\bar{\vec{p}}_i). \tag{8}$$

One should note here that the $H^{(n)}$ defined by Grad are not ordinary Hermite polynomials. The $H^{(n)}$ are eigenfunctions of $\hat{O}(\vec{P})$. In the particular case $n = 2$, if $A_{1,ij} = P_{ij}$, the pressure, then the solution of (7), according to (8), is

$$\phi_{1,ij} = \frac{1}{4}\frac{\kappa T}{V} \sum_{i=1}^{N} H_{ij}^{(2)}(\bar{\vec{p}}_k). \tag{9}$$

In the kinetic theory formulated by Grad [16], the pressure and heat flux of a perfect gas are represented by tensor Hermite functions with $n = 2$ and $n = 3$, respectively, with a single contraction in the case of heat flux $\vec{Q}$. Thus

$$V\hat{Q}_i = \frac{1}{2}m^{-\frac{1}{2}}(\kappa T)^{3/2} \sum_{j=1}^{N} \bar{p}_{ji}\left(p_j^{-2} - 5\right)$$

$$= \frac{1}{2}m^{-\frac{1}{2}}(\kappa T)^{3/2} \sum_{j,k} H^{(3)}{}_{ikk}(\bar{\vec{p}}_j) \qquad (i = x, y, z). \tag{10}$$

The corresponding ϕ_1 satisfying (7) is then proportional to the sum on the right-hand side of (10), in the same way that (9) follows when $\hat{A}_1$ is a sum of $H^{(2)}$ functions.

Accordingly, in a dilute gas, as long as $\{\hat{A}_i\}$ are represented as in the Grad theory by tensor Hermite functions $H^{(n)}(\bar{\vec{p}}_k)$, ϕ_i is proportional to $\hat{A}_i$ $(1 \leqslant i \leqslant \nu)$. This is precisely the result we obtain in the linearized Jaynes distribution [5] with ψ_J having the form (6) and with a Lagrange multiplier satisfying

$$\tilde{\lambda}_J = -\lambda_F/n_i \qquad (1 \leqslant i \leqslant \nu). \tag{11}$$

λ_F is the Lagrange multiplier in the Fisher distribution when we measure the same set $\{\hat{A}_i\}$.

Thus we have shown that if the Jaynesian multipliers are related to the Fisher ones by (11), then $f_F = F_J + O(\lambda^2)$ is an exact solution of the Fisher Euler equation (3a) to terms linear

in λ. The functions f_F and f_J are the same, neglecting $O(\lambda^2)$, if the specified information is the same. In section 3 we show that the technique of Robertson [11] can be used to derive an equation for $\partial f_F/\partial t$ which is solved exactly by the solution of the Euler equation. To terms linear in λ, this equation will be the same as the existing equation derived [16] for $\partial f_J/\partial t$. By examining the latter, we can see whether the coefficients in the moment equation for $\partial \vec{Q}/\partial t$ satisfy the conditions for validity of the entropy principle when $\dot{S}_F$ is calculated from (4).

3. Exact equations for $\partial f_F/\partial t$ and $\mathrm{d}\vec{Q}/\mathrm{d}t$

Once one has obtained, by solving (3a) to an arbitrary order in λ, a phase-space distribution $f_F(x)$, the Robertson method [11] readily yields an equation for $\partial f_F/\partial t$ satisfied exactly by this f_F to the same order in λ. Let

$$\dot{f} = -\mathrm{i}\hat{L}f \tag{12}$$

be the Liouville equation, where $\hat{L}$ is the Liouville operator. Let the operators $\{\hat{A}_i(\vec{r}, x)\}$ represent a set of variables such as heat flux or pressure at point $\vec{r}$ in a non-uniform fluid. For an arbitrary integrable phase function $\chi(x)$, define the Robertson operator

$$\hat{P}_{RF}\chi(x) \equiv \sum_i \int \mathrm{d}\vec{r}\{\delta f_F/\delta A_i(t, \vec{r})\}\mathrm{Tr}\{\hat{A}_i(\vec{r}, x)\chi\}. \tag{13}$$

Given that f_F depends on time through its dependence on the variables $\{A_i(t, \vec{r})\}$, we have

$$\dot{f}_F = \sum_i \int \mathrm{d}\vec{r}\{\delta f_F/\delta A_i(t, \vec{r})\}(\partial/\partial t)\mathrm{Tr}\{\hat{A}_i(\vec{r}, x)f\} = \hat{P}_{RF}\dot{f}. \tag{14}$$

Operating with $\hat{P}_{RF}$ on (12), we can find an exact equation for the time derivative of the function f_F obtained by solving (3a).

