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Fisher and Jaynesian statistics compared in the description of classical fluids

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Abstract

Fisher statistics provides an information measure which, like that of Shannon, is a functional of a distribution f . The latter solves an Euler equation to minimize the functional. To make comparison with statistical derivations of extended thermodynamics, calculations by Frieden, Plastino, and collaborators are specialized to the case where f is a phase-space distribution approximating a solution of the Liouville equation. The Euler equations are solved subject to conditions specifying values of internal energy and fluxes, e.g. of heat and momentum. The solution is compared with that of Jaynes which, with information theory, provides an entropy model. The Fisher and Jaynes entropies are identical only in equilibrium. The distributions agree in linear approximation for a restricted set of variables. This set is large enough to embrace all those needed in the classical non-equilibrium description of simple fluids. Fisher–Euler solutions are not unique in non-equilibrium.

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1. Introduction

Information theory, as developed by Jaynes [1], maximizes the Shannon information entropy [2] subject to constraints which constitute the ‘information’, yielding an optimal distribution consistent with these constraints. It has been found [3] that this procedure does not always lead to a useful distribution, and so an alternative variational calculation has been put forward [3, 4] based on the information measure of Fisher [5].

As a functional of $f(x)$, the desired distribution for a variable x , the Fisher information is [5]

$$I = \int dx f^{-1} (df/dx)^2. \quad (1)$$

If I is minimized subject to specification of energy $E = \int dx f(x)E(x)$, one obtains the usual Boltzmann distribution [3]. The statistical theory based on minimizing I is called ‘estimation theory’ [6]. It agrees with other approaches in equilibrium thermodynamic systems and gives

interesting results in other cases, e.g. where the exact microscopic distribution obeys a diffusion equation, for which case one can prove an H -theorem [7].

The distributions agree in linear approximation for a restricted set of variables. This set is large enough to embrace all those needed in the classical non-equilibrium description of simple fluids. The Fisher–Euler solutions are not unique in non-equilibrium.

We proceed to specialize (1) to the case of a pure, N -particle fluid whose phase-space distribution f depends on the configuration coordinates $\vec{R} \equiv \{\vec{r}_i\}$ and momenta $\vec{P} \equiv \{\vec{P}_i\}$ ($1 \leq i \leq N$) of the N particles. Such a system has been used in conjunction with the Shannon–Jaynes approach to provide a statistical entropy model. This model can be used [8–10] to derive the phenomenological equations [11] of non-equilibrium thermodynamics from the Liouville equation via a formalism of Robertson [12] which is exact.

Here we consider the distribution obtained by minimizing the Fisher information (1). Under circumstances where this f agrees with Jaynes in linear approximation, the previous work [11, 12] will still hold to the same level of approximation. It is necessary, however, before drawing conclusions concerning the applicability of earlier statistical results to specify for what choice of variables, e.g. χ in (3), the Jaynes distribution solves approximately the Euler equation of Fisher theory.

We shall find that if the normalization of I is chosen so that the Fisher f agrees with standard results in equilibrium, then the non-equilibrium linearized Fisher and Jaynes distributions will agree for e.g. kinetic components of heat and momentum fluxes in liquids and gases. If collisional transfer components are included, disagreement with Jaynes will occur unless they are treated as separate, independent variables. There are essential differences between Fisher and Jaynes in the predicted thermodynamic potentials and equations of state, and we shall try to bring these out in what follows. Fisher statistics shows promise of predicting the outcome of measurements of quantities that are not thermodynamic. These predictions are in the form of equations of state relating the predicted value of a variable to be measured to known values of a set of variables already measured.

To cast (1) in a form appropriate to an N -particle fluid, we write

$$I[f] = \Gamma_p \int dx f^{-1} [\partial f / \partial \vec{P}]^2 + \Gamma_c \int dx f^{-1} [\partial f / \partial \vec{R}]^2 \quad (2)$$

where $\partial f / \partial \vec{P}$ and $\partial f / \partial \vec{R}$ are the $3N$ -dimensional vectors whose components are, respectively, $\partial f / \partial \vec{P}_i^\alpha$ and $\partial f / \partial \vec{r}_i^\alpha$ ($1 \leq i \leq N$; $\alpha = x, y, z$). The dimensional constants Γ_p and Γ_c are determined in what follows such that minimization of $I[f]$ subject to specification of N and internal energy E will yield an equilibrium result in agreement with other statistical equilibrium models in the classical and thermodynamic limits. This agreement is discussed in section 3. It does not entail the agreement between linearized Fisher and Jaynes distributions in non-equilibrium. That agreement occurs for certain variables which are eigenfunctions of the differential operators in the Euler equation.

