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Fisher information, the Hellmann–Feynman theorem, and the Jaynes reciprocity relations

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ABSTRACT

We explore intriguing links connecting Hellmann–Feynman's theorem to a thermodynamics information-optimizing principle based on Fisher's information measure.

1. Introduction

The connection Information Theory ⇔ Thermodynamics + Statistical Mechanics was established by Jaynes half a century ago [1,2], its core being a variational approach that entails extremization of Shannon's information measure subject to the constraints imposed by the *a priori* knowledge one may possess concerning the system of interest. In this way, the whole of statistical mechanics can be elegantly reformulated, if one chooses Boltzmann's constant as the informational unit and identifies Shannon's measure with the thermodynamic entropy. The concomitant methodology is referred to as the *Maximum Entropy Principle (MaxEnt)* [1,2]. More recently, a similar program was successfully developed that replaces Shannon's information measure S by Fisher's one (FIM) I (see, for instance,

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[3–11]). Such an approach provides a new viewpoint within the so-called Wheeler program of establishing an information-theoretical foundation for the basic theories of physics [12]. Indeed, much effort is being focused upon FIM applications. A not exhaustive small sample is that of [13–25].

In the two cases just mentioned, the connection with thermodynamics is made by means of a set of first-derivative reciprocity relations that involve

- the Lagrange multipliers that emerge from the variational process,
- the information quantifier (S or I), and
- the expectation values that constitute the prior knowledge regarding the system of interest that are provided as input information within the formalism.

In the Fisher case, a Schrödinger-like equation is involved [6,8,26], a fact the will be employed below to pave the way for the construction of an intriguing connection with the celebrated Hellmann–Feynman theorem of quantum mechanics.

2. Hellmann–Feynman theorem

The Hellmann–Feynman theorem (HFT) [27–31] demonstrates the relationship between perturbations in an operator on a complex inner product space and the corresponding perturbations in the operator's eigenvalue. The theorem establishes that to evaluate the derivative of an eigenvalue with respect to a parameter of the above-mentioned operator, we only need the concomitant eigenvector and the derivative of the operator. The Hellmann–Feynman theorem states that a non-degenerate eigenvalue $E_i(b)$ of a parameter-dependent Hermitian operator $H(b)$, with associated (normalized) eigenvector $\psi_i(b)$, changes with respect to the parameter b according to the formula

$$\frac{\partial E_i}{\partial b} = \langle \psi_i(b)| \frac{\partial H}{\partial b} |\psi_i(b)\rangle. \tag{1}$$

The HFT has a distinguished history, and it plays a central role in many areas of applied quantum mechanics [28]. In particular, it plays a central role in the quantum mechanical evaluation of forces in chemical systems. The FHT holds both for exact eigenstates and also for approximate eigenstates determined via variational methods [29]. 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 in the Appendix.

3. 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 [1,2], 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

$$S(f) = -\int \mathrm{d}x f(x) \ln f(x), \tag{2}$$

subject to the constraints given by the M conditions

$$\langle A_j\rangle = \int \mathrm{d}x f(x) A_j(x), \tag{3}$$

together with normalization

$$\int \mathrm{d}x f(x) = 1, \tag{4}$$

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 customary in appealing to information theory tools (like S) to regard the accompanying probability distribution functions

(PDFs) as being dimensionless quantities. In any case, because of normalization, $\mathrm{d}xf(x)$ must be dimensionless. Additionally, in the case of Fisher's information (see below), one deals with derivatives of the form $\frac{\partial}{\partial\theta}\left[\ln f(x;\theta)\right] = \frac{1}{f}\frac{\partial f}{\partial\theta}$, which can obviously be expressed without explicitly using the ln function. Consequently, the units of f pose no problem here.

