Fisher-based thermodynamics: Its Legendre transform and concavity properties

B. R. Frieden,¹ A. Plastino,^{1,2,3} A. R. Plastino,^{2,3} and B. H. Soffer^{1,*}
 ¹Optical Sciences, University of Arizona, Tucson, Arizona 85721
 ²Universidad Nacional de La Plata, C.C. 727, 1900 La Plata, Argentina
 ³Argentine National Research Center (CONICET), Buenos Aires, Argentina
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It is shown that the Legendre-transform structure of thermodynamics can be replicated without any change if one replaces the entropy S by Fisher's information measure I. Also, the important thermodynamic property of concavity is shown to be obeyed by I. By this use of the Fisher information measure we develop a thermodynamics that seems to be able to treat equilibrium and nonequilibrium situations in a manner entirely similar to the conventional one. [S1063-651X(99)03707-1]

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I. INTRODUCTION

One of the salient contributions of Shannon's information theory (IT) is a recipe for ascertaining in precise and unambiguous terms the amount of information (the *information measure*) that an observer possesses concerning a given phenomenon in terms of a probability distribution function (PDF). The information content of a normalized probability distribution P(i) (i=1,...,N), where the index *i* runs over the states of the system one is trying to study, is given by Shannon's information measure (IM) [1]

$$S = -\sum_{i=1}^{N} P(i) \ln[P(i)],$$
 (1)

where the choice of the logarithm basis is used to fix the information units. If the basis is 2, then *S* is measured in *bits*.

Jaynes [1] has shown that if one chooses Boltzmann's constant as the informational unit and identifies Shannon's IM with the thermodynamic entropy, then the whole of statistical mechanics can be elegantly reformulated, without any reference to the notion of ensemble, by extremization of Shannon's S, subject to the constraints imposed by the a priori information one may possess concerning the system of interest (the maximum entropy principle) [1]. Now, the phenomenal success of thermodynamics and statistical physics crucially depends upon certain necessary mathematical relationships involving energy and entropy (Legendretransform structure). We will show here that these relationships are also valid if one replaces S by Fisher's information measure (FIM) [2]. As pointed out above, the Legendre structure of thermodynamics constitutes its essential mathematical ingredient, so that it should be of interest to study that structure within a FIM context.

Indeed, much effort has been focused recently upon FIM. The work of Frieden and co-workers [3–11], Silver [12], and Plastino et al. [13-16]. has shed much light upon the manifold physical applications of Fisher's information measure. In that vein we mention that Frieden and Soffer have shown that FIM provides one with a powerful variational principle that yields the canonical Lagrangians of theoretical physics [10]. Additionally, I has been shown to characterize an "arrow of time" with reference to the celebrated Fokker-Planck equation [14]. Moreover, interesting relationships exist that connect FIM and the relative Shannon information measure invented by Kullback [17,18]. These have been shown to have some bearing on the time evolution of arbitrary systems governed by quite general continuity equations [15,16]. Finally, a rather general I-based H theorem has recently been proved [19,20]. FIM is then an important quantity that is involved in many aspects of the theoretical description of nature.

II. FISHER'S INFORMATION MEASURE FOR TRANSLATION FAMILIES

The investigation of the properties and applications of Fisher's information measure to diverse problems in theoretical physics is much in vogue nowadays, mainly due to the pioneering work of Frieden and co-workers [3-11], who have unveiled the manifold physical applications of FIM and clarified its relation to Shannon's logarithmic information measure.

Consider a system that is specified by a physical parameter θ and let $g(x, \theta)$,

$$\int dxg(x,\theta) = 1,$$
 (2)

describe the PDF for this parameter. Fisher's information measure I is of the form

^{*}Mailing address: 665 Bienveneda Avenue, Pacific Palisades, CA 90272.

$$I = \int dx g(x,\theta) \left[\frac{\partial g/\partial \theta}{g(x,\theta)} \right]^2.$$
(3)

The special case of *translation families* deserves special mention. These are monoparametric families of distributions of the form $g(x - \theta)$ which are known up to the shift parameter θ . Following Mach's principle, all members of the family possess identical shape (there are no absolute origins), and here FIM adopts the appearance

$$I = \int dx \frac{1}{g} \left[\frac{\partial g}{\partial x} \right]^2.$$
 (4)

This form of Fisher's measure constitutes the main ingredient of a powerful variational principle devised by Frieden and Soffer [10], which gives rise to a substantial portion of canonical physics. In particular, the existence of a thermodynamics based entirely on Fisher's information has recently been predicted [10,20]. In the considerations that follow we shall restrict ourselves to the form (4) of Fisher's information measure and confirm the above mentioned prediction.