In terms of $\hat{P}_{RF}$, we can define $\hat{T}_F(t, t')$ which solves

$$\partial \hat{T}_F(t, t')/\partial t' = \mathrm{i}\hat{T}_F(t, t')[1 - \hat{P}_{RF}(t')]\hat{L}. \tag{15}$$

Then from (13)–(15) it follows [17] that

$$\dot{f}_F = -\mathrm{i}\hat{P}_{RF}(t)\hat{L}f_F(t) - \int_0^t \mathrm{d}t'\,\hat{P}_{RF}(t)\hat{L}(t)\hat{T}_F(t, t')[1 - \hat{P}_{RF}(t')]\hat{L}(t)f_F(t'). \tag{16}$$

Multiplying (16) by $\hat{A}_i(\vec{r}, x)$ and integrating over phase space, we obtain rate equations for $\{\dot{A}_i(\vec{r}, t)\}$ which, taken together with the solution of the Fisher Euler equation, provide an exact solution to (16).

In the particular cases described in section 2, e.g. a dilute gas in equilibrium with a heat bath, where $\hat{A}_i = \hat{A}_i(\vec{P})$, it is pointed out that $f_F = f_J$ to leading order in λ. Therefore, to this order $\hat{P}_{RF} = \hat{P}_{RJ}$, and equation (16) is identical to an earlier result [17] for f_J derived from Robertson's work [11]. The linear approximation to (16) and the moment equation for $\vec{Q}$, which suffice for our purposes, have been shown [18] to be more exact than is apparent from the Robertson approach.

Applying the earlier result to a dilute gas where the heat flux operator is given by (10), we multiply (16), in which $\hat{P}_{RF} = \hat{P}_{RJ}$, by $\hat{\vec{Q}}$, given by

$$\hat{\vec{Q}}(\vec{r}, x) = \sum_{i=1}^N \left\{(p_i^2/2m) - \frac{5}{2}\kappa T(\vec{r}_i)\right\}(\vec{p}_i/m)\delta(\vec{r}_i - \vec{r}) \tag{17}$$

to obtain an equation for $\partial \vec{Q}/\partial t$, where $\vec{Q} \equiv \int f \hat{\vec{Q}} \, dx$. The linearized $f_J = f_F + O(\lambda^2)$ has the form (6). To obtain the term in $\dot{\vec{Q}}$ linear in $\nabla_{\vec{r}} T$, we substitute $f_J = \psi_J^2 = \psi_0^2 \left[1 - \int d\vec{r} \tilde{\lambda}_Q(\vec{r}) \hat{\vec{Q}}(\vec{r}, x) \right] + O(\tilde{\lambda}_Q^2)$, with

$$\psi_0^2 = Z^{-1} \exp\left[-\int d\vec{r} \beta(\vec{r}, t) \hat{H}(\vec{r}, x) \right] \tag{18a}$$

$$\hat{H}(\vec{r}, x) = \sum_{j=1}^{N} \left(p_j^2 / 2m \right) \delta(\vec{r}_j - \vec{r}) \tag{18b}$$

into the first term on the right-hand side in (16). Z is a normalization factor, and $\beta(\vec{r}, t) = [\kappa T(\vec{r}, t)]^{-1}$. If $\vec{Q}(\vec{r}, t)$ and $T(\vec{r}, t)$ are the only variables, the linearized moment equation for $\vec{Q}$ obtained from (16) after substitution of (18a) has the form [19]

$$\dot{\vec{Q}} = -(1/\tau_Q)\vec{Q} - K_Q T^{-1} \nabla_{\vec{r}} T \tag{19a}$$

$$K_Q \equiv 5N(\kappa T)^2 / 2Vm. \tag{19b}$$

$\nabla_{\vec{r}} T$ is assumed small, and T in $K_Q T^{-1}$ is a constant average temperature. Equation (19a) is the Cattaneo–Vernotte equation of extended thermodynamics [9].