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 [1]. $f(x)$, the classical MaxEnt PDF, associated to the Boltzmann–Gibbs–Shannon logarithmic entropy S, is given by [1,2]

$$f(\mathrm{MaxEnt}) = f(x) = \exp\left\{-\left[\Omega + \sum_{i=1}^{M}\lambda_i A_i(x)\right]\right\}, \tag{5}$$

with [1,2]

$$\Omega(\lambda_1, \ldots, \lambda_M) = \ln\left\{\int \mathrm{d}x\left(\exp\left[-\sum_{i=1}^{M}\lambda_i A_i(x)\right]\right)\right\} \equiv -\lambda_o, \tag{6}$$

$$\frac{\partial\Omega(\lambda_1, \ldots, \lambda_M)}{\partial\lambda_j} = -\langle A_j\rangle, \quad (j = 1, \ldots, M), \tag{7}$$

and

$$S = \Omega + \sum_{i=1}^{M}\lambda_i\langle A_i\rangle, \tag{8}$$

entailing

$$\mathrm{d}S = \sum_{i=1}^{M}\lambda_i d\langle A_i\rangle. \tag{9}$$

The Euler theorem holds [2]:

$$\frac{\partial S}{\partial\lambda_i} = \sum_k \lambda_k\frac{\partial\langle A_k\rangle}{\partial\lambda_i}, \tag{10}$$

and, using (8), one arrives at

$$\mathrm{d}S = \sum_{i=1}^{M}\lambda_i d\langle A_i\rangle \Longrightarrow \frac{\partial S}{\partial\langle A_i\rangle} = \lambda_i$$
$$S = S(\langle A_1\rangle, \ldots, \langle A_M\rangle). \tag{11}$$

Effecting now the Legendre transform

$$\Omega = \Omega(\lambda_1, \ldots, \lambda_M) = S - \sum_{i=1}^{M}\lambda_i\langle A_i\rangle, \tag{12}$$

one immediately ascertains that reciprocity holds;, namely,

$$\frac{\partial S}{\partial\langle A_j\rangle} = \lambda_j \quad \text{and} \quad \frac{\partial\Omega}{\partial\lambda_j} = -\langle A_j\rangle; \quad j = 1, \ldots, M, \tag{13}$$

where the second set of equations, together with (6), yields the Lagrange multipliers as a function of the input information regarding expectation values [2]. The reciprocity relations (13) are a manifestation of the Legendre-invariant structure of thermodynamics and also its most salient structural mathematical feature.

4. Extremizing Fisher's information measure

Consider a system that is described by a normalized probability density (PDF)

$$f(x;\theta) = \psi(x;\theta)^2, \tag{14}$$

characterized by a fixed physical parameter θ and an amplitude ψ. Information measures are functionals of the PDF that assign to it a real number indicative of its information content. In particular, Fisher's information measure (FIM) I is defined as [4]

$$I = \int \mathrm{d}x f(x;\theta) \left\{ \frac{\partial}{\partial\theta} \ln[f(x;\theta)] \right\}^2. \tag{15}$$

The idea for employing it refers to an estimation of the value of θ on the basis of measurements of x [4]. Suppose that the PDF f is unknown, and one wishes to determine it. An observer makes a measurement and obtains a value, say x_1, of x. The observer has to best infer θ from this isolated measurement, and calls the resulting estimate $\theta_{\mathrm{est}} = \theta_{\mathrm{est}}(x_1)$. One wonders how well θ can be determined. Estimation theory asserts [4] that the best possible estimator $\theta_{\mathrm{est}}(x)$, after a very large number of samples (x-values) is examined, suffers a mean-square error e^2,

$$e^2 = \int \mathrm{d}x f(x,\theta)[\theta - \theta_{\mathrm{est}}(x)]^2, \tag{16}$$

that obeys a relationship, called the Cramer–Rao bound, involving Fisher's information measure I. One has [4]

$$e^2 \geq 1/I. \tag{17}$$

Eq. (16) gives the variance Var$x$ of x. If one defines a "Fisher length" $\delta x = \frac{1}{\sqrt{I}}$, 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

$$\Delta x \geq \delta x \tag{18}$$

for the root-mean-square deviation Δx of x.