There are two different approaches in current use that employ Fisher's information measure, namely, minimum Fisher information (MFI) [6] and extreme physical information (EPI) [10]. The approaches differ in how the constraint information is used to modify FIM. However, in the following we do not distinguish between the two treatments since for our present purposes they lead to the same result.

III. VARIATIONAL APPROACHES APPLIED TO EXTREMIZING FISHER'S INFORMATION

Our present considerations assume one is dealing with vectors x that belong to \mathcal{R} . Let us focus our attention upon the positive-definite, normalized density (of probability) function $f(x, \theta)$,

$$\int dx f(x,\theta) = 1,$$
(5)

and consider the concomitant *Fisher's information measure* for translation families:

$$I[f] = \int dx F_{\text{Fisher}}(f), \qquad (6)$$

with the functional F_{Fisher} in the particular form

$$F_{\text{Fisher}}(f) = f(x) \left[\frac{\partial f}{\partial x} \middle/ f \right]^2.$$
⁽⁷⁾

Further, assume that for *M* functions $A_i(x)$ the mean values $\langle A_i \rangle$,

$$\langle A_i \rangle = \int dx A_i(x) f(x) \quad (i=1,\ldots,M),$$
 (8)

are *known*, stressing here the fact that the $\langle A_i \rangle$'s depend in a linear fashion upon *f*. These mean values will play the role of thermodynamical variables.

It will be of importance below to assume that our foreknowledge [the M x moments (8)] represents information at some appropriate (fixed) time t. The analysis will use MFI (or EPI) to find the probability distribution $f \equiv f_{MFI}$ that extremizes I subject to prior conditions $\langle A_i \rangle$, Eqs. (5)–(8). The pertinent result will be shown below to be given by the solutions of a Schrödinger-like equation.

Jaynes used the Shannon functional $(F = -f \ln f)$ [1] so that

$$S[f] = -\int dx f \ln f.$$
(9)

This is to be constrained by data inputs using the Lagrange multiplier technique. *Our* Fisher-based extremization problem adopts the appearance

$$\delta_f \Biggl\{ I(f) - \alpha \langle 1 \rangle - \sum_{i}^{M} \lambda_i \langle A_i \rangle \Biggr\} = 0, \qquad (10)$$

i.e.,

$$\delta_f \left\{ \int dx \left(F_{\text{Fisher}}(f) - \alpha f - \sum_{i}^{M} \lambda_i A_i f \right) \right\} = 0, \quad (11)$$

where we have introduced the (M+1) Lagrange multipliers $(\alpha, \lambda_1, \ldots, \lambda_M)$. Variation leads now to

$$\int dx \,\delta f \left\{ (f)^{-2} \left(\frac{\partial f}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left[(2/f) \frac{\partial f}{\partial x} \right] + \alpha + \sum_i^M \lambda_i A_i \right\} = 0$$
(12)

and, on account of the arbitrariness of δf ,

$$\left\{ (f)^{-2} \left(\frac{\partial f}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left[(2/f) \frac{\partial f}{\partial x} \right] + \alpha + \sum_i^M \lambda_i A_i \right\} = 0.$$
(13)

It is clear that the normalization condition on f makes α a function of the λ_i 's. Let then $f_I(x, \vec{\lambda})$ be a solution of Eq. (13), where obviously, $\vec{\lambda}$ is an M (Lagrange multiplier) vector. Our extreme Fisher information is

$$I = \int dx f_{\rm MFI}^{-1} \left[\frac{\partial f_{\rm MFI}}{\partial x} \right]^2.$$
(14)

In what follows and for the sake of a simpler notation, we write

$f_{\rm MFI} \equiv f_I$.

