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Fisher Information and Quantum Mechanics

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ABSTRACT

A suggestive relation links Fisher' information measure (FIM) *I* and Schrödinger equation (SE). The connection is based upon the fact that the constrained minimization of *I* leads to a SE. This, in turn, is the origin of intriguing relationships between various aspects of SE, on the one hand, and the formalism of statistical mechanics derived from Jaynes's maximum entropy principle (MaxEnt), on the other one. The link entails the existence of a Legendre transform structure underlying the SE, which allows for the emergence of two first-order differential equations that must, respectively, be satisfied by i) the Fisher measure and ii) the SE energy eigenvalues. The complete A) *I*-solution and B) energy-solution are both obtained bypassing the SE and, furthermore, linked by the Legendre structure.

Keywords: Fisher information; MaxEnt; legendre structure; reciprocity relations; Virial theorem; Hellmann-Feynman theorem.

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1. INTRODUCTION

The bridge linking Information Theory and Thermodynamics - Statistical Mechanics was erected by Jaynes half a century ago (Jaynes, 1957; Katz, 1967). It is supported by a variational approach that entails extremization of Shannon's information measure subject to the constraints posed by the *a priori* knowledge one may possess concerning the system of interest. The entire edifice of statistical mechanics can be constructed if one chooses Boltzmann's constant as the informational unit and identifies Shannon's information measure S with the thermodynamic entropy. The concomitant methodology is referred to as the *Maximum Entropy Principle* (*MaxEnt*) (Jaynes, 1957; Katz, 1967). In the 90's a similar program was successfully developed that replaces Shannon's information measure S by Fisher's one (FIM) I (see, for instance (Frieden, 1990; Nikolov and Frieden, 1994; Frieden and Soffer, 1995; Plastino and Plastino, 1995,1996,1997; Plastino et al., 1997; Plastino et al., 1998; Frieden, 1998, 2004; Frieden et al., 1999; Flego et al., 2003)). A new viewpoint was in this way provided within the so-called Wheeler's program of establishing an information theoretical foundation for the basic theories of physics (Wheeler, 1991). Much effort has been expended upon FIM-applications. A not exhaustive small sample is that of refs.(Pennini and Plastino, 2005; Nagy, 2006, 2007; Sen et al., 2007; Lopez-Rosa et al., 2008; Frieden and Soffer, 2009; Ubriaco, 2009; Pennini et al., 2009a, 2009b; Hernando et al., 2009, 2010; Olivares et al., 2010; Kapsa et al., 2010).

Now, the thermodynamical formalism is characterized by its Legendre transform structure (Callen, 1960; Desloge, 1968). Legendre transformations allow one to express fundamental thermal equations in terms of a set of independent variables chosen to be convenient for a given problem (Callen, 1960; Desloge, 1968). In a more general context, Legendre transform structures arise naturally in physical theories or models that are based upon entropic or information theoretical optimization principles. An example is that of references (Curado and Plastino, 2005, 2007; Plastino and Curado, 2006; Curado et al., 2010), that purport to rederive, on such a basis, the principles of statistical mechanics. At its core one finds a variational technique involving extremization of Shannon's logarithmic information measure S subject to constraints imposed by the *a priori* knowledge at one's disposal. The concomitant procedure is automatically endowed with the Legendre-transform structure of thermodynamics (Plastino and Plastino, 1997), that in fact constitutes its essential formal ingredient (Desloge, 1968).

Here we will review the Fisher's information measure (FIM) I-counterpart of the entropy-linked MaxEnt approach. The two approaches, Shannon's and Fisher's, are seen to result in a set of first-derivative relations (the Legendre structure) that involve i) the Lagrange multipliers that emerge from the variational process, ii) the information quantifier (S or I), and iii) the expectation values that constitute the input, a-priori information on the system of interest.

We emphasize that in the Fisher's case a Schrödinger-like equation is involved (Reginatto,1998; Frieden et al., 1999; Flego et al., 2003), a fact of paramount importance which is employed to pave the way for going way beyond thermodynamics by constructing an intriguing connection with celebrated theorems of quantum mechanics (Flego et al., 2011b, 2011c, 2011d, 2011e, 2011f). One of the more intriguing result appears when fundamental consequences of the Schrödinger equation (SE), such as the Hellmann-Feynman and Virial theorems, can be re-interpreted in terms of a special kind of reciprocity relations between relevant physical quantities similar to the ones exhibited by the thermodynamics' formalism (Flego et al., 2011b). This fact demonstrates that a Legendre-transform structure (LTS) underlies the non-relativistic Schrödinger equation.

The LTS, in turn, has been proved to lead in natural fashion to a differential equation for *I* (Flego et al., 2011c). Such equation can be analytically solved. The solution encodes the available prior knowledge concerning the system at hand in terms of adequately selected expectation values. Thus, such solution adds to the rather large Fisher literature a general, explicit expression for that particular FIM I_{Extr} that arises out of any constrained *I*-extremization problem. Note that, once in possession of this I_{Extr}, one does not need to ever address any explicit extremization task nor to solve the FIM-associated Schrödinger equation.

To better understand why this is of importance one should recall that Fisher's information and Shannon's entropy play complementary roles (Frieden, 1998, 2004). The former is convex, the later concave. When one grows, the other diminishes, etc. The associated Shannon's MaxEnt problem has as its solution, always, an exponential form that contains those physical quantities whose mean values are a priori known. The solution of the FIM minimization problem is instead a Schrödinger like differential equation (Reginatto, 1998; Frieden et al., 1999), whose solutions exhibit panoply of mathematical forms. A universal form for I_{Extr}, expressed in terms of those mean values that are a priori known, filling thus a gap in the literature of the physics of information. Moreover, the connection between the Fisher's Information measure via Schrödinger's wave equation to the Hellmann-Feynman theorem lead to the conclusion that a lot of quantum problems have got associated one FIM (Flego et al., 2011d) and the Legendre structure allows one to obtain a first-order differential equation that energy eigenvalues must necessarily satisfy (Flego et al., 2011e). From this particular equation a complete (in mathematical terms) solution for SE's eigenvalues can be obtained. By appeal to the Cramer Rao bound (Rao, 1945; Cramer, 1946) it is possible to Fisher-infer that particular solution that yields the eigenvalues without explicitly having to solve Schrödinger's equation. Remarkably enough, and in contrast with standard SE-variational approaches, the present procedure does not involve any free (fitting) parameter (Flego et al., 2011f). Once in possession of the extremal *I*, one does not need to ever address any explicit *I* -extremization task nor solve the FIM-associated Schrödinger equation, a fact that should be of interest to the Fisher practitioners.

2. CONNECTIONS BETWEEN SHANNON'S AND FISHER'S MEASURES

Consider the normalized probability density (PDF) describing a system of interest

$$f(x;\theta) = \psi(x;\theta)^2 \tag{1}$$

characterized by a given physical parameter θ and a probability-amplitude ψ. Generally speaking, information measures are functionals of the PDF that assign to it a real number indicative of its informational content. Specifically, Fisher's Information Measure (FIM) I was defined in the 20's as (Frieden, 1998, 2004)

$$I = \int dx\, f(x;\theta)\left\{\frac{\partial}{\partial\theta}\ln[f(x;\theta)]\right\}^2 . \tag{2}$$

The idea for using it is to estimate the value of θ on the basis of measurements of *x* (Frieden, 1998, 2004). Consider that the PDF *f* is unknown. One wishes to determine it, makes a measurement, and obtains a value, say x_1, of *x*. Now we have to best infer θ from this isolated measurement. Let us call the resulting estimate $\theta_{est} = \theta_{est}(x_1)$. How well θ can be determined? Estimation theory asserts (Frieden, 1998, 2004) that the best possible estimator $\theta_{est}(x)$, after a very large number of samples (*x*-values) is examined, suffers a mean-square error e^2

$$e^2 = \int dx\, f(x,\theta)[\theta - \theta_{est}(x)]^2, \tag{3}$$

that obeys a relationship, called the Cramer-Rao bound, involving Fisher's Information Measure I. One has (Frieden, 1998, 2004)

$$e^2 \geq 1/I. \tag{4}$$

Eq. (3) gives the variance *Var(x)* of *x*. If one defines a ``Fisher length'' $\delta x = 1/\sqrt{I}$, that quantifies the length scale over which *f* varies in a significant fashion, the Cramer-Rao bound may then be recast as a length inequality

$$e \geq \delta x \tag{5}$$

for the root mean square deviation *e* of x.
The simplest and most fundamental $\theta-$instance is that of translational families, mono-parametric distribution families of the type

$$f(x + ò). \tag{6}$$

Given any *f(x)* we generate a translational family consisting of the densities $f(x + ò)$ resulting from uniform translations of the original density *f(x)*. Since here the parameter ε is additive with respect to *x*, the parameter-derivative appearing in the *I*-definition reduces to the derivative *f(x)* of *f* with respect to itself. Accordingly, this FIM does not explicitly involve any structural parameters (of *f*). Now FIM adopts the form (remember $f = \psi^2$ according to (1)) (Frieden, 1998, 2004)

$$I = \int dx\, f(x) \left\{ \frac{\partial}{\partial x} \ln[f(x)] \right\}^2 = 4 \int dx\, \vec{\nabla} \psi \cdot \vec{\nabla} \psi . \tag{7}$$