More recent formulations of Fisher statistics have used derivatives with respect to the mean values $\{\theta_i\}$ of variables $\{x_i\}$ in the functional I rather than derivatives $\partial f / \partial x_i$. The latter can be used if $f = f(\{x_i - \theta_i\})$. This condition is implicit in what follows. In the fluid that we discuss, the mass centre is fixed and the mass velocity zero, so the $\{\theta_i\}$ vanish.

Once $I[f]$ has been minimized subject to conditions which specify the values of thermodynamic state variables, and we have obtained the optimal distribution f_μ , we might expect that $S_F = -\kappa I[f_\mu]$ ($\kappa =$ Boltzmann constant) is a statistical analogue of thermodynamic entropy. If this is so, then S_F must obey a Gibbs equation relating dS_F to dU and to the differentials of any additional state variables. Such an equation will be given in section 2, based on existing literature. In section 3, the Euler equation for minimization

is derived and solved in equilibrium where f is shown to agree with Boltzmann statistics in the thermodynamic limit. In section 4, a linearized solution to the Euler equation is found for certain non-equilibrium problems, e.g. momentum and heat flow in a dilute gas where the linearized optimal distribution agrees with Shannon–Jaynes.

In a fluid where collisional transfer in transport is taken into account, it is shown, for the case of pressure, that Fisher and Shannon information measures yield differing distributions and, in general, differing physical predictions. It is demonstrated in section 5 that disagreement between the two statistical approaches can be avoided if the kinetic and collisional transfer components are taken to be independent variables and if we modify the usual operator representation for the collisional transfer component in non-equilibrium.

When the distributions differ, so do the non-equilibrium entropies. A discussion is given in section 6. There it is pointed out that whether the Fisher or Jaynes entropy model is to be preferred in non-equilibrium thermodynamics can best be decided by deriving from the Liouville equation dynamical equations for rates of change of state variables and checking consistency with the entropy principle. That will be the subject of a subsequent paper.

2. Gibbs equation

Let us suppose that the thermodynamic description of the system is formulated in terms of a set of state variables

$$r_i = \int f(x) A_i(x) dx \quad (0 \leq i \leq v) \quad (3)$$

where $f(x)$ is a solution of the Liouville equation and the set $\{A_i(x)\}$ are dynamical functions of the phase coordinates collectively denoted by x . In thermodynamics, the set $\{A_i\}$ must include the Hamiltonian \hat{H} so that the $\{\eta_i\}$ include the internal energy. The values $\{\eta_i\}$ are obtained empirically, and the optimal distribution $f_\mu(x)$ minimizes $I[f]$ whilst satisfying conditions (3).

The variational problem for calculation of f can be formulated as

$$\delta I[f] - \int dx \delta f \left[\alpha + \sum_{i=0}^v \lambda_i A_i(x) \right] = 0. \quad (4)$$

Here α and the $\{\lambda_i\}$ are Lagrange multipliers, with the $\{\lambda_i\}$ determined such that, when the variational solution f_μ is substituted into equation (3), the latter are satisfied identically. α provides for the normalization of f_μ . Equation (4) determines the functional derivative of $I[f]$ when $f = f_\mu$. It will continue to hold with $f = f_\mu$ and with δf caused by changes in the variables η_i . Thus

$$dI[f_\mu] = \int dx \delta I / \delta f|_{f=f_\mu} df_\mu = \sum_{i \geq 0} \lambda_i \int dx A_i(x) df_\mu = \sum_{i \geq 0} \lambda_i d\eta_i. \quad (5)$$

For the case of a simple fluid in equilibrium with a heat bath and having a fixed number N of particles in a fixed volume \tilde{V} , there is just one variable, the internal energy U , and one associated function, $A_0 = \hat{H}(x)$, the Hamiltonian, and one Lagrange multiplier, $\lambda_0 = -\beta = -(\kappa T)^{-1}$. However, as a statistical estimation procedure, minimization of $I[f]$ is not limited to equilibrium, and so equation (5) will hold when there are additional state variables $\{\eta_i\}$ ($i > 0$). The $\{\lambda_i\}_{i>0}$ and $\{\eta_i\}_{i>0}$ will vanish in equilibrium. In the formulation known as ‘extended thermodynamics’ [11] these additional variables can include the fluxes of heat, momentum, and particle diffusion in a mixture.