4. Failure of S_F to satisfy the entropy principle in heat conduction

The heat flux $\vec{Q}(\vec{r}, t)$ at $\vec{r}$ is both a variable and a thermodynamic flux in the formalism of extended thermodynamics [9]. From the matching conditions (1) in which we use the linearized f_J, we find [19] the linearized relation

$$\vec{Q}(\vec{r}, t) = -K_Q \tilde{\lambda}_Q / \beta. \tag{20}$$

Comparison of (19a) and (20) shows that if the thermodynamic force associated with $\vec{Q}$ were $\tilde{\lambda}_Q/\beta$ as in Jaynesian statistics, then the phenomenological coefficient linking the flux $\dot{\vec{Q}}(\vec{r}, t)$ to $\tilde{\lambda}_Q/\beta$ is the negative of the coefficient linking $\dot{\vec{Q}}$ to $-T^{-1}\nabla T$. This anti-reciprocal relation is a necessary condition for positive definiteness of the irreversible entropy production, $\dot{S}_{J,\text{irrev}}$. The Jaynesian entropy production $\dot{S}_J$ is calculated from the Gibbs equation

$$T \, dS_J = \sum_i (\tilde{\lambda}_i / \beta) \, dA_i. \tag{21}$$

From (11) and (20), we deduce

$$\tilde{\lambda}_Q = -\lambda_Q / n = -\lambda_Q / 3 = \beta \phi_{QF} / 3 \tag{22}$$

since $n = 3$. $\phi_{QF} = -\lambda_Q / \beta$ is the thermodynamic force associated with $\vec{Q}$ in Fisher statistics, according to (4). The factor $1/3$ in (22) means that if (22) is substituted into (20), the coefficient of ϕ_{QF} in (20) is not without the coefficient of $T^{-1}\nabla_{\vec{r}} T$ in (19a), and so $\dot{S}_{F,\text{irrev}}$ calculated from (4) will not be positive definite. A similar result follows for the momentum flux, P. We have $\partial P/\partial t$ coupled to the gradient $\nabla \vec{u}$ of mass velocity and also P proportional to $\lambda_P = \beta \phi_{PF}/2$, by analogy with (22).

Thus we conclude that, for heat conduction in a fluid, S_F cannot be used as a statistical model for non-equilibrium thermodynamic entropy. If the phenomenological description does

not involve flows of heat, momentum or particles, this difficulty does not arise. In this case, suppose that

$$\dot{S}_J = \sum_k (\tilde{\lambda}_{Jk}/\beta)\dot{A}_k = \sum_{k,p} \beta^{-2}(\tilde{\lambda}_{Jk} L_{kp} \tilde{\lambda}_{Jp})$$

$$= \sum_{k,p} \beta^{-2}(\tilde{\lambda}_{Fk} L_{kp} \lambda_{Fp}/n_k n_p) \geqslant 0. \tag{23}$$

Then we cannot in general expect that

$$\dot{S}_F = \sum_{k,p} \beta^{-2}\lambda_{Fk} L_{kp} \lambda_{Fp}/n_p \tag{24}$$

will be $\geqslant 0$. Therefore, if the phenomenological equations couple thermodynamic forces associated with variables which are contractions of tensors of different tensorial order, $\dot{S}_F$ will not, in general, satisfy the entropy principle if $\dot{S}_J$ does.

5. Fisher and Jaynes statistics in fluctuation space

Since it has been found in the previous section that $\dot{S}_F$ will not satisfy the entropy principle in many cases, we are led to ask whether this is consistent with the observation [12] that $I_F[\tilde{f}]$ may, for some processes, obey an H-type theorem if $\tilde{f}$ satisfies, to a sufficiently good approximation, a Fokker–Planck equation. The H-theorem in gas kinetic theory is often taken as an embodiment of the second law of thermodynamics in non-equilibrium [20]. To examine this question, we are led to study a distribution occurring in the statistical mechanics of fluids which obeys a Fokker–Planck equation approximately, leading to an approximate H-type theorem very similar to that used in the work of Plastino and Plastino [12].