This particular FIM-form is very important in physical applications. Indeed, it constitutes the main ingredient of a powerful variational principle devised by Frieden and Soffer (FS), that gives rise to a substantial part of (today's known) Physics ((Frieden, 1998, 2004) and references therein). Here we employ these translational families in implementing the principle according to which FIM is extremized with adequate constraints, the so-called minimum Fisher information (MFI) approach (see refs. Frieden, 1998, 2004; Frieden et al., 1999, for more details). Consequently, one assumes that the pertinent PDF is of the form (6).

Some interesting relationships have been recently established between Fisher's and Shannon's measures. The information measure of Fisher's places an upper bound to the entropy increase for a wide variety of processes, namely, those in which the pertinent probability distribution is governed by a continuity equation, as shown by Plastino and Plastino in (Plastino and Plastino, 1995). The bound is of the form

$$\left|\frac{dS}{dt}\right| \leq constant\ \sqrt{I}. \tag{8}$$

Consider now diffusion equations (the paradigm of irreversible behavior). Plastino, Plastino, and Miller have uncovered some important relationships (Frieden et al., 1999). For instance,

$$\frac{dS}{dt} = I \geq 0, \tag{9}$$

and

$$\frac{d^2S}{dt^2} = \frac{dI}{dt} \leq 0, \tag{10}$$

from which one gathers that (Frieden et al., 1999)

$$S_{t=0} \leq S(t) \leq S_{t=0} + (t-t_0)\, I_{(t=0)}\ . \tag{11}$$

Thus, *S* and *I* are intimately related. It is clear that *I* regulates the entropy growth. Parenthetically, it should be mentioned that a direct relationship links *I* to the Kullback-Leibler relative entropy *K* between two probability distributions *f(x)* and *f(x+ε)*. One has (Frieden, 1998, 2004)

$$K[f(x+\epsilon) \,||\, f(x)] \propto \epsilon^2 I + \text{higher order terms in } \epsilon. \tag{12}$$

3. EXTREMIZING FISHER'S INFORMATION MEASURE

In the remainder of the paper we will consider a system that is specified by a set of *M* parameters μ_k which are the mean values of *M* relevant physical quantities,

$$\mu_k = \langle A_k \rangle \qquad \text{with} \qquad A_k = A_k(x) \quad (k = 1,...,M).$$

The set of μ_k-values constitute the prior knowledge. This is empirical information that someone has measured. Let the pertinent probability distribution function (PDF) be *f(x)*. Then,

$$\langle A_k \rangle = \int dx\, A_k(x) f(x), \qquad k = 1,\ldots,M. \tag{13}$$

In this context, it is well-known (Frieden et al., 1999) that the relevant PDF *f(x)* extremizes the FIM (7) subject to i) the prior conditions (13) and, of course, ii) the normalization condition

$$\int dx\, f(x) = 1. \tag{14}$$

The reader may perhaps wonder why do we extremize *I* instead of Shannon's *S*. This is because in the latter case the PDF-result is always of Gaussian form. This is good enough for many purposes, but nor for all. For instance, power-law PDFs are excluded in this way. Working with *I* allows for a much greater degree of versatility because the variational process leads to a differential equation and not to a fixed functional form (Frieden et al., 1999). Consequently, we briefly review now the formalism developed in ref. (Frieden et al., 1999). The MFI approach adopts the appearance

$$\delta\left(I-\alpha\int dx\, f(x)-\sum_{k=1}^{M}\lambda_k\int dx\, A_k(x)\, f(x)\right)=0 \quad (15)$$

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

$$\left[\frac{1}{f^2}\left(\frac{\partial f}{\partial x}\right)^2+\frac{\partial}{\partial x}\left(\frac{2}{f}\frac{\partial f}{\partial x}\right)\right]+\alpha+\sum_{k=1}^{M}\lambda_k\, A_k(x)=0 \quad (16)$$

To put the above equation into a more manageable form (Richards, 1959; Silver, 1992; Frieden et al., 1999), we introduce the function $\psi(x)$ via the identification $f(x)=|\psi(x)|^2$ so that Eq.(16) acquires the SE-aspect

$$-\frac{1}{2}\nabla^2\psi-\sum_{k=1}^{M}\frac{\lambda_k}{8}A_k\,\psi=\frac{\alpha}{8}\,\psi, \quad (17)$$

which can be formally interpreted as a Schrödinger wave equation (SE) for a particle of unit mass moving in the potential

$$U=U(x)=-\frac{1}{8}\sum_{k=1}^{M}\lambda_k\, A_k(x)\,. \quad (18)$$

We see that in order to find the adequate PDF one has to solve the above wave-equation. In it the Lagrange multiplier ($\alpha/8$) plays the role of an energy eigenvalue $E=\alpha/8$. The Lagrange parameters λ_k are fixed following Jaynes, of course (Katz, 1967), by recourse to the available prior information. Notice that the eigen-energy $\alpha/8$ yield automatically the value of the Lagrange multiplier associated to normalization. The solutions ψ provide us with the desired PDF via

$$|\psi(x)|^2=f(x)\,. \quad (19)$$

3.1 Finding a Convenient Way of Actually Manipulating FIM

In one dimensional scenarios (or for the ground state of a real potential in N dimensions (Bates, 1961; Greiner and Müller, 1988)) $\psi(x)$ is guaranteed to be real, a fact useful for establishing a new way of expressing Fisher's information measure as a function of ψ. One substitutes $f(x)=\psi(x)^2$ into Eq. (7) to find

$$I=\int dx\,\psi^2\left(\frac{\partial\ln\psi^2}{\partial x}\right)^2=4\int dx\left(\frac{\partial\psi}{\partial x}\right)^2=-4\int\psi\frac{\partial^2}{\partial x^2}\psi\, dx \quad (20)$$

Now, using the SE (17) one discovers that

$$I=\int \psi \left(\alpha+\sum_{k=1}^{M} \lambda_k A_k\right)\psi\, dx. \quad (21)$$

Finally, the prior conditions (13) and the normalization condition (14) allow one to express *I* in the quite convenient fashion

$$I=\alpha+\sum_{k=1}^{M} \lambda_k \left\langle A_k \right\rangle. \quad (22)$$

4. FISHER THERMODYNAMICS

4.1 The Reciprocity Relations

The reciprocity relations given in the Appendix A (see (112)) and their Fisher-counterparts are an expression of the so-called Legendre-transform structure of thermodynamics (Plastino and Plastino, 1997; Pennini and Plastino, 2005) that indeed constitute its essential formal ingredient (Desloge, 1968). It has been proved by us that they also hold for the Fisher treatment. Standard thermodynamic makes use of the derivatives of the entropy *S* with respect to both the λ_k and $\langle A_k \rangle$ quantities (for instance, pressure and volume, respectively).

As just stated, analogous properties of $\partial\alpha / \partial\lambda_k$ and $\partial I / \partial\langle A_k \rangle$ are valid as well (Frieden et al., 1999). To see why, we start recasting (22) in a fashion that emphasizes the role of the relevant independent variables

$$I(\langle A_1 \rangle,\ldots,\langle A_M \rangle) = \alpha+\sum_{k=1}^{M} \lambda_k \langle A_k \rangle . \quad (23)$$

The Legendre transform changes the identity of the relevant variables, and as for we have

$$\alpha(\lambda_1,\ldots,\lambda_M) = I-\sum_{k=1}^{M} \lambda_k \langle A_k \rangle , \quad (24)$$

so that we encounter the three reciprocity relations proved in (Frieden et al., 1999)

$$\frac{\partial\alpha}{\partial\lambda_i}=-\langle A_i \rangle \; ; \qquad \frac{\partial I}{\partial\langle A_k \rangle} = \lambda_k \; ; \qquad \frac{\partial I}{\partial\lambda_i}=\sum_{k}^{M} \lambda_k \frac{\partial\langle A_k \rangle}{\partial\lambda_i}, \quad (25)$$

noting that the last one being a generalized Fisher-Euler theorem. It is instructive to have a look at the Appendix A at this point to check that entirely similar relations are obeyed by the ordinary Gibbs-Boltzmann entropy *S*. On the basis of such an observation, it seems natural to consider that the three reciprocity relations above should allow one to speak of a ``Fisher-thermodynamics" (Flego et al., 2003).