If we suppose that $-\kappa I[f_\mu] = S_F$ is a statistical analogue of thermodynamic entropy, equation (5) becomes

$$T dS_F = dU - \sum_{i>0} (\lambda_i/\beta) d\eta_i \quad (6)$$

which is the usual expression [11] of the Gibbs equation for a fluid confined within rigid boundaries. The thermodynamic ‘forces’ are $\phi_i = -\lambda_i/\beta$ ($1 \leq i \leq \nu$). Equations (5) and (6) have essentially been obtained by Frieden *et al* [13] who show that one can effect a Legendre transformation from U and the set $\{\eta_i\}$ to the $\{\lambda_i\}_{i \geq 0}$ as the set of independent variables. However, such a result is far from conclusive evidence that S_F can be used in non-equilibrium as a thermodynamic entropy analogue. We have shown that S_F is consistent with (6) which is a fundamental postulate of extended non-equilibrium thermodynamics. Much of the mathematics has already been done [13]. What is done here is to define the variables and parameters used in what follows and to cast the results in thermodynamic language.

3. Euler equations for the minimization procedure and equilibrium solution

If we substitute from (2) into (4) and effect a partial integration, we obtain the condition for an extremum:

$$\begin{aligned} \Gamma_p [f^{-2} (\partial f / \partial \vec{P})^2 + (\partial / \partial \vec{P}) \{2f^{-1} (\partial f / \partial \vec{P})\}] + \Gamma_c [f^{-2} (\partial f / \partial \vec{R})^2 \\ + (\partial / \partial \vec{R}) \{2f^{-1} (\partial f / \partial \vec{R})\}] + \alpha + \sum_{i=0}^{\nu} \lambda_i A_i(x) = 0. \end{aligned} \quad (7)$$

The structure of this equation has been discussed in the literature [13]. The form given here is appropriate to the case of an N -particle fluid where the $\{A_i\}$ are the Hamiltonian $\hat{H}(x)$ and additional variables such as fluxes of momentum and energy. We can seek equilibrium and non-equilibrium solutions for f and compare them with the Jaynesian maximum-entropy distribution. Substituting the solutions into the Fisher and Jaynesian entropy functionals, we can see how these differ. In particular, we can see whether, when Γ_p and Γ_c are determined so as to make the equilibrium solutions agree, the Jaynesian f is a solution of (7).

Equation (7) can be simplified in equilibrium, where $i = 0$ is the only term in the sum, if we set [13]

$$f \equiv \psi^2 \quad (8a)$$

$$(4\Gamma_p/\psi) \partial^2 \psi / \partial \vec{P}^2 + (4\Gamma_c/\psi) \partial^2 \psi / \partial \vec{R}^2 + \alpha + \sum_{i=0}^{\nu} \lambda_i A_i(x) = 0. \quad (8b)$$

In equilibrium,

$$\lambda_0 = -\beta = -(\kappa T)^{-1} \quad (9a)$$

$$A_0(x) = \hat{H}(x) = K(\vec{P}) + V(\vec{R}) \quad (9b)$$

$$\lambda_i = 0 \quad (i > 0) \quad (9c)$$

where K and V are respectively kinetic and potential energy functions. The derivatives in (8b) are $3N$ -dimensional Laplacians.

When (9a)–(9c) are used in (8), the equation is separable. We set

$$\psi = \psi_p(\vec{P}) \psi_c(\vec{R}) \quad (10a)$$

$$4\Gamma_p \partial^2 \psi_p / \partial \vec{P}^2 + \{\alpha - \beta K(\vec{P})\} \psi_p = C_\psi \psi_p \quad (10b)$$

$$4\Gamma_c \partial^2 \psi_c / \partial \vec{R}^2 - \beta V(\vec{R}) \psi_c = -C_\psi \psi_c \quad (10c)$$

where C_ψ is a constant, independent of the phase coordinates.