Consider a fluid which is isolated, so that its phase-space distribution obeys the Liouville equation (12). Here we do not introduce a heat bath which is not essential to the argument. If the measured values are represented by a set $\{\hat{A}_i(x)\}$ of phase functions, the probability $g(a)\,da$ that $\hat{A}_i$ is observed to have a value between a_i and $a_i + da_i$ $(1 \leqslant i \leqslant v)$ has been given by Zwanzig [21] as

$$da \equiv \prod_{i=1}^{v} da_i \tag{25a}$$

$$g(a,t) = \int f(x,t)\psi_a\,dx \tag{25b}$$

$$\psi_a \equiv \prod_{i=1}^{v} \delta(\hat{A}_i - a_i) \tag{25c}$$

$\delta(\hat{A}_i - a_i)$ in (25c) is a Dirac delta, and $f(x,t)$ solves the Liouville equation. The phase-space integration in (25b) is over an energy shell centred at the surface $\hat{H}(x) = E$, where $\hat{H}(x)$ is the Hamiltonian. The equilibrium distributions f_0, g_0 are given by

$$f_0(x) = \tilde{V}_E^{-1} \tag{26a}$$

$$g_0(a) = \tilde{V}_E^{-1} \int \psi_a\,dx \equiv \tilde{V}_E \Gamma(a) \tag{26b}$$

where $\tilde{V}_E$ is the volume of the energy shell. The space of vectors $(a_1, \ldots, a_v)$ will be called 'fluctuation space'. The observed values of the set $\{\hat{A}_i(x)\}$ will fluctuate around the set $\{A_i(t)\}$,

and $g(a, t)$ will be the probability amplitude for observing the values $(a_1, \ldots, a_\nu)$ at time t. We have

$$A_i(t) = \int g(a) a_i \, da = \int \hat{A}_i(x) f(x, t) \, dx \qquad (1 \leqslant i \leqslant \nu). \tag{27}$$

An exact Fokker–Planck-type equation for $\partial g / \partial t$ has been derived by Grabert [22] from the Liouville equation. The derivation introduces the Zwanzig–Grabert projection operators,

$$\hat{P}_Z \chi(x) = \int da \, g_0^{-1} \, \mathrm{Tr}(f_0 \psi_a \chi) \psi_a(x) \tag{28a}$$

$$\hat{P}_Z^T \chi(x) = f_0 \int da \, g_0^{-1} \, \mathrm{Tr}(\psi_a \chi) \psi_a(x) \tag{28b}$$

and the initial condition,

$$\hat{P}_Z f(x, 0) = f(x, 0). \tag{29}$$

One obtains [22]

$$(\partial/\partial t) g(a, t) = -\sum_i (\partial/\partial a_i) \{v_i(a) g(a, t)\} + \int_0^t ds \sum_{i,j} (\partial/\partial a_i)$$

$$\times \int da' \, D_{ij}(a, a', t - s) g_0(a') (\partial/\partial a'_j) \{g(a', x)/g_0(a')\} \tag{30a}$$

$$v_i(a) \equiv \mathrm{Tr}(f_0 \dot{A}_i \psi_a)/g_0(a) \tag{30b}$$

$$\dot{A}_i(x) \equiv i \hat{L} \hat{A}_i(x) \tag{30c}$$

$$D_{ij}(a, a', t - s) \equiv \{g_0(a')\}^{-1} \mathrm{Tr}\{f_0 R_i(a, t) R_j(a', s)\} \tag{30d}$$

$$R_i(a, t) \equiv (1 - \hat{P}_Z)[\exp\{i\hat{L}(1 - P_Z)t\} \dot{A}_i \psi_a]. \tag{30e}$$

In addition to a Fokker–Planck-type equation for $g(a, t)$ which, as we shall point out in the following section, can have a diffusion kernel D_{ij} which is positive definite for some processes, we need an information measure $I(g)$ in a-space. This can be used, via mathematical arguments analogous to those previously discussed [12], to prove an H-type theorem applicable to the processes in question.

Let us consider first the Jaynes distribution $g_J(a)$. In phase space [5],

$$f_J(x) = f_0 Z^{-1} \exp\left[-\sum_k \tilde{\lambda}_k \hat{A}_k\right] \tag{31}$$

where $\{\tilde{\lambda}_k\}$ are the Lagrange multipliers. From (25b), the corresponding distribution in a-space is

$$g_J(a) = \int f_J(x) \psi_a \, dx = g_0 Z^{-1} \exp\left[-\sum_k \tilde{\lambda}_k a_k\right]. \tag{32}$$

This distribution is obtained by minimizing

$$I_J(g) = \int g \ln(g/g_0) \, da \tag{33}$$

subject to

$$A_i(t) = \int g(a) a_i \, da = \int g_J(a) a_i \, da \qquad (1 \leqslant i \leqslant \nu). \tag{34}$$

Thus information measures and associated distributions can exist in a-space which are consistent with (25b).