FIM expresses a relation between the independent variables or control variables (the prior information) and a dependent value *I*. Such information is encoded into the functional form of $I = I(\langle A_1 \rangle,\ldots,\langle A_M \rangle)$. For later convenience, we will also denote such a relation or encoding as $\{I,\langle A_k \rangle\}$. We see that the Legendre transform FIM-structure involves eigenvalues of the information-Hamiltonian, which neatly display the information encoded in *I* via Lagrange multipliers, $\alpha = \alpha(\lambda_1,...\lambda_M)$:

$$\{I, \langle A_k \rangle\} \quad \leftrightarrow \quad \{\alpha, \lambda_k\}.$$

4.2 Connecting the SE's Solutions to Thermodynamics

The connection between the solutions of Eq. (17) and thermodynamics has been established in refs.(Frieden et al., 1999; Flego et al., 2003). We summarize now the main details. One is assumedly dealing with an equilibrium gas of mass density ρ_o. In this context, *x* is velocity ($x \to v$). Moreover, one will focus on non-equilibrium thermodynamics' facets. Accordingly, the velocity-space Schrödinger (SE) reads

$$-\frac{1}{2\rho_o}\frac{\partial^2}{\partial v^2}\psi(v) - \frac{1}{8}\sum_{k=1}^{M}\lambda_k\, A_k(v)\psi(v) = \frac{\alpha}{8}\psi(v)\,, \tag{26}$$

The prior knowledge is chosen to be the temperature characterizing the equilibrium state. The equipartition theorem allows one calculate the average value of the squared velocity mean value for the equilibrium state $\langle v^2 \rangle_o$. Consequently, choosing $A_1(v) = v^2$ and writing $\lambda_1' = \rho_o / (2\omega_o^2)$, $\alpha / 8 = E / \omega_o^2$, the ensuing time-independent Schrödinger wave equation turns out to be

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial v^2} + \frac{\rho_o^2}{2\omega_o^2}v^2\right]\psi = \frac{\rho_o E}{\omega_o^2}\psi\,. \tag{27}$$

At this point one splits the hamiltonian *H* into the unperturbed hamiltonian H_o plus a perturbation part *H'*,

$$H = H_o + H' \quad , \quad H\psi = E\psi \quad , \quad H_o\phi = E^o\phi$$

H_0 can be identified with the harmonic oscillator's hamiltonian,

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial v^2} + \frac{\rho_o^2}{2\omega_o^2}v^2\right]\phi(v) = \frac{\rho_o E^o}{\omega_o^2}\phi(v)\,, \tag{28}$$

So that the ground state solution becomes a Gaussian function,

$$\phi_o = \left(\frac{\rho_o}{\pi\omega_o}\right)^{3/4} exp\left(-\frac{\rho_o}{2\omega_o}v^2\right). \tag{29}$$

The *excited solutions* $\psi(v)$ to the Fisher-based SE can be obtained using an appropriate, standard approximation method for stationary states (Cassels, 1970; Frieden et al., 1999; Flego et al., 2003; Tannor, 2007). The expansion coefficients are computed using the $\langle A_k \rangle$ of (13), by recourse to Hermite polynomials (It is important to remark that Hermite-Gaussian polynomials are orthogonal with respect to a Gaussian kernel, i.e. *the equilibrium distribution*. No other set of functions is orthogonal (and complete) with respect to a Gaussian kernel function.). The total number of them that one needs depends upon how far from equilibrium we are.

Note that the coefficients are computed at the fixed time *t* at which the input data $\langle A_k \rangle$ are collected. At equilibrium there is only one such coefficient. The premise of the constrained Fisher information approach is that its input constraints are correct, since *they come from experiment*. Summing up, the approach of (Frieden et al.,1999) yields solutions *at the fixed (but arbitrary) time t*. Schrödinger's wave equation approach gives solutions valid at discrete time-points *t*. In other words, for any other time value *t** we need to input new $\langle A_k \rangle$ values, appropriate for *this* time, but this does not compromise the validity of the Fisher-Schrödinger approach. In ref. (Flego et al., 2011a) we showed that the procedure can be extended to the three-dimensional scenario.

5. A QUANTAL- FISHER CONNECTION

Eq. (17) is an ordinary Schrödinger wave equation for a particle of unit mass in which the Lagrange multiplier ($\alpha/8$) plays the role of an energy eigenvalue $E=\alpha/8$. Remark that $U(x)$ is taken now to be an actual, physical potential, not an effective ``information" one. The FIM *I* (20) is now seen to be proportional to the expectation value of the Laplace operator, namely,

$$I = -4\int \psi \frac{\partial^2}{\partial x^2}\psi \, dx = -4\left\langle \frac{\partial^2}{\partial x^2} \right\rangle, \tag{30}$$

where the real functions ψ are the eigenfunctions of the SE (17). The potential function $U(x)$ belongs to L_2 and thus admits of a series expansion in x, x^2, x^3, etc. (Bates, 1961; Greiner and Müller, 1988). The $A_k(x)$ themselves belong to L_2 as well and can be series-expanded in similar fashion. This enables one to base future considerations on the assumption that the a priori knowledge refers to moments x^k of the independent variable, i.e.

$$\langle A_k \rangle = \langle x^k \rangle , \tag{31}$$

and that one possesses information on *M* moment-mean values $\langle x^k \rangle$. The ``information" potential *U* then reads

$$U(x) = -\frac{1}{8}\sum_k \lambda_k \, x^k . \tag{32}$$

Thus, the A_k in the preceding Sections become here x^k – moments and one assumes that the expansion is good enough if M terms of them are included. The λ_k are now the expansion-coefficients and not Lagrange multipliers. A Fisher's measure is to be constructed with these coefficients.

Enters here, as essential new ingredient in the present considerations, the celebrated virial theorem that of course applies in this Schrödinger-scenario (see Appendix C). This theorem states that

$$\left\langle -\frac{\partial^2}{\partial x^2} \right\rangle = \left\langle x \frac{\partial}{\partial x} U(x) \right\rangle . \tag{33}$$

and allows one to immediately obtain

$$\left\langle \frac{\partial^2}{\partial x^2} \right\rangle = \frac{1}{8} \sum_{k=1}^{M} k\, \lambda_k \langle x^k \rangle . \tag{34}$$

Thus, via (30) and (34) a very useful, virial-related expression for Fisher's information measure can be arrived at,

$$I = -\sum_{k=1}^{M} \frac{k}{2} \lambda_k \langle x^k \rangle , \tag{35}$$

which is an explicit function of the *M* physical parameters $\langle x^k \rangle$ and their respective Lagrange multipliers λ_k. Eq. (35) encodes the information provided by the Virial theorem. Now, replacing (35) into (24) one finds

$$\alpha = -\sum_{k=1}^{M} \left(\frac{k}{2} + 1 \right) \lambda_k \langle x^k \rangle , \tag{36}$$

The last two equations above constitute one important result of ref. (Flego et al., 2011b).

5.1 Hellmann-Feynman and Virial Theorems Imply Reciprocity Relations

In this subsection we are going to show that eqs. (35), (36), and the Hellmann-Feynman theorem (eq. (113) in Appendix B) jointly lead to Fisher-reciprocity relations.

Recalling that in the one-dimensional scenarios, the eigenfunctions $\psi(x)$ of (17) are real. We can then appeal to the *Hellmann-Feynman theorem* and obtain

$$\frac{\partial}{\partial \lambda_k}\left(\frac{\alpha}{8} \right) = \left\langle \psi \left| \frac{\partial H}{\partial \lambda_k} \right| \psi \right\rangle = \left\langle \psi \left| -\frac{1}{8} x^k \right| \psi \right\rangle \qquad \longrightarrow \qquad \frac{\partial \alpha}{\partial \lambda_k} = -\langle x^k \rangle , \tag{37}$$

thus discovering that the HF theorem immediately implies the reciprocity relation (25).