Equations with the structure of (10b), (10c) are found in the literature [13]. They permit us to derive results consistent with the canonical ensemble if Γ_p and Γ_c are appropriately defined. The canonical momentum distribution is

$$\psi_p = C_p \exp \left[-\beta \sum_{i=1}^N (p_i^2/4m) \right] \quad (11)$$

where m is the particle mass. This is a solution of (10b) provided that

$$\beta\Gamma_p = \frac{1}{2}m \quad (12a)$$

$$-\alpha + C_\psi = -3N. \quad (12b)$$

Equation (10c) is a stationary Schrödinger equation, describing a system with energy ε_β , if

$$C_\psi = \beta\varepsilon_\beta \quad (13a)$$

$$4\Gamma_c = \hbar^2\beta/2m. \quad (13b)$$

In the thermodynamic limit, the energy distribution multiplied by the density of states is sharply peaked, and ε_β corresponds to the most probable energy which depends on β . The canonical ensemble in the thermodynamic limit permits calculation of configuration-space averages using ψ_c^2 as the configuration-space distribution, with ψ_c satisfying (10c). Since the classical and quantum density matrices approach each other as $\hbar \rightarrow 0$ and $\beta \rightarrow 0$ [15], we obtain an $f = \psi^2$ consistent with the classical canonical distribution in these limits.

Equation (10c) has been derived by Frieden *et al* [13]. Here we find the equilibrium solution in order to evaluate Γ_p , Γ_c for use in the non-equilibrium case discussed in section 4. Since we are evaluating Γ_c in (13b) to obtain agreement with alternative approaches, the Euler equations given here are not a statistical derivation of quantum mechanics. $\psi_p^2\psi_c^2$ is a classical distribution in both \vec{P} - and \vec{R} -space, and the derivation given here applies only to the classical limit.

Since in equilibrium the result of minimizing the Fisher information agrees with the result of maximizing the Shannon entropy, one should expect the Fisher and Shannon functionals in equilibrium to be equivalent in the classical and thermodynamic limits. From (2), with $f = \psi^2$, we find that

$$\begin{aligned} -\kappa I[f] &= -4\kappa\Gamma_p \int d\vec{P} (\partial\psi_p/\partial\vec{P}) - 4\kappa\Gamma_c \int d\vec{R} (\partial\psi_c/\partial\vec{R})^2 \\ &= 4\kappa\Gamma_p \int \psi_p \nabla_{\vec{P}}^2 \psi_p d\vec{P} + 4\kappa\Gamma_c \int \psi_c \nabla_{\vec{R}}^2 \psi_c d\vec{R} \\ &= \kappa\beta \int \psi_p^2 K(\vec{P}) d\vec{P} - 3N\kappa + \kappa\beta \int \psi_c^2 V(\vec{R}) d\vec{R} - \kappa C_\psi \\ &= \kappa\beta \int f_\mu^{(0)} (K(\vec{P}) + V(\vec{R})) dx - 3N\kappa - \kappa C_\psi \end{aligned} \quad (14)$$

where $f_\mu^{(0)} \equiv \psi_p^2\psi_c^2$ is the equilibrium Fisher distribution. Here we have invoked (10b), (10c). The canonical partition function, when the energy distribution is sharply peaked, is approximately

$$z \cong v_\beta(\varepsilon_\beta) \exp(-\beta\varepsilon_\beta) \quad (15)$$

where v_β is a small number of terms whose energies are close to the peak. If the classical and quantum distributions are equivalent in the $\hbar \rightarrow 0$, $\beta \rightarrow 0$ limits, we should have, with S_J the Jaynesian entropy,

$$f_{\mu}^{(0)}(\vec{P}, \vec{R}) = Z^{-1} \exp(-\beta K(\vec{P}) - \beta V(\vec{R})) \quad (\hbar \rightarrow 0, \beta \rightarrow 0) \quad (16a)$$

$$-\ln f_{\mu}^{(0)} = \kappa\beta(K + V) + \kappa \ln Z \quad (16b)$$

$$\begin{aligned} S_J &= -\kappa \int f^{(0)} \ln f^{(0)} dx = \kappa\beta \int f^{(0)}(K + V) dx + \kappa \ln Z \\ &= -\kappa I[f^{(0)}] + 3N\kappa + \kappa \ln v_{\beta}(\varepsilon_{\beta}). \end{aligned} \quad (16c)$$

In (16c) we have used (14). In equilibrium the Fisher and Shannon entropy functionals differ by a constant, since $v_{\beta} \ll N$.