6. H-type theorems in fluctuation space

Consider the functional

$$\tilde{I}_J[g] \equiv \int da(g^2/g_0). \tag{35}$$

$\tilde{I}_J$ may be said to approximate I_J in the sense that minimizing $\tilde{I}_J$ subject to conditions (34) yields the same result as (33) and (34) with accuracy $O(\tilde{\lambda})$. Higher orders in $\tilde{\lambda}$ are not generally significant in a simple fluid where non-linear effects have been predicted to be negligibly small [23, 24] save in viscoelasticity at high shear rates. As we shall point out in the following section, $\tilde{I}_J$ is the Tsallis information model [14] corresponding to Tsallis parameter $q = 2$.

From (30a) and (36),

$$(\partial/\partial t)\tilde{I}_J[g] = 2 \int da(g/g_0)(\partial g/\partial t) = -2 \sum_i \int (g/g_0)(\partial/\partial a_i)\{v_i(a)g(a,t)\}\, da$$

$$+ 2 \int_0^t ds \int da \sum_{i,j}(g/g_0) \int da'(\partial/\partial a_i)D_{ij}(a,a',t-s)g_0(a')$$

$$\times (\partial/\partial a'_j)\{g(a',s)/g_0(a')\}. \tag{36}$$

Using (30b), we can put the first term on the right-hand side in (36) in the form

$$\int -2 \sum_i (g/g_0)(\partial/\partial a_i)(v_i g)\, da = f_0 \int \sum_i \int (\partial/\partial a_i)(g/g_0)^2 \mathrm{Tr}(\dot{A}_i \psi_a)\, da$$

$$= f_0 \int (g/g_0)^2 \mathrm{Tr}(i\hat{L}\psi_a)\, da = 0. \tag{37}$$

A partial integration serves to put the remaining terms in (36) in the form

$$(\partial/\partial t)\tilde{I}_J = -2 \int_0^t ds \int da \sum_{i,j}(\partial/\partial a_i)(g/g_0) \int da' D_{ij}(a,a',t-s)g_0(a')$$

$$\times (\partial/\partial a'_j)\{g(a',s)/g_0(a')\}. \tag{38}$$

It has been shown by Grabert [22] that

$$D_{ij}(a,a',t-s) = \partial(a-a')[g_0(a)]^{-1}\mathrm{Tr}[f_0\{\dot{A}_i(t)-v_i(a)\}\{A_j(s)-v_j(a)\}] + O(\dot{A}^3). \tag{39}$$

$O(\dot{A}^3)$ is small if the particle interactions are weak.

If $\{\hat{A}_i\}$ are all even under inversion in configuration or momentum space, then all $\{v_i(a)\}$ vanish. We can imagine a process in which D_{ij} is proportional to the integral of a time correlation function $\langle \dot{A}_i(t)\dot{A}_j(t-s)\rangle$. The $\{\hat{A}_i\}$ can be constructed as sums of orthogonal functions, e.g. sinusoidal, so that $D_{ij} = 0$ if $i \neq j$ and so that the time integral of the correlation is $\geqslant 0$. Since $g(a,t)$ is a distribution, $g \geqslant 0$, and so from (36)

$$(\mathrm{d}/\mathrm{d}t)\tilde{I}_J[g] \leqslant 0. \tag{40}$$

The reasoning of (35)–(40) resembles closely that of Plastino and Plastino [12] which can be carried over to prove a similar theorem for $I_F[g]$ provided g belongs to a family of two-parameter solutions to (30a). Suppose that the parameters are ζ_1 and ζ_2 and that the solutions are $g(a, \zeta_1, \zeta_2)$. Take

$$I_F[g] \equiv \Gamma_1 \int da\, g^{-1}(\partial g/\partial \zeta_1)^2 + \Gamma_2 \int da(\partial g/\partial \zeta_2)^2. \tag{41}$$

From the fact that g, $\partial g/\partial \zeta_1$ and $\partial g/\partial \zeta_2$ are all solutions of (30a), then from [12] it follows that if $\Gamma_1 > 0 < \Gamma_2$, then the time derivatives of the terms in $I_F[g]$ are both $\leqslant 0$, and thus $(\mathrm{d}/\mathrm{d}t)I_F[g] \leqslant 0$.