It is clear that differentiating (36) with respect to λ_n yields

$$\frac{\partial \alpha}{\partial \lambda_n} = -\left(\frac{n}{2} + 1 \right) \langle x^n \rangle - \sum_{k=1}^{M} \left(\frac{k}{2} + 1 \right) \lambda_k \frac{\partial \langle x^k \rangle}{\partial \lambda_n} . \tag{38}$$

The two relations (37) and (38) converge in yielding

$$\frac{n}{2}\langle x^n\rangle = -\sum_{k=1}^{M}\left(\frac{k}{2}+1\right)\lambda_k\frac{\partial\langle x^k\rangle}{\partial\lambda_n}. \tag{39}$$

At this point one goes back to (35) and differentiates it with respect to λ_n to arrive at

$$\frac{\partial I}{\partial\lambda_n} = -\frac{n}{2}\langle x^n\rangle - \sum_{k=1}^{M}\frac{k}{2}\lambda_k\frac{\partial\langle x^k\rangle}{\partial\lambda_n}. \tag{40}$$

At this stage, recourse to the relation (39) allows one to recover the Euler relations

$$\frac{\partial I}{\partial\lambda_n} = \sum_{k=1}^{M}\lambda_k\frac{\partial\langle x^k\rangle}{\partial\lambda_n}. \tag{41}$$

One also has

$$\frac{\partial I(< x^1 >,\ldots,< x^M >)}{\partial\lambda_n} = \sum_{k=1}^{M}\frac{\partial I}{\partial\langle x^k\rangle}\frac{\partial\langle x^k\rangle}{\partial\lambda_n}, \tag{42}$$

so that, comparing (41) and (42), we immediately obtain

$$\frac{\partial I}{\partial\langle x^n\rangle} = \lambda_n. \tag{43}$$

The three expressions (37), (41) and (43), obtained by the joint application of the Hellmann-Feynman and Virial theorems to Fisher's information measure, are reciprocity relations that, in turn, constitute a manifestation of an underlying SE-Legendre-invariant structure, analogous to that of thermodynamics. This constitutes the main result of ref. (Flego et al., 2011b).

6. A DIFFERENTIAL FIM-EQUATION

Inserting the reciprocity relations (43) into (35) one arrive to

$$\frac{\partial I}{\partial\langle x^k\rangle} = \lambda_k \qquad \longrightarrow \qquad I = -\sum_{k=1}^{M}\frac{k}{2}\langle x^k\rangle\frac{\partial I}{\partial\langle x^k\rangle}. \tag{44}$$

Eq. (44) constitutes an important result. We have now at our disposal a differential FIM-equation. Dealing with it should allow one to find *I* in terms of the $\langle x^k\rangle$ without passing first through a Schrödinger equation, a commendable achievement. This is a linear partial differential equation that an extremal *I* must necessarily comply with. This discovery is one main result of ref. (Flego et al., 2011c). For convenience, let us recast the key relations above using dimensionless magnitudes

$$\forall \langle A_k \rangle \equiv \langle x^k \rangle \neq 0 \quad , \qquad \mathrm{I} = \frac{I}{[I]} = \frac{I}{[x]^2}, \qquad \langle \mathrm{X}_k \rangle = \frac{\langle x^k \rangle}{[\langle x^k \rangle]} = \frac{\langle x^k \rangle}{[x]^k} \ , \tag{45}$$

where $[I]$ and $[\langle x^k \rangle]$ denote the dimension of I and $\langle x^k \rangle$, respectively. Thus, the differential equation that governs the FIM-behavior, i.e. (44), can be translated into

$$\mathrm{I} = -\sum_{k=1}^{M} \frac{k}{2} \langle \mathrm{X}_k \rangle \frac{\partial \mathrm{I}}{\partial \langle \mathrm{X}_k \rangle} \quad , \qquad \mathrm{I} = \mathrm{I}\ (\langle \mathrm{X}_1 \rangle, \cdots, \langle \mathrm{X}_M \rangle), \tag{46}$$

which is a first order linear nonhomogeneous equation with *M* independent variables.

All first order, linear PDEs possess a solution that depends on an arbitrary function, called the general solution of the PDE. In many physical situations this solution if less important than other solutions called complete ones (Courant and Hilbert, 1962; Kambe, 1965; Rhee et al., 1986; Evans, 1998; Polyanin et al., 2002; Polyanin, 2002). Such complete solutions are particular PDE solutions containing as many arbitrary constants as intervening independent variables. One should then look for a complete solution for the PDE (46). Set first

$$\mathrm{I} = \sum_{k=1}^{M} \mathrm{I}_k = \sum_{k=1}^{M} \exp\left[g(\langle \mathrm{X}_k \rangle) \right], \tag{47}$$

and substituting (47) into (46) leads to

$$\mathrm{I} = -\sum_{k=1}^{M} \frac{k}{2} \langle \mathrm{X}_k \rangle\, g'(\langle \mathrm{X}_k \rangle) \mathrm{I}_k \,. \tag{48}$$

The above relation entails

$$g'(\langle \mathrm{X}_k \rangle) = -\frac{2}{k \langle \mathrm{X}_k \rangle} \qquad \longrightarrow \qquad g(\langle \mathrm{X}_k \rangle) = -\frac{2}{k} \ln\left| \langle \mathrm{X}_k \rangle \right| + c_k \,, \tag{49}$$

where c_k is an integration constant. Finally, substituting (49) into (47) one arrives at

$$\mathrm{I}\ (\langle \mathrm{X}_1 \rangle, ..., \langle \mathrm{X}_M \rangle) = \sum_{k=1}^{M} C_k \ \left| \langle \mathrm{X}_k \rangle \right|^{-2/k} \quad , \qquad C_k = e^{c_k} > 0 \ , \tag{50}$$

or, in function of the original input-quantities (45)

$$I(\langle x^1 \rangle, ..., \langle x^M \rangle) = \sum_{k=1}^{M} C_k \ \left| \langle x^k \rangle \right|^{-2/k} \ , \tag{51}$$

an intriguing result. It implies the existence of a universal prescription, a linear PDE, that FIM must necessarily comply with. Eq. (51) is a significant result of ref. (Flego et al., 2011c). Some important features deserve special mention.
The I -domain is,

$$D_I = \left\{(\langle x^1\rangle,...,\langle x^M\rangle)\,/\,\langle x^k\rangle \in \Re_o\right\}.$$

Also, for $\langle x^k\rangle > 0$, I is a monotonically decreasing function of $\langle x^k\rangle$ and, as one expects from a ``good'' information measure (Frieden, 1998, 2004), the Fisher measure is a convex function.

One may obtain λ_k from the reciprocity relations (25). For $\langle x^k\rangle > 0$ one gets,

$$\lambda_k = \frac{\partial I}{\partial\langle x^k\rangle} = -\frac{2}{k} C_k \; \langle x^k\rangle^{-(2+k)/k} < 0\,. \quad (52)$$

and then, using (24), one happily arrives to the α-normalization Lagrange multiplier's expression.

The general solution for the I-PDE does exist. Moreover its uniqueness has been proven (see (Flego et al., 2011c)).

7. A DIFFERENTIAL α – EQUATION

Since $\langle x^k\rangle$ is given by (25) as $[-\partial\alpha/\partial\lambda_k]$, expression (36) adopts the appearance

$$\alpha = \sum_{k=1}^{M} \left(1+\frac{k}{2}\right)\lambda_k \frac{\partial\alpha}{\partial\lambda_k}. \quad (53)$$

Eq. (53) constitutes another pivotal result. One has found a *linear, partial differential equation (PDE)* for α, whose variables are $U(x)$'s series-expansion's coefficients. The equation's origins are two information-sources, namely, i) the Legendre structure and ii) the Virial theorem. Dealing with this new equation might allow one to find α in terms of the λ_k *without passing before through a Schrödinger equation*, a commendable achievement. See below, however, the pertinent caveats.