4. Linear non-equilibrium solution and comparison with Jaynes

In the previous section an equilibrium distribution $\psi_0 = \psi_p \psi_c$ has been obtained and Γ_p, Γ_c determined to make ψ_0 consistent with the canonical ensemble in the thermodynamic limit. It is now possible to consider the case where, in addition to $\lambda_0 = -\beta$, there is a $\lambda_1 \neq 0$ and an associated $A_1(x)$ whose average $\eta_1 = \langle A_1 \rangle$ is a non-equilibrium state variable which, like λ_1 , vanishes in equilibrium. Under these circumstances, equation (8b) becomes

$$(4\Gamma_p/\psi)\partial^2\psi/\partial\vec{P}^2 + (4\Gamma_c/\psi)\partial^2\psi/\partial\vec{R}^2 = -\alpha + \beta(K + V) - \lambda_1 \odot A_1. \quad (17)$$

In general, λ_1 and A_1 are tensors of the same order, with $\lambda_1 \odot A_1$ a fully contracted tensor product. For example, A_1 in the case of pressure is a tensor of rank two and, in the case of heat flux, it is a vector obtained by contraction of a tensor of rank three. If A_1 is pressure, λ_1, η_1 are traceless.

If the solution to (17) can be expanded in powers of λ_1 , the linearized non-equilibrium form should be

$$\psi = \psi_0[1 + \lambda_1 \odot \phi_1] \quad (18)$$

with ϕ_1 a tensor to be determined by substituting the ansatz (18) into (17) and comparing terms linear in λ_1 . In a dilute gas, the dissipative fluxes used as non-equilibrium state variables depend only on \vec{P} . Remembering that ψ_0 solves the terms in (17) which are zero order in λ_1 , we obtain

$$4\Gamma_p[\partial^2\phi_1/\partial\vec{P}^2 - (\beta/m)\vec{P} \cdot \partial\phi_1/\partial\vec{P}] = -A_1. \quad (19)$$

In the Grad theory of dilute gases [16], the heat and momentum fluxes are represented by tensor Hermite functions. To draw general conclusions about the solution of (19) in cases where such a representation is used, let

$$A_1 = \sum_{i=1}^N \bar{c}(\kappa T)^{n/2} H^{(n)}(\vec{p}) \quad (20a)$$

$$\vec{p}_j \equiv \vec{p}_j(m\kappa T)^{-\frac{1}{2}} \quad (20b)$$

where \bar{c} is a constant and $H^{(n)}$ is a Hermite tensor function of order n which may be contracted. In terms of dimensionless momenta, equation (19) becomes

$$2 \sum_{i=1}^N [\partial^2\phi_1/\partial\vec{p}_i^2 - \vec{p}_i \cdot \partial\phi_1/\partial\vec{p}_i] = -\bar{c}(\kappa T)^{n/2} \sum_j H^{(n)}(\vec{p}_j). \quad (21)$$

A particular solution to (21) is found immediately in the form

$$\phi_1 = (\bar{c}/2n)(\kappa T)^{n/2} \sum_j H^{(n)}(\vec{p}_j) = (2n)^{-1} A_1. \quad (22)$$

In this case, A_1 is an eigenfunction of the differential operator in (21), exemplifying the solution considered in equation (8). As Grad has shown [16], all the variables needed to describe the non-equilibrium state and transport in dilute gases can be found by choosing the tensor Hermite functions to represent A_1 . The same Hermite functions can represent the kinetic components of fluxes of momentum and energy in a dense fluid. To find λ_1 to leading order in $\eta_1 \equiv \langle A_1 \rangle$, we substitute (22) into (18) and use the result to calculate λ_1 from (3). This gives, to terms linear in λ_1 ,

$$\eta_1 = \int \psi^2 A_1(\vec{P}) d\vec{P} = n^{-1} \int \psi_0^2 \lambda_1 \cdot A_1 A_1 d\vec{P}. \quad (23)$$

Equation (23) is almost the same as the equation that we obtain via the Shannon–Jaynes approach. The latter yields a linearized distribution of the form (18) if we make the replacements $\lambda_1 \rightarrow -\gamma_1$ in (18) and (6) and $\phi_1 \rightarrow n\gamma_1$, with γ_1 the Lagrange multiplier introduced in maximizing the Shannon entropy. The Jaynesian approach gives (23) with $\lambda_1 \rightarrow -\gamma_1$ and without the factor n^{-1} . Thus

$$-\kappa^{-1}(\partial S_F/\partial n_1) = \lambda_1 = -n\gamma_1 = -n\kappa^{-1}(\partial S_J/\partial n_1) \quad (24)$$

relates the derivatives of the Fisher entropy S_F and the Jaynes entropy S_J when these are used as statistical models of non-equilibrium thermodynamic entropy. If there are several variables η_1, η_2, \dots having different associated values of n , the $O(\eta_j^2)$ non-equilibrium term in S_F will be the corresponding term in S_J multiplied by n_j , and n_j will depend on j . The non-equilibrium $O(\eta^2)$ contributions to S_F and S_J involving Hermite tensors of different tensorial order have different proportionality constants.