IV. RICCATI EQUATION

Let us now find the general solution of Eq. (13). For the sake of simplicity let us define

$$G(x) = \alpha + \sum_{i}^{M} \lambda_{i} A_{i}(x), \qquad (15)$$

and recast Eq. (13) as

$$\left[\frac{\partial \ln f_I}{\partial x}\right]^2 + 2\frac{\partial^2 \ln f_I}{\partial x^2} + G(x) = 0.$$
(16)

We introduce now the identification [12] $f_I = (\psi)^2$ and the new variable,

$$v(x) = \frac{\partial \ln \psi(x)}{\partial x}; \qquad (17)$$

then Eq. (16) becomes (the prime stands for derivative with respect to x)

$$v'(x) = -\left\{\frac{G(x)}{4} + v^2(x)\right\},$$
 (18)

which is a Riccati equation [21]. Introduction further of [21]

$$u(x) = \exp\left\{\int^{x} dx[v(x)]\right\},$$
(19)

i.e.,

$$u(x) = \exp\left\{\int^{x} dx \frac{d\ln\psi}{dx}\right\} \equiv \psi,$$
 (20)

makes Eq. (16) become a Schrödinger-like equation [21]

$$-(1/2)\psi''(x) - (1/8)\sum_{i}^{M} \lambda_{i}A_{i}(x)\psi(x) = \alpha\psi(x)/8, \quad (21)$$

where the Lagrange multiplier $\alpha/8$ plays the role of an energy eigenvalue, and the sum of the $\lambda_i A_i(x)$ is an effective potential function

$$U(x) = (1/8) \sum_{i}^{M} \lambda_{i} A_{i}(x).$$
 (22)

It is to be remarked here that Fisher's information measure corresponds to the expectation value of the kinetic energy of Schrödinger's equation. This point has been appropriately discussed in Ref. [3]. In a similar vein, an extensive analysis, within the framework of functional density theory, can also be found in [22].

Notice that Eq. (21) has multiple solutions, in contrast with the unique solution one obtains when employing Shannon's entropy in place of FIM [1]. The question is then, which solution to choose? Our solutions will, of course, depend upon the form of the effective potential function U(x). It seems reasonable to assume that the solution leading to the lowest I value is the equilibrium one. The following argument supports such a conclusion.

Consider that x is a velocity and concentrate our attention upon a very simple case of the Boltzmann equation [23]: space-homogeneous solutions f(v,t) that depend only upon the velocity v and the time t. Focus attention upon the number $f(v_1)dv_1$ of particles in the element dv_1 of the space of velocities. This number is decreased by all collisions for which one of the two pertinent initial velocities belongs to dv_1 [the other velocity (v_2) and the kind of collision may be arbitrary]. Conversely, $f(v_1)dv_1$ is increased by all collisions for which one of the final velocities belongs to dv_1 . Here the other final velocity (v_2) and the kind of collision may also be arbitrary. In mathematical terms this reads

$$\frac{\partial}{\partial t}f(v_1)dv_1 = \int_{v_2} (dn' - dn).$$
(23)

Substituting for the numbers dn and dn' the expressions given by Maxwell's ansatz [25] we obtain the simplest instance of Boltzmann's equation, namely [23,26],

$$\frac{\partial}{\partial t}f(v_1) = \int_{v_2} \alpha |v_1 - v_2| [f(v_1')f(v_2') - f(v_1)f(v_2)] dv_2,$$
(24)

where one must remember that v'_1 and v'_2 depend upon v_1 and v_2 (conservation of energy and momentum), and α takes care of units [23].

Now, it is clear that, in equilibrium, $(\partial/\partial t)f(v_1,t)=0$. This implies that f(v) cannot have zeros. Obviously, if, for some v_1 , $f(v_1)=0$, one of the two terms in the integrand above vanishes and the derivative on the left hand side (LHS) cannot vanish for that v_1 value. As a consequence of the multiple solutions of Eq. (21), we are forced to select the one with no nodes. It is a theorem that the ground state solution of Schrödinger equations has no nodes (see, e.g., Ref. [24]). According to the variational equation (10), this solution that we are here choosing has a stationary I value.

V. RECIPROCITY RELATIONS

Standard thermodynamics makes use of derivatives of the entropy *S* with respect to both λ_i and $\langle A_i \rangle$ parameters (for instance, pressure and volume, respectively). In the same way, we are led to investigate analogous properties of $\partial I/\partial \lambda_i$ and $\partial I/\partial \langle A_i \rangle$. It will be seen that Euler's theorem [27] still holds whithin this new, Fisher context.