For convenience we recast now the key relations using dimensionless magnitudes

$$\mathrm{A} = \frac{\alpha}{[\alpha]} = \frac{\alpha}{[x]^{-2}} \quad , \qquad \Lambda_k = \frac{\lambda_k}{[\lambda_k]} = \frac{\lambda_k}{[x]^{-(2+k)}} \quad , \quad (54)$$

where $[\alpha]$ and $[\lambda_k]$ denote the dimensions of α and λ_k, respectively. Thus, the differential equation that governs the energy-behavior, i.e. (53), can be translated into

$$\mathrm{A} = \sum_{k=1}^{M} \left(1+\frac{k}{2}\right)\Lambda_k \frac{\partial \mathrm{A}}{\partial\Lambda_k}, \quad (55)$$

and is easy to obtain a solution as follows. One first sets

$$\mathrm{A} = \sum_{k=1}^{M} \mathrm{A}_k = \sum_{k=1}^{M} \exp\left[h(\Lambda_k) \right], \tag{56}$$

and substitution of (56) into (55) then leads to

$$\mathrm{A} = \sum_{k=1}^{M} \left(1 + \frac{k}{2}\right) \Lambda_k \, h'(\Lambda_k) \mathrm{A}_k \, . \tag{57}$$

The above relation entails

$$h'(\Lambda_k) = \frac{2}{(2+k)} \frac{1}{\Lambda_k} \qquad \longrightarrow \qquad h(\Lambda_k) = \frac{2}{2+k} \ln|\Lambda_k| + d_k \,, \tag{58}$$

where d_k is an integration constant. Finally, inserting (58) into (56) one gets

$$\mathrm{A}(\Lambda_1, ..., \Lambda_M) = \sum_{k=1}^{M} D_k \, |\Lambda_k|^{2/(2+k)} \,, \qquad D_k = e^{d_k} > 0 \,, \tag{59}$$

or, as a function of the original input-quantities (54)

$$\alpha(\lambda_1, ..., \lambda_M) = \sum_{k=1}^{M} D_k \, |\lambda_k|^{2/(2+k)} \, . \tag{60}$$

Again, another universal prescription has been encountered; a linear PDE that energy eigenvalues must necessarily comply with. Eq. (60) is, of course, one main result of ref. (Flego et al., 2011e). Its solution poses a necessary but not (yet) sufficient condition for α to be an energy-eigenvalue. Some important energy-properties deserve special mention.

The α -domain is $D_\alpha = \{(\lambda_1, \cdots, \lambda_M) \,/\, \lambda_k \in \Re\} = \Re^M$. Also, eq.(60) states that for $\lambda_k < 0$, α is a monotonically decreasing function of the λ_k , and as one expect from the Legendre transform of I , one end up with a concave function.

One may obtain the $\langle x^k \rangle$ s from the reciprocity relations (25). For $\lambda_k < 0$ one gets

$$\langle x^k \rangle = -\frac{\partial \alpha}{\partial \lambda_k} = \frac{2}{(2+k)} D_k \, |\lambda_k|^{-k/(2+k)} > 0. \tag{61}$$

and then, using (23) one is able to build up I .

The general solution for α - PDE exists and uniqueness is proved from an analysis of the associated Cauchy problem (Flego et al., 2011e).

8. THE INTEGRATION CONSTANTS C_k AND D_k

The mathematical structure associated to the Legendre transform (see (23), (24) and (25)) implies the existence of a relation between the integration constants C_k and D_k associated, respectively, to the $I-$ and $\alpha-$expressions. It is given by (51) and (60). Thus, both expressions can be expressed in function of just one unique set of parameters F_k ,$(k=1...M)$. Accordingly, since FIM is constrained to obey the CR-bound (3) (Frieden, 1998, 2004), the best estimator is the one that exhibits the optimal CR-relation. Consequently, the reference quantities F_k should be chosen in such a manner that they lead to the optimal bound. Moreover, the reference quantities F_k should contain important information concerning the referential system with respect which prior conditions are experimentally determined. It is thus convenient to start proceedings by choosing an appropriate referential system. Such is our next topic.

8.1 The Mathematical Structure of the Legendre Transforms

In this section we discuss in some detail the mathematical structure associated to the Legendre transform (see (23), (24) and (25)) which establishes an interesting relation between the integration constants C_k and D_k (pertaining, respectively, to the I and α expressions given by (51) and (60)). One can study such relation in the two scenarios, $\{\alpha,\lambda_k\}$ and $\{I,\langle x^k\rangle\}$. Remember that the Lagrange multipliers are here simply $U(x)$'s series-expansion's coefficients.

In a $\{I,\langle x^k\rangle\}-$scenario, the λ_k are functions that depend on the $\langle x^k\rangle$-values. Taking into account (52), the energy (60) and the potential U, expressed as functions of the independent $\langle x^k\rangle-$values, take the form

$$\alpha=\sum_{k=1}^{M} D_k \left|\lambda_k\right|^{2/(2+k)}=\sum_{k=1}^{M} D_k \left(\frac{2}{k}C_k\right)^{2/(2+k)} \left|\langle x^k\rangle\right|^{-2/k} , \tag{62}$$

$$\sum_{k=1}^{M}\lambda_k\langle x^k\rangle=-\sum_{k=1}^{M}\frac{2}{k}C_k\left|\langle x^k\rangle\right|^{-2/k} . \tag{63}$$

Substituting (51), (62) and (63) into (23) one obtains

$$\sum_{k=1}^{M}C_k\left|\langle x^k\rangle\right|^{-2/k}=\sum_{k=1}^{M} D_k \left(\frac{2}{k}C_k\right)^{2/(2+k)} \left|\langle x^k\rangle\right|^{-2/k}-\sum_{k=1}^{M}\frac{2}{k}C_k\left|\langle x^k\rangle\right|^{-2/k},$$

which can be recast as

$$\sum_{k=1}^{M}\left\{D_k\left(\frac{2}{k}C_k\right)^{2/(2+k)} - \frac{2+k}{k}C_k\right\}\left|\langle x^k\rangle\right|^{-2/k}=0\ . \tag{64}$$

The above equation is automatically fulfilled if one imposes that

$$D_k\left(\frac{2}{k}C_k\right)^{2/(2+k)} = \frac{2+k}{k}C_k \quad ,$$

which leads to

$$D_k\, C_k^{-k/(2+k)}=\frac{(2+k)}{2}\left(\frac{k}{2}\right)^{-k/(2+k)}\ . \tag{65}$$

In the $\{\alpha,\lambda_k\}-$scenario, the $\langle x^k\rangle$ are functions that depend on the λ_k-values. Taking into account i) (61) and ii) the FIM-relation (51), the FIM and the information-potential, expressed as a function of the independent λ_k-values, adopt the appearance

$$I=\sum_{k=1}^{M}C_k\ \left|\langle x^k\rangle\right|^{-2/k}=\sum_{k=1}^{M}\left(\frac{2}{2+k}\right)^{-2/k}C_k\, D_k^{-2/k}\left|\lambda_k\right|^{2/(2+k)}\ , \tag{66}$$

$$\sum_{k=1}^{M}\lambda_k\langle x^k\rangle=-\sum_{k=1}^{M}\frac{2}{(2+k)}D_k\ \left|\lambda_k\right|^{2/(2+k)}. \tag{67}$$

Substituting (60), (66) and (67) into (24) one obtains

$$\sum_{k=1}^{M}C_k\left(\frac{2\,D_k}{2+k}\right)^{-2/k}\left|\lambda_k\right|^{2/(2+k)}=\sum_{k=1}^{M}D_k\left|\lambda_k\right|^{2/(2+k)}-\sum_{k=1}^{M}\ \frac{2}{(2+k)}D_k\left|\lambda_k\right|^{2/(2+k)}\ ,$$

which can be recast as

$$\sum_{k=1}^{M}\left\{C_k\left(\frac{2\,D_k}{2+k}\right)^{-2/k}-\frac{k}{(2+k)}D_k\right\}\left|\lambda_k\right|^{2/(2+k)}=0\ .$$

The above equation is automatically fulfilled if one enforces

$$C_k\left(\frac{2\,D_k}{2+k}\right)^{-2/k}=\frac{k}{(2+k)}D_k\ ,$$

which leads to

$$C_k\, D_k^{-(k+2)/k} = \frac{k}{2}\left(\frac{2+k}{2}\right)^{-(k+2)/k} . \tag{68}$$

From eqs. (65) or (68) one can write

$$C_k = \frac{k}{2}\bar{C}_k \ , \qquad D_k = \frac{k+2}{2}\bar{D}_k \ , \qquad \bar{D}_k^{(2+k)} = \bar{C}_k^{\,k} \equiv F_k^2. \tag{69}$$