However, to terms linear in η_1 , ψ_F and ψ_J are identical. We have to linear terms

$$\psi_F = \psi_0[1 + \lambda_1 \odot \phi_1] = \psi_0[1 - \gamma_1 \odot (n\phi_1)] = \psi_J. \quad (25)$$

So long as we do not identify S_F in non-equilibrium with thermodynamic entropy, the linearized Fisher and Jaynes formalisms give the same physical predictions for a dilute gas. We have shown here only that S_F and S_J disagree as thermodynamic entropy models in non-equilibrium. To choose between them for the calculation of thermodynamic functions, we must derive via the Liouville equation the dynamical equation for $\dot{\eta}_1$ as has been done [8] in the case of Jaynesian entropy. One can then see whether the irreversible part of \dot{S}_F is positive definite.

Whilst the procedures of Fisher and Jaynes yield the same linearized non-equilibrium distribution in the case of dilute gases, where the $\{A_i(x)\}$ can be represented by tensor Hermite functions of \vec{P} , this is no longer the case when $A_i(x)$ depends on the configuration \vec{R} . To see this, consider the potential $\chi_{ij} = \chi(\vec{r}_{ij})$, with $\vec{r}_{ij} \equiv \vec{r}_j - \vec{r}_i$ the position of j relative to i . When A_1 is an operator for pressure, we have $A_1 = A_1^K(\vec{P}) + A_1^R(\vec{R})$, $\phi_1 = \phi_1^K + \phi_1^R$, and A_1 is given by (20a) with $n = 2$ whilst

$$A_1^R = -\frac{1}{2} \sum_{i,j} \vec{r}_{ij} \vec{F}_{ij} + \sum_i \vec{\delta}(i) \kappa T \quad (26a)$$

$$\vec{F}_{ij} = -\nabla_{\vec{r}_i} \chi_{ij} \quad (26b)$$

$$4\Gamma_c [\partial^2 \phi_1^R / \partial R^{\odot 2} - \beta(\partial V / \partial \vec{R}) \cdot (\partial \phi_1^R / \partial R)] = -A_1^R(\vec{R}). \quad (26c)$$

$\vec{\delta}(i)$ is a unit tensor in the configuration space of particle i . To arrive at (26a), we start with the operator (momentum flux multiplied by \vec{V})

$$\hat{P} = \sum_i m^{-1} \vec{p}_i \vec{p}_i - \frac{1}{2} \sum_{i,j} \vec{r}_{ij} \vec{F}_{ij} = \kappa T_i H^{(2)}(\vec{p}_i) + A_1^R(\vec{R}). \quad (27)$$

Thus if $A_1^K(\vec{P})$ is taken proportional to $\sum_i H^{(2)}(\vec{p}_i)$ as in (15), then A_1^R is given by (26a).

Equation (26c) has the solution:

$$\phi_1^R = -(\kappa T/8\Gamma_c) \sum_i \vec{r}_i \vec{r}_i = -(m/h^2)(\kappa T)^2 \sum_i \vec{r}_i \vec{r}_i. \quad (28)$$

This solution is not proportional to $A_1^R(\vec{R})$, and so we do not obtain a distribution in agreement with the Jaynesian one. One can add to ϕ_1^R two solutions, with arbitrary multiplicative constants, of the result of equating to zero the left-hand member of (26c). Predictions of the Fisher approach can be made, by adjusting the constants, to agree with Jaynes in particular cases or with other results such as the fluctuation-dissipation theorem. However, if one can make $\lambda_1 = -\gamma_1$ in this way, then the present result cannot be extrapolated to high dilution. If A_1 is not an eigenfunction of the \vec{p} -dependent operator in the Euler equation, physical predictions of the Fisher and Jaynes distributions will not in all cases be the same, even in linear approximation. This is not wholly unexpected. The question of whether Fisher or Jaynes statistics represents better the behaviour of measured properties of the system is not at issue here, since that needs to be settled experimentally.