Starting from Eq. (14) and after a single integration by parts, we find

$$\frac{\partial I}{\partial \lambda_i} = \int dx \frac{\partial f_I}{\partial \lambda_i} \bigg\{ -f_I^{-2} \bigg(\frac{\partial f_I}{\partial x} \bigg)^2 - \frac{\partial}{\partial x} \bigg[(2/f_I) \frac{\partial f_I}{\partial x} \bigg] \bigg\}.$$
(25)

Comparing Eq. (13) to Eq. (25) we immediately gather that

$$\frac{\partial I}{\partial \lambda_i} = \int dx \frac{\partial f_I}{\partial \lambda_i} \left\{ \alpha + \sum_j^M \lambda_j A_j \right\}, \qquad (26)$$

which, on account of normalization, yields

$$\frac{\partial I}{\partial \lambda_i} = \sum_{j}^{M} \lambda_j \frac{\partial}{\partial \lambda_i} \int dx f_I A_j(x), \qquad (27)$$

i.e.,

$$\frac{\partial I}{\partial \lambda_i} = \sum_j^M \lambda_j \frac{\partial}{\partial \lambda_i} \langle A_j \rangle, \qquad (28)$$

which is a generalized Fisher-Euler theorem [28]. The thermodynamic counterpart of Eq. (28) is the derivative of the entropy with respect to the mean values. We easily find

$$\sum_{i} \frac{\partial I}{\partial \lambda_{i}} \frac{\partial \lambda_{i}}{\partial \langle A_{j} \rangle} = \sum_{i} \sum_{k} \lambda_{k} \frac{\partial \langle A_{k} \rangle}{\partial \lambda_{i}} \frac{\partial \lambda_{i}}{\partial \langle A_{j} \rangle}, \qquad (29)$$

$$\frac{\partial I}{\partial \langle A_j \rangle} = \lambda_j \,, \tag{30}$$

as expected. The Lagrange multipliers and mean values are seen to be conjugate variables, related as is typical of λ_i vs $\langle A_i \rangle$ variables in thermodynamics.

It is also clear that

$$f_I \equiv f_I(\lambda_1, \dots, \lambda_M), \tag{31}$$

since, based on the M mean values that constitute our *a priori* knowledge, the extremization process renders f_I a function of the Legendre multipliers only.

VI. LEGENDRE STRUCTURE

In thermodynamics it is equivalent to have as input information either the chemical potential or the number of moles, the pressure or the volume, etc. This is so because of the characteristic Legendre structure of thermodynamics. Now, as our density f_I formally depends upon M+1 Lagrange multipliers, normalization

$$\int dx f_I = 1 \tag{32}$$

makes α a function of the *M* remaining λ 's:

$$\alpha = \alpha(\lambda_1, \ldots, \lambda_N). \tag{33}$$

It is also of importance to stress that, of course, the λ 's and the $\langle A_i \rangle$'s play reciprocal (symmetrical) roles within thermodynamics [29,30]. It is thus possible to assume, as initial conditions, that the input information refers to the λ 's and not to the $\langle A_i \rangle$'s [29,30]. The *M* Lagrange multipliers and the *M* mean values are then on an equal footing for the purpose of determining *I*.

Introduce now the generalized thermodynamic potential (the Legendre transform of I)

$$\lambda_J(\lambda_1,\ldots,\lambda_N) = I(\langle A_1 \rangle,\ldots,\langle A_N \rangle) - \sum_{i=1}^N \lambda_i \langle A_i \rangle, \quad (34)$$

i.e., the Legendre transform of FIM [27]. We have

$$\frac{\partial \lambda_J}{\partial \lambda_i} = \sum_{j=1}^M \frac{\partial I}{\partial \langle A_j \rangle} \frac{\partial \langle A_j \rangle}{\partial \lambda_i} - \sum_{j=1}^M \lambda_j \frac{\partial \langle A_j \rangle}{\partial \lambda_i} - \langle A_i \rangle = -\langle A_i \rangle,$$
(35)

where Eq. (30) has been used.

With the latest relation the Legendre structure here described can be summed up as follows:

$$\lambda_{J} = I - \sum_{i=1}^{M} \lambda_{i} \langle A_{i} \rangle,$$
$$\frac{\partial \lambda_{J}}{\partial \lambda_{i}} = - \langle A_{i} \rangle,$$

$$\frac{\partial I}{\partial \langle A_i \rangle} = \lambda_i,$$

$$\frac{\partial \lambda_i}{\partial \langle A_j \rangle} = \frac{\partial \lambda_j}{\partial \langle A_i \rangle} = \frac{\partial^2 I}{\partial \langle A_i \rangle \partial \langle A_j \rangle},$$
(36)

$$\frac{\partial \langle A_j \rangle}{\partial \lambda_i} = \frac{\partial \langle A_i \rangle}{\partial \lambda_i} = -\frac{\partial^2 \lambda_J}{\partial \lambda_i \partial \lambda_i}.$$
(37)

As a consequence of the last relation we can recast Eq. (28) in the form

$$\frac{\partial I}{\partial \lambda_i} = \sum_j^M \lambda_j \frac{\partial}{\partial \lambda_j} \langle A_i \rangle. \tag{38}$$

The Legendre-transform structure of thermodynamics is thus seen to be entirely translated into the Fisher context.