Now expressions (51) and (60) take the form,

$$I = \sum_{k=1}^{M} \frac{k}{2}\bar{C}_k \left|\langle x^k \rangle\right|^{-2/k} = \sum_{k=1}^{M} \frac{k}{2}\left[\frac{F_k}{\langle x^k \rangle}\right]^{2/k} , \tag{70}$$

$$\alpha = \sum_{k=1}^{M} \frac{k+2}{2}\bar{D}_k \ \left|\lambda_k\right|^{2/(2+k)} = \sum_{k=1}^{M} \frac{k+2}{2}\left[F_k \left|\lambda_k\right|\right]^{2/(2+k)} . \tag{71}$$

and the reciprocity relations (52) and (61) can be condensed into

$$F_k^{\ 2} = \left|\lambda_k\right|^k \langle x^k \rangle^{(2+k)}. \tag{72}$$

8.2 FIM and Cramer Rao - Bound

The essential FIM feature is undoubtedly its being an estimation measure known to obey the Cramer Rao (CR) bound (Frieden, 1998, 2004). Accordingly, since the partial differential equation has multiple solutions, it is natural to follow Jaynes's MaxEnt ideas and select amongst them the one that optimizes the CR bound. We utilize then the bound here as the operative constraint in the Fisher manipulations. Of course, Jaynes needs to maximize the entropy instead. One can also, without loss of generality, re-normalize the reference quantities F_k. This procedure is convenient because it allows one to regard the $F_k -$ quantities as statistical weights that optimize the CR-bound (3). In other words, the procedure entails extremization of

$$g(F_1,\cdots,F_M) = I\,\langle x^2 \rangle = \sum_{k=1}^{M} \frac{k}{2}\left[\frac{F_k}{\left|\langle x^k \rangle\right|}\right]^{2/k} \langle x^2 \rangle \tag{73}$$

with the constraint

$$\phi(F_1,\cdots,F_M) = \sum_{k=1}^{M} F_k^{\ 2/k} = 1. \tag{74}$$

The preceding considerations were applied in ref. (Flego et al., 2011f) so as to obtain the eigenvalues of the quartic anharmonic oscillator. Our theoretical, parameter-free results, obtained without passing first through a Schrödinger equation, are in a quite good agreement with those of the literature. In Section 9 we are going to tackle simple situations that illustrate the concomitant procedure.

8.3 The Appropriate Referential System

As conjectured in (Flego et al., 2011c), the reference-quantities F_k should contain important information concerning the referential system with respect which prior conditions are experimentally determined. Following ideas advanced in (Flego et al., 2011c) we will look for the `` $x-$space point" at which the potential function achieves a minimum, because it turns out to be convenient to incorporate at the outset, within the $I-$ and $\alpha-$mathematical forms, information concerning this minimum of the information potential. Assume that

$$U(x) = -\frac{1}{8}\sum_{x=1}^{M} \lambda_k x^k,$$

achieves its absolute minimum at the ``critical point" $x=\xi$

$$U'(\xi)=0\ , \qquad U_{min}=U(\xi). \tag{75}$$

Now, effecting the translational transform $u = x-\xi$ leads us to

$$I = -\sum_{k=1}^{M} \frac{k}{2}\lambda_k \langle x^k\rangle = -\sum_{k=1}^{M} \frac{k}{2}\lambda_k^* \langle u^k\rangle', \tag{76}$$

with (see below in Appendix D)

$$\lambda_k^* = -\frac{8}{k!}U^{(k)}(\xi)\ , \qquad \langle u^k\rangle' = \langle (x-\xi)^k\rangle, \tag{77}$$

where $U^{(k)}(\xi)$ is the k^{th} derivative of $U(x)$ evaluated at $x=\xi$ and $\langle\ \rangle'$ indicates that the relevant moment (expectation) is computed with translation-transformed eigenfunctions.

Summing up:

► The corresponding FIM-explicit functional expression is built up with the $N-$non-vanishing momenta ($N<M$, $\langle u^k\rangle' \neq 0$) and is given by

$$I = \sum_{k=2}^{N} \frac{k}{2}\bar{C}_k \left|\langle u^k\rangle'\right|^{-2/k} = \sum_{k=2}^{N} \frac{k}{2}\bar{C}_k \left|\langle (x-\xi)^k\rangle\right|^{-2/k}\ , \tag{78}$$

where one kept in mind that $\lambda_1^* = -8U'(\xi)=0$. A glance at the above FIM-expression suggests that we re-arrange things in the fashion

$$I = \bar{C}_2 \left|\langle (x-\xi)^2 \rangle\right|^{-1} + \sum_{k=3}^{N} \frac{k}{2} \bar{C}_k \left|\langle (x-\xi)^k \rangle\right|^{-2/k} \ . \quad (79)$$

Taking now into account that

$$\begin{cases} \langle x-\xi \rangle \ \ = 0 \\ \langle (x-\xi)^2 \rangle = \langle x^2 \rangle - 2\xi\langle x \rangle + \xi^2 \end{cases} \longrightarrow \begin{cases} \langle x \rangle = \xi \\ \langle (x-\xi)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \sigma^2 \end{cases} \quad (80)$$

we get

$$I = \bar{C}_2 \, \sigma^{-2} + \sum_{k=3}^{N} \frac{k}{2} \bar{C}_k \left|\langle (x-\xi)^k \rangle\right|^{-2/k} \ , \quad (81)$$

from which one obtains

$$I \, \sigma^2 = \bar{C}_2 + \sigma^2 \sum_{k=3}^{N} \frac{k}{2} \bar{C}_k \left|\langle (x-\xi)^k \rangle\right|^{-2/k} \geq 1 \ . \quad (82)$$

Therefore, if no moment $k \geq 3$ is a priori known, in forcing I to preserve the well-known Cramer-Rao $I-$bound (Frieden and Soffer, 1995) $I\sigma^2 \geq 1$, we need that

$$\bar{C}_2 = 1 \qquad \longrightarrow \qquad \bar{C}_2 = \bar{D}_2 = F_2 = 1.$$

► The corresponding α-explicit functional expression is constructed with the $N-$non-vanishing momenta ($N<M$) ($\langle u^k \rangle' \neq 0$) and is given by

$$\alpha = 8U(\xi) + \sum_{k=2}^{N} \frac{k+2}{2} \bar{D}_k \left|\lambda_k^*\right|^{2/(k+2)} \ . \quad (83)$$

For the harmonic oscillator it is well known that (Flego et al., 2011c)

$$U(x) = -\frac{1}{8} \lambda_2 \, x^2 \ , \qquad \lambda_2 = -4\omega^2. \quad (84)$$

The minimum of the potential function is obtained at the origin $\xi = 0$,

$$U'(\xi) = -\frac{1}{4} \lambda_2 \, \xi = 0 \qquad \longrightarrow \qquad \xi = 0.$$

Thus, using the α -expression (71) con $\bar{D}_2 = 1$, we have

$$\alpha = 2|\lambda_2|^{1/2} = 4\omega \ . \tag{85}$$

as one should expect since $(\alpha/8)$ plays the role of an energy eigenvalue (Cf. Eq.(13)) and we took Planck's constant equal to unity.

9. A COUPLE OF PHYSICAL EXAMPLES

So as to illustrate the above considerations we are going to consider simple and instructive examples. We take the mass $m=1$ and $\hbar = 1$.

►Harmonic oscillator (HO) in $\{I, \langle x^k \rangle\}$ – scenario

The prior information is given by

$$\langle x^2 \rangle = \frac{1}{2\omega} \ , \qquad M = 1 \ , \qquad k = 2 \ . \tag{86}$$

The minimum of the potential function obtains at the origin $\xi = 0$,

$$U(x) = -\frac{1}{8}\lambda_2 x^2 \quad \longrightarrow \quad U'(\xi) = -\frac{1}{4}\lambda_2 \xi = 0 \quad \longrightarrow \quad \xi = 0.$$

The pertinent FIM can be obtained using (78) with $u = x - \xi = x$,

$$I = I(\langle x^2 \rangle) = C_2 \langle x^2 \rangle^{-1} \ ,$$

and, the CR bound is saturated when $C_2 = 1$,

$$\langle x^2 \rangle = C_2 = 1 \qquad \longrightarrow \qquad I = \langle x^2 \rangle^{-1} \ . \tag{87}$$

The corresponding Lagrange multiplier can be obtained by recourse to the reciprocity relation (43) and (87),

$$\lambda_2 = \frac{\partial I}{\partial \langle x^2 \rangle} = -\langle x^2 \rangle^{-2} \tag{88}$$

The prior-knowledge (86) is encoded into the FIM (87), and the Lagrange multiplier λ_2 (88),

$$I = \langle x^2 \rangle^{-1} = 2\omega; \qquad \lambda_2 = -\langle x^2 \rangle^{-2} = -4\omega^2 \ . \tag{89}$$

Finally, the α – value can be obtained from (24),

$$\alpha = I - \lambda_2 \langle x^2 \rangle = 4\omega. \quad (90)$$

► Harmonic oscillator in a uniform external-field. The $\{I, \langle x^k \rangle\}$ – scenario.