The reason that the Fisher and Jaynes distributions are not the same, when collisional transfer is included in the pressure, is that $A_1^R(\vec{R})$ is not an eigenfunction of the differential operator in (26c). $A_1^R(\vec{R})$ could be expanded in eigenfunctions of the operator on the left, and the eigenfunctions taken to be variables. Then, however, there would be an infinity of variables, whereas a thermodynamic description comprises a small number which are measurable. In the following section, we find it possible to represent the collisional pressure by an operator which multiplies A_1^R by a function of \vec{P} . The result is an eigenfunction of the differential operator in (21). Equation (26c) yields a solution of (17) in the form of a sum of powers of \hbar . Terms with \hbar^n ($n \geq 1$) approach zero in the classical limit.

5. Representation for collisional transfer components leading to agreement between linearized Jaynes and Fisher distributions

We have seen in the preceding section that when the collisional transfer component A_1^R is included in the operator A_1 , we do not get an eigenfunction of the operator in (26c). A way around this difficulty is found if we take the kinetic and collisional transfer components of pressure to be independent variables, represented respectively by \hat{P}_k and \hat{P}_c . \hat{P}_k is the operator in (20a), and

$$\hat{P}_c \equiv -\frac{1}{2}m\kappa T \sum_{i,j} (\vec{p}_i^2 - 3)\{\vec{r}_{ij} \vec{F}_{ij} - \frac{1}{3}\vec{r}_{ij} \cdot \vec{F}_{ij} \vec{\delta}\}. \quad (29)$$

$\hat{P}_c \equiv \langle \hat{P}_c \rangle$ is taken to be traceless, so that it relaxes to zero in equilibrium.

If we initially ignore Γ_c and terms $O(\hbar^2)$ in the Euler equation, with a view to taking eventually the classical limit $\hbar > 0$, we find that a solution to the Euler equation (17) is obtained in the form

$$\psi = \psi_0[1 + \lambda_1 \phi_1 + \lambda_c \phi_c] + O(\hbar^2) \quad (30a)$$

$$\phi_c = -\frac{1}{8}m\kappa T \sum_{i,j} \vec{p}_i^2 \{\vec{r}_{ij} \vec{F}_{ij} - \frac{1}{3}\vec{r}_{ij} \cdot \vec{F}_{ij} \vec{\delta}\} \quad (30b)$$

with a term $\lambda_c \hat{P}_c$ now appearing in the right-hand member of the Euler equation, since \hat{P}_c is now an independent variable. λ_c , like λ_1 , is a traceless tensor. \hat{P}_c can be used as a measure of the traceless collisional pressure, $P_c \equiv \langle -\frac{1}{2} \sum_{i,j} \vec{r}_{ij} \vec{F}_{ij} - \frac{1}{3} \vec{r}_{ij} \cdot \vec{F}_{ij} \vec{\delta} \rangle$ since

$$\begin{aligned}\langle \hat{\mathbf{P}}_c \rangle &= 2\lambda_c \sum \psi_0^2 \phi_c \hat{\mathbf{P}}_c \, dx = (\lambda/8)N \langle p_i^2 \rangle_0 (p_i^2 - 3m\kappa T) (\vec{r} \vec{f})^0 \\ &= \frac{3}{4} \lambda N (m\kappa T)^2 (\vec{r} \vec{f})^0 \cong m\kappa T \langle \hat{\mathbf{P}}_c \rangle = m\kappa T \mathbf{P}_c\end{aligned}\quad (31)$$

where $\langle \hat{\mathbf{P}}_c \rangle$ is the traceless collisional pressure and $(\vec{r} \vec{f})^0$ is a traceless dyadic. To terms linear in the λ_s , $\langle \hat{\mathbf{P}}_c \rangle$ proportional to $\langle \hat{\mathbf{P}}_c \rangle$ can be represented by an operator which enters in the same way into both the Jaynes and Fisher distributions. We can prove a similar result for \vec{Q}_c , the collisional component of heat flux. The corresponding operator is

$$\tilde{V} \vec{Q}_c = \sum_i \left[\frac{1}{2} \sum_j \phi_{ij} \vec{\delta} - \frac{1}{2} \sum_j \vec{r}_{ij} \vec{F}_{ij} - \vec{h} \vec{\delta} \right] \cdot \vec{p}_i / m \quad (\vec{h} \equiv \text{enthalpy/particle}) \quad (32)$$

which is a contracted product of the second-rank tensor in square brackets with $m^{-1} H_i^{(1)} = \vec{p}_i / m$. This will be an eigenfunction of the operator in (21) with $n = 1$. If \vec{Q}_c is taken as an independent variable with its own Lagrange multiplier λ_c^q , then (30a) will acquire terms $\lambda_K \hat{\vec{Q}}_K + \lambda_c \hat{\vec{Q}}_c$. Since \vec{Q}_K is a contracted tensor with $n = 3$ and \vec{Q}_c has $n = 1$, we cannot obtain a Jaynesian distribution for a single variable, i.e. $\vec{Q}_K + \hat{\vec{Q}}_c$ with a single Lagrange multiplier. To obtain the Jaynesian λ_s , we must divide λ_K by 3 and λ_c^q by 1.