VII. CONCAVITY OR MIXING PROPERTY

In order to be able to construct a thermodynamics based upon I, it is necessary to examine the concavity or convexity nature of I [27]. We prove below that I is a concave functional [17] of the probability distribution p. Therefore, I exhibits the desirable mixing property.

Let a, b be two real scalars such that a+b=1, p_1, p_2 two normalized probability distributions, and consider

$$\psi = \sqrt{ap_1 + i\sqrt{bp_2}},\tag{39}$$

so that

$$|\psi|^2 = ap_1 + bp_2. \tag{40}$$

We study now the properties of a third probability distribution

$$P = |\psi|^2 = ap_1 + bp_2, \tag{41}$$

whose associated Fisher information for translation families reads (the prime stands for derivative with respect to x)

$$I(P) = \int dx P^{-1} P'^{2} = 4 \int dx \frac{d|\psi|^{2}}{dx}.$$
 (42)

In order to investigate the convexity question we must find the relationship relating I(P) to $aI(p_1)+bI(p_2)$ [17]. If we set now

$$\psi(x) = R(x) \exp[iS(x)], \qquad (43)$$

R,S two real functions in \mathbb{R} , we immediately find

$$I(P) = 4 \int dx R'^2 = \int dx P(x) \left[\frac{R'(x)}{R(x)} \right]^2 = 4 \left\langle \left[\frac{R'}{R} \right]^2 \right\rangle.$$
(44)

Now, it is easy to see that

$$\frac{d\psi}{dx} = (1/2)(\sqrt{a/p_1}p_1' + i\sqrt{b/p_2}p_2'), \qquad (45)$$

so that

$$\left|\frac{d\psi}{dx}\right|^2 = (1/4)[(a/p_1)(p_1')^2 + (b/p_2)(p_2')^2], \quad (46)$$

which implies

$$aI(p_1) + bI(p_2) = 4 \int dx \left| \frac{d\psi}{dx} \right|^2$$
. (47)

Now, on account of Eq. (43), it is clear that

$$\left|\frac{d\psi}{dx}\right|^{2} = R'^{2} + R^{2}S'^{2} = R'^{2} + |\psi|^{2}S'^{2}, \qquad (48)$$

which leads to

$$aI(p_1) + bI(p_2) = I(P) + 4 \int dx [|\psi|^2 S'^2].$$
(49)

The integral on the RHS of the preceding equation is clearly ≥ 0 , which allows one to assert that

$$aI(p_1) + bI(p_2) \ge I(ap_1 + bp_2);$$
 (50)

i.e., Fisher information for translation families is indeed a concave functional of the probability distributions. A generalization of the last equation easily follows. Assume $b_1 + b_2 = 1$ and

$$p_2 = b_1 p_{21} + b_2 p_{22}. \tag{51}$$

Then, Eq. (50) implies

$$I(ap_1+bb_1p_{21}+bb_2p_{22}) \leq aI(p_1)+bb_1I(p_{21})+bb_2I(p_{22}),$$
(52)

since $a + b(b_1 + b_2) = 1$.

The RHS of Eq. (50) represents the net probability, after mixing, of two distinct systems. It should be mentioned here that the approach can be generalized in the same fashion to a mixture theorem for N systems. We see that I displays the same mixing property as does Boltzmann's entropy. The inequality (50) is a special instance of Fisher's I theorem,

$$\frac{dI}{dt} \leq 0, \tag{53}$$

predicted in [31] and proved in [19].

VIII. CONCLUSIONS

The entire Legendre-transform structure of thermodynamics has been expressed using Fisher information in place of Boltzmann's entropy. In general, this abstract Legendre structure constitutes an essential ingredient that allows one to build up a statistical mechanics. Fisher information I allows then for such a construction. The desired concavity property obeyed by I further demonstrates its utility as a statistical mechanics generator.

It is becoming increasingly evident [3-6,10,13,14,19,20] that Fisher information is vital to the fundamental structure of physics. In this paper we have shown how the concept lays the foundation for a thermodynamics, as well. In the same way that Boltzmann entropy is normally used to define extrinsic parameters such as temperature, etc., so we can likewise expect Fisher information to define its own extrinsic parameters [20]. The two sets of parameters will be different in general. This will be the subject of future publications.

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