We consider a charged unit-mass particle moving in the HO potential. The electrical charge is q and there is a uniform electric field ε, in the x – direction. Our prior knowledge is given by (Bates, 1961; Greiner and Müller, 1988)

$$\langle x \rangle = \frac{q\varepsilon}{\omega^2}, \qquad \langle x^2 \rangle = \frac{1}{2\omega} + \left(\frac{q\varepsilon}{\omega^2}\right)^2. \quad (91)$$

We look first for the ξ-point at which $U(x)$ is minimal.

$$U'(\xi) = 0 \qquad \longrightarrow \qquad \xi = -\frac{\lambda_1}{2\lambda_2}. \quad (92)$$

The translational transform $u = x - \xi$ implies that

$$\langle u \rangle' = \langle x - \xi \rangle = \langle x \rangle - \xi, \qquad \langle u^2 \rangle' = \langle (x-\xi)^2 \rangle = \langle x^2 \rangle - 2\xi \langle x \rangle + \xi^2. \quad (93)$$

The translation-transformed FIM is now given by

$$I = C_2 \langle u^2 \rangle'^{-1}. \quad (94)$$

and, the CR bound is saturated when $C_2 = 1$,

$$I \langle u^2 \rangle' = C_2 = 1 \qquad \longrightarrow \qquad I = \langle u^2 \rangle'^{-1}. \quad (95)$$

The reciprocity relations now lead us to

$$\lambda_1 = \frac{\partial I}{\partial \langle x \rangle} = \frac{\partial I}{\partial \langle u^2 \rangle'} \frac{\partial \langle u^2 \rangle'}{\partial \langle x \rangle} = -\langle u^2 \rangle'^{-2} \, (-2\xi), \quad (96)$$

$$\lambda_2 = \frac{\partial I}{\partial \langle x^2 \rangle} = \frac{\partial I}{\partial \langle u^2 \rangle'} \frac{\partial \langle u^2 \rangle'}{\partial \langle x^2 \rangle} = -\langle u^2 \rangle'^{-2}. \quad (97)$$

From the prior knowledge (91) and using (93) we thus have

$$\langle x \rangle = \xi = \frac{q\varepsilon}{\omega^2}, \quad (98)$$

$$\langle u^2 \rangle' = \langle x^2 \rangle - \xi^2 = \frac{1}{2\omega} + \left(\frac{q\varepsilon}{\omega^2}\right)^2 \left(\frac{q\varepsilon}{\omega^2}\right)^2 = \frac{1}{2\omega}. \quad (99)$$

Proceeding to insert (98) and (99) into (95)-(97) we get

$$I = \langle u^2 \rangle'^{-1} = \left(\frac{1}{2\omega} \right)^{-1} = 2\omega, \tag{100}$$

$$\lambda_1 = 2\xi \langle u^2 \rangle'^{-2} = 2\frac{q\varepsilon}{\omega^2}\,(2\omega)^2 = 8q\varepsilon \tag{101}$$

$$\lambda_2 = -\langle u^2 \rangle'^{-2} = -(2\omega)^2 = -4\omega^2 \tag{102}$$

The corresponding translational transform $\bar{\alpha}-$value can be obtained substituting (100)-(102) into (24),

$$\bar{\alpha} = I - \lambda_1 \langle x \rangle - \lambda_2 \langle x^2 \rangle = 2\omega - 8q\varepsilon \frac{q\varepsilon}{\omega^2} + 4\omega^2 \left(\frac{1}{2\omega} + \left(\frac{q\varepsilon}{\omega^2} \right)^2 \right) = 4\omega\,,$$

and the corresponding $\alpha-$value is given by (see appendix D),

$$\alpha = \bar{\alpha} + 8U(\xi) = 4\omega - 4\frac{q^2\varepsilon^2}{\omega^2}, \tag{103}$$

as we expect.

10. CONCLUSIONS

In this work we have shown that, if Fisher's measure *I* is associated to a Schrödinger wave equation (SE), as it happens whenever one extremizes *I* subject to appropriate constraints, two theorems intimately linked to quantum mechanics, the Hellmann-Feynman and Virial ones, automatically lead to Jaynes-like reciprocity relations involving the coefficients of the series-expansion of the potential function. One is then authorized to assert that a Legendre-transform structure underlies the one-dimensional non-relativistic Schrödinger's equation, a rather surprising finding.

Also, the insertion of Virial theorem-tenets into this Legendre structure leads to a differential equation for *I*. The equation is analytically solvable and its solution provides us with a general, explicit new expression for *I* in terms of the input-information contained in the M expectation values $\langle x^k \rangle$ from which we can directly codify the information provided by such set of expectation values in an *I* -form without previous appeal to a Schrödinger equation. An application to simple examples has illustrated these considerations. Of course, as is the case in the MaxEnt environment, the usefulness of (51) depends on how adequate is our input information for describing the situation at hand. Maximal entropy or minimum FIM are just the best ways to exploit that knowledge.

Additionally, on the basis of a variational principle based on Fisher's information discover a first order differential equation for the Schrödinger energy-eigenvalues. Its general solution exists and is unique. The particular solution that one obtains imposing the condition that the associated FIM be minimal leads, for some well-known problems, to $\alpha -$values which are in good agreement with those of the literature.

Note that, once in possession of the minimal *I*, one does not need to ever address any explicit *I* - minimization task nor solve the FIM-associated Schrödinger equation, a fact that should be of interest to the large number of Fisher practitioners. This constitutes a new illustration of the power of information-related tools in analyzing physical problems.

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Authors have declared that no competing interests exist.

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APPENDIX

1. MAXENT AND RECIPROCITY RELATIONS

Statistical mechanics and thereby thermodynamics can be formulated on the basis of Information Theory if the concomitant density distribution $f(x)$ is obtained by recourse to MaxEnt (Jaynes, 1957; Katz, 1967), which asserts that assuming that your prior knowledge about the system is given by the values of M expectation values $\langle A_1\rangle,\ldots,\langle A_M\rangle$, then $f(x)$ is uniquely fixed by extremizing $S(f)=-\int dx\, f(x)\ln f(x)$ subject to the constraints given by the M conditions $\langle A_j\rangle=\int dx\, f(x)\, A_j(x)$, entailing the introduction of M Lagrange multipliers λ_i. Here x stands for a point in the relevant (micro)state space associated with the system under consideration (it is usual in appealing to information theory tools (like S) to regard the accompanying PDFs as being dimensionless quantities). In the process of applying the MaxEnt principle one discovers that the information quantifier S can be identified with the equilibrium entropy of thermodynamics if our prior knowledge $\langle A_1\rangle,\ldots,\langle A_M\rangle$ refers to extensive quantities. $S(maximal)$, once determined, yields complete thermodynamical information with respect to the system of interest (Jaynes, 1957). $f(x)$, the classical MaxEnt probability distribution function (PDF), associated to Boltzmann-Gibbs-Shannon's logarithmic entropy S, is given by (Jaynes, 1957; Katz, 1967)

$$f(MaxEnt)=f(x)=\exp\left\{-\left[\Omega+\sum_{i=1}^{M}\lambda_i\, A_i(x)\right]\right\}, \tag{104}$$

with (Jaynes, 1957; Katz, 1967)

$$\Omega(\lambda_1,\ldots,\lambda_M)=\ln\left\{\int dx\left(\exp\left[-\sum_{i=1}^{M}\lambda_i\, A_i(x)\right]\right)\right\}\equiv-\lambda_o, \tag{105}$$

$$\frac{\partial\Omega(\lambda_1,\ldots,\lambda_M)}{\partial\lambda_j}=-\langle A_j\rangle,\qquad (j=1,\ldots,M), \tag{106}$$

and

$$S=\Omega+\sum_{i=1}^{M}\lambda_i\,\langle A_i\rangle, \tag{107}$$

entailing

$$dS=\sum_{i=1}^{M}\lambda_i\, d\langle A_i\rangle. \tag{108}$$

The Euler theorem holds (Katz, 1967)

$$\frac{\partial S}{\partial \lambda_i} = \sum_k \lambda_k \frac{\partial \langle A_k \rangle}{\partial \lambda_i}, \tag{109}$$

and, using (107), one arrives to

$$\begin{aligned} dS &= \sum_{i=1}^{M} \lambda_i \, d\langle A_i \rangle \\ S &= S(\langle A_1 \rangle, \ldots, \langle A_M \rangle) \end{aligned} \qquad \longrightarrow \qquad \frac{\partial S}{\partial \langle A_i \rangle} = \lambda_i. \tag{110}$$

Effecting now the Legendre transform

$$\Omega = \Omega(\lambda_1, \ldots, \lambda_M) = S - \sum_{i=1}^{M} \lambda_i \langle A_i \rangle, \tag{111}$$

one immediately ascertains that reciprocity holds, namely,

$$\frac{\partial S}{\partial \langle A_j \rangle} = \lambda_j \qquad \text{and} \qquad \frac{\partial \Omega}{\partial \lambda_j} = -\langle A_j \rangle; \qquad j = 1, \ldots, M, \tag{112}$$

where the second set of equations, together with (105), yield the Lagrange multipliers as a function of the input information regarding expectation values (Katz, 1967). The reciprocity relations (112) are a manifestation of the Legendre-invariant structure of thermodynamics and its most salient structural mathematical feature.