Accordingly, it is seen that if kinetic and collisional terms for components of dissipative fluxes are treated as independent variables, then in a dense fluid, the linearized Fisher and Jaynes distributions for these variables will agree in non-equilibrium. However, if $\hat{\mathbf{P}}_K + \hat{\mathbf{P}}_c$ and $\hat{\vec{Q}}_K + \hat{\vec{Q}}_c$ are treated in each case as a single independent variable, the linearized Fisher and Jaynes distributions will disagree. If we substitute the $\hbar \rightarrow 0$ solution into the $O(\hbar^2)$ terms in the Euler equation, we obtain a perturbation quantum correction which we need not take into account in a purely classical calculation.

In the following section, we shall point out that if variables are chosen such that the solutions of the Fisher–Euler equations do not solve those of Jaynes, then, in general, the entropy principle will not be satisfied, and so the Fisher entropy will not be a valid model of thermodynamic entropy. In the linear case, we can do this without deriving the general, nonlinear evolution equations of Fisher statistics.

6. Discussion

The foregoing sections describe the application of Fisher statistics [5] to classical fluids with the ultimate objective of possibly using the Fisher information as an entropy model from which we can calculate other thermodynamic potentials. The mathematical properties of Fisher distributions have been discussed extensively in the literature [3–5, 7, 13], and so the original contribution of sections 1–3 of the present paper resides in specializing the variational calculation to the case of a classical n -particle fluid where the arguments of f are \vec{R} and \vec{P} .

It has been established that, for a special set of variables sufficiently broad to comprise all those needed in the existing literature on non-equilibrium thermodynamics of classical fluids, the Jaynesian distribution will solve, in linear approximation, the Euler equation of Fisher statistics as $\hbar \rightarrow 0$.

At this point, we must consider the fact that the linear approximate solutions of Jaynes type are not unique solutions of the Euler equation. To these solutions can be added a solution to the homogeneous equation obtained by equating to zero the right-hand member of (21). This addition can introduce two adjustable parameters into ϕ_1 yielding a distribution non-Jaynesian in linear approximation. Such a distribution, after adjustment of the added parameters such that it predicts observed values of quantities such as relaxation times or transport coefficients,

may yield improved predictions of still other variables $\{\langle X_j \rangle\}$ not appearing in the Jaynesian distribution and not previously measured. The non-Jaynesian solutions of (21) may be statistically useful, but this must be established empirically.

However, if ψ is a linear sum of terms $\lambda_i \phi_i$, as in (30a), one can carry out [8, 12] an exact calculation of linearized evolution equations for the variables $\{\hat{Y}_i\}$, with \hat{Y}_i the operators in the right-hand side of (17). The coefficients in these equations are time correlations of Kubo–Green type. These will fail, in general, to exhibit Onsager symmetry if ϕ_i is not proportional to \hat{Y}_i , since the correlations $\langle \phi_i \hat{Y}_i \rangle$ are asymmetric. Therefore, in an experiment in which we observe the evolution of a small number of state variables, we need to use Jaynesian solutions if the evolution equations are to agree with irreversible thermodynamics. The non-Jaynesian ϕ_i may be useful in predicting the outcome of measurements of additional variables observed in a separate experiment performed under similar conditions.

In the present paper, we have examined solutions of the Euler equation for the Fisher distribution f , and we have found that, in general, the choice of variables for which Jaynes-type solutions are found is the only one consistent with non-equilibrium thermodynamics. Other choices give phenomenological coefficients not consistent, in general, with Onsager–Casimir reciprocity. This does not answer the question of whether Fisher’s information measure is proportional to a model for thermodynamic entropy. To do that, one has to calculate dS_F/dt and show that it is ≥ 0 in a closed system (entropy principle). That will be the subject of a subsequent paper.

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