ζ_1 and ζ_2 should be parameters suggested by the symmetries of (30a). We can note from (25b) that if $f = f(x, \zeta_1, \zeta_2)$, then $g = g(a, \zeta_1, \zeta_2)$. Since the Liouville equation is invariant under translations in momentum and configuration space, ζ_1 and ζ_2 can represent these translations. Therefore, an H-type theorem for $I_F[f]$ can exist even where $I_F[f_F]$ is not consistent with the entropy principle.

7. Discussion

It has not been shown that I_F in a fluid never obeys the entropy principle and never has all the properties of thermodynamic entropy. The heat conduction counterexample in section 4 does not apply in a uniform system or when we are not concerned with transport. The demonstration of (22) and (23) will not apply if the set $\{\dot{A}_i\}$ does not involve contracted tensors whose order was different before contraction. What has been shown in earlier work is that the Jaynesian entropy satisfies the anti-reciprocity relation violated by having $n = 3$ in (22) and gives the usual fluctuation–dissipation theorem result for thermal conductivity [25]. Therefore S_J is useful in commonly-encountered cases where S_F is not.

While an H-type theorem applies to $I_F[g]$ and not to the thermodynamic entropy model $I_F[g_F]$ and thus does not support use of the latter, the H-type theorem testifies to the stability of certain solutions of the Fokker–Planck equation which are relevant to the particular processes in question. It has never been possible to show that D_{ij} is positive definite for all exact solutions of the Zwanzig–Grabert equation (37), and the second law of thermodynamics does not appear to imply that all exact solutions must be stable. It has been possible to show [26] that I_J increases in irreversible processes observed over timescales encountered in practice. The relevant distribution is f_J which depends on a finite number of variables which are measured in any given experiment. The H-type theorems refer to a distribution $\tilde{f}$ from which we can calculate an infinite number of moments. Thus in gas-kinetic theory the Boltzmann H-theorem expresses the second law for the case where we can measure an infinite number of moments [27], which does not happen in practice.

Although $I_F[f_F]$, where f_F is the optimal distribution calculated from (3a), is not, in general, a model for thermodynamic entropy, there is no indication in preceding sections that Fisher statistics is not a useful method of statistical inference. $S_F = -\kappa I_F[f_F]$ is required to obey the entropy principle if it is to be used as a model in calculating thermodynamic entropy in one of the formulations of irreversible thermodynamics for which positive definiteness of irreversible entropy production is a basic postulate. There is no such requirement on $I_F[\tilde{f}]$ which is minimized to give f_F. f_F can be used to make useful predictions. f_F from (3a) agrees with f_J to O(λ) for a set $\{A_i\}$ of variables large enough for the linear non-equilibrium description of a classical fluid in equilibrium with a heat bath. One can add to the solution of (3a) a solution of the homogeneous part, which is not dependent on α and $\{\lambda_i\}$. This solution contains adjustable constants whose values can be fitted to information of a different type from the kind contained in specification of $\{A_i\}$, e.g. the measured values of rate constants or relaxation times.

The information measure $\tilde{I}_J[g]$ has been presented as an approximation to I_J in the sense that minimization of $\tilde{I}_J$ yields the Jaynes f_J to terms linear in λ. There is an indication, however, that $\tilde{I}_J$ may have thermodynamic significance in its own right. The 'purity' in a system where W_n is the probability of state n is

$$P_w(\{W_n\}) \equiv \sum_n W_n^2. \tag{42}$$

There is a correspondence [14] between minima of P_w and of I_J, and indeed P_w may at times serve as an effective thermodynamic potential. P_w agrees, to an additive constant, with the Tsallis entropy [14],

$$S_q = \{k/(q-1)\}\left[1 - \sum_n W_n^q\right] \tag{43}$$

for the case $q = 2$.[1] The Tsallis S_2 has been used [18] in obtaining a linearized version of the Robertson formalism [11] which argues that the linear approximation to (16) is more exact than is apparent from the reasoning of Robertson. It has also been shown [28] that by maximizing S_q, one obtains a statistical analogue of the thermodynamic Gibbs equation.

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