2. HELLMANN-FEYNMAN THEOREM

The Hellmann-Feynamn theorem (HFT) (Hellmann, 1933; Feynman, 1939; Griffiths, 1995; Namgung, 1998) demonstrates the relationship between perturbations in an operator on a complex inner product space and the corresponding perturbations in the operator's eigenvalue. It shows that to compute the derivative of an eigenvalue with respect to a parameter of the operator, we need only to know the corresponding eigenvector and the derivative of the operator. More to the point, the Hellmann-Feynman theorem assures that a non-degenerate eigenvalue $E_i(\lambda)$ of a parameter-dependent hermitian operator $H(\lambda)$, with associated (normalized) eigenvector $\psi_i(\lambda)$, varies with respect to the parameter λ according to the formula

$$\frac{\partial E_i}{\partial \lambda} = \langle \psi_i(\lambda) | \frac{\partial H}{\partial \lambda} | \psi_i(\lambda) \rangle. \tag{113}$$

The theorem has a rich history and is of paramount importance in many areas of applied quantum mechanics (Wallace, D.W. (2005). An introduction to Hellmann-Feynman theory. Master Thesis, University of Central Florida, Orlando, Florida, (unpublished).). In particular, it plays a central role in the quantum mechanical evaluation of forces in chemical systems. The HFT can be proved to hold for exact eigenstates and also for variationally determined states (Namgung, 1998). The proof of the theorem is well known. However, since the HFT plays a vital role in the present considerations, for the sake of clarity and completeness we include a brief sketch of the proof.

Let ψ' stand for $(\partial\psi/\partial\lambda)$ and remember that

$$H\,|\,\psi_i(\lambda)\rangle = E_i\,|\,\psi_i(\lambda)\rangle \quad and \quad \langle\psi_i(\lambda)\,|\,\psi_i(\lambda)\rangle = 1 \quad \Rightarrow \frac{d}{d\lambda}\langle\psi_i(\lambda)\,|\,\psi_i(\lambda)\rangle = 0 \tag{114}$$

Then,

$$\begin{aligned}\frac{\partial E_i(\lambda)}{\partial\lambda} &= \langle\psi_{i'}(\lambda)\,|\,H\,|\,\psi_i(\lambda)\rangle + \langle\psi_i(\lambda)\,|\,H\,|\,\psi_{i'}(\lambda)\rangle + \langle\psi_i(\lambda)\,|\,\partial H/\partial\lambda\,|\,\psi_i(\lambda)\rangle = \\ &= \langle\psi_{i'}(\lambda)\,|\,E_i(\lambda)\,|\,\psi_i(\lambda)\rangle + \langle\psi_i(\lambda)\,|\,E_i(\lambda)\,|\,\psi_{i'}(\lambda)\rangle + \langle\psi_i(\lambda)\,|\,\partial H/\partial\lambda\,|\,\psi_i(\lambda)\rangle = \\ &= E_i(\lambda)(d/d\lambda)\langle\psi_i(\lambda)\,|\,\psi_i(\lambda)\rangle + \langle\psi_i(\lambda)\,|\,\partial H/\partial\lambda\,|\,\psi_i(\lambda)\rangle = \\ &= 0 + \langle\psi_i(\lambda)\,|\,\partial H/\partial\lambda\,|\,\psi_i(\lambda)\rangle.\end{aligned}$$

where, obviously, the differentiability of E_i, H and ψ_i with respect to λ was assumed.

The HFT, and others derived from it, have been used in many areas of physics and specially in solid state and molecular physics after the pioneering work of Feynman (Feynman, 1939).

3. VIRIAL THEOREM

For any quantum system in stationary state, with a Hamiltonian that does not have explicit time dependence,

$$H = -\frac{\vec{p}^{\,2}}{2m} + U(\vec{x}) \tag{115}$$

the Virial theorem states that (Bates, 1961; Greiner and Müller, 1988)

$$\left\langle -\frac{\hbar^2}{m}\vec{\nabla} \right\rangle = \left\langle \vec{x}\,.\,\vec{\nabla}U(\vec{x}) \right\rangle \tag{116}$$

where the expectation value is taken for stationary states of the Hamiltonian.

4. FIM'S TRANSLATIONAL TRANSFORMATION

The potential function

$$U(x) = -\frac{1}{8}\sum_{k=1}^{M}\lambda_k x^k.$$

can be Taylor-expanded about $x = \xi$

$$U(x)=\sum_{k=0}^{M}\frac{U^{(k)}(\xi)}{k\ !}(x-\xi)^k .$$

The shift $u=x-\xi$ leads to

$$\bar{U}(u)=U(u+\xi)=\sum_{k=0}^{M}\frac{U^{(k)}(\xi)}{k\ !}u^k , \tag{117}$$

which can be recast as

$$\bar{U}(u)=-\frac{1}{8}\sum_{k=0}^{M}\lambda_k^* u^k \ , \tag{118}$$

with

$$\lambda_k^* \equiv -8\frac{U^{(k)}(\xi)}{k\ !}=-\frac{8}{k!}\sum_{j=1}^{M} j(j-1)(j-2)\cdots(j-k+1)\lambda_j\, \xi^{j-k} \ . \tag{119}$$

The shifted-FIM corresponding to $u=x-\xi$ is obtained from (20) in the fashion (note that $\langle\ \rangle'$ indicates that the pertinent moment is calculated with translation-transformed eigenfunctions)

$$I=-4\int\psi\frac{\partial^2}{\partial x^2}\psi\, dx=-4\int\bar{\psi}\frac{\partial^2}{\partial u^2}\bar{\psi}\, du=-4\left\langle\frac{\partial^2}{\partial u^2}\right\rangle' , \tag{120}$$

where $\bar{\psi}=\bar{\psi}(u)$ is the TF of $\psi(x)$. Now, using the TF of (14) one easily finds

$$I=\int\bar{\psi}_n\left(\alpha+\sum_{k=0}^{M}\lambda_k^* u^k\right)\bar{\psi}_n\, du \ , \tag{121}$$

and one realizes that

$$I=\alpha+\sum_{k=0}^{M}\lambda_k^*\langle u^k\rangle'=\bar{\alpha}+\sum_{k=1}^{M}\lambda_k^*\langle u^k\rangle' , \tag{122}$$

where

$$\bar{\alpha}=\alpha+\lambda_0^*=\alpha-8U(\xi). \tag{123}$$

Also, the Virial theorem (33) leads to

$$I=4\left\langle\frac{\partial^2}{\partial u^2}\right\rangle'=-4\left\langle u\frac{\partial}{\partial u}\bar{U}(u)\right\rangle'=-\sum_{k=1}^{M}\frac{k}{2}\lambda_k^*\langle u^k\rangle'. \tag{124}$$

The TF moments $\langle u^k\rangle'$ are related to the original moments as

$$\langle u^k \rangle' = \int u^k \, \bar{\psi}^2(u)\,du = \int u^k \, \psi^2(u+\xi)\,du = \int (x-\xi)^k \, \psi^2(x)\,dx = \langle (x-\xi)^k \rangle.$$

By recourse to the Newton-binomial we write

$$\int (x-\xi)^k \, \psi^2(x)\,dx = \sum_{j=1}^{k} (-1)^j \binom{k}{j} \xi^j \int x^{k-j} \, \psi^2(x)\,dx, \tag{125}$$

and then we finally have

$$\langle u^k \rangle' = \langle (x-\xi)^k \rangle = \sum_{j=1}^{k} (-1)^j \binom{k}{j} \xi^j \, \langle x^{k-j} \rangle. \tag{126}$$