The simplest and arguably most fundamental θ-instance is that of translational families. These are mono-parametric distribution families of the form

$$f(x+\epsilon). \tag{19}$$

Given any probability density $f(x)$, we can generate a translational family consisting of the densities $f(x+\epsilon)$ resulting from uniform translations of the original density $f(x)$. In this case, since the parameter ϵ is additive with respect to x, the parameter derivative appearing in the I definition reduces to the derivative $f'(x)$ of the density f with respect to the coordinate x itself. That is, this FIM does not explicitly involve any structural parameters of f. Now, this FIM adopts the form (remember $f = \psi^2$ according to (14)) [4]:

$$I = \int \mathrm{d}x f(x) \left\{ \frac{\partial}{\partial x} \ln[f(x)] \right\}^2 = 4 \int \mathrm{d}x \nabla\psi \nabla\psi. \tag{20}$$

This particular form of Fisher's information is specially important in physical applications because it constitutes the main ingredient of a powerful variational principle devised by Frieden and Soffer (FS), which gives rise to a substantial portion of (the thus far known) physics ([4] and references therein). In this work, we use the special instance of the principle in which FIM is minimized with adequate constraints, the so-called minimum Fisher information (MFI) approach (see Refs. [4,6] for more details). Consequently, one assumes that the relevant PDF is always of the form (19).

It is worth mentioning that some interesting relationships have been recently established between Fisher's and Shannon's measures that are to be mentioned here. As a first result, we mention that Fisher's information measure places an upper bound on 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 [32]. This bound is of the form

$$|(\mathrm{d}S/\mathrm{d}t)| \leq \text{ constant } \sqrt{I}. \tag{21}$$

In the case of diffusion equations (the paradigm of irreversible behavior), Plastino, Plastino, and Miller have demonstrated some additional important relationships [33]. These are

$$(\mathrm{d}S/\mathrm{d}t) = I \geq 0, \tag{22}$$

and

$$(\mathrm{d}S^2/\mathrm{d}t^2) = (\mathrm{d}I/\mathrm{d}t) \leq 0, \tag{23}$$

from which one deduces the fact that [33]

$$S_{t=0} \leq S(t) \leq S_{t=0} + (t - t_0)I(t = 0). \tag{24}$$

S and I are intimately related, and it is clear that I regulates the entropy growth. Parenthetically, it is worth stating a direct relationship that links I to the celebrated Kullback–Leibler relative entropy K between two probability distributions $f(x)$ and $f(x+\epsilon)$. It reads [4]

$$K[f(x+\epsilon) \parallel f(x)] \propto \epsilon^2 I + \text{higher order terms in } \epsilon. \tag{25}$$

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,

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

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

$$\langle A_k \rangle = \int \mathrm{d}x A_k(x) f(x), \quad k = 1, \ldots, M. \tag{26}$$

These mean values play here the role of extensive thermodynamical variables [6]. In this context, it is well known [6] that the relevant PDF $f(x)$ extremizes the FIM (20) subject to (i) the prior conditions (26) and, of course, (ii) the normalization condition

$$\int \mathrm{d}x f(x) = 1. \tag{27}$$

Why do we extremize I instead of Shannon's S? Because in the latter case the PDF result is always of an exponential form. This is good enough for many purposes, but nor for all. For instance, power-law PDFs do not arise naturally 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 [6]. Consequently, we now briefly review the formalism developed in Ref. [6]. The MFI approach adopts the appearance

$$\delta\left(I - \alpha \int \mathrm{d}x f(x) - \sum_{k=1}^{M} \lambda_k \int \mathrm{d}x A_k(x) f(x)\right) = 0, \tag{28}$$

where we have introduced the $(M+1)$ Lagrange multiplier. Variation leads to

$$\left[\frac{1}{f^2}\left(\frac{\partial f}{\partial x}\right)^2 + \frac{\partial}{\partial x}\left(\frac{2}{f}\frac{\partial f}{\partial x}\right)\right] + \alpha + \sum_{k=1}^{M} \lambda_k A_k(x) = 0. \tag{29}$$

To put the above equation in a more manageable form [34,6,35], we introduce the function $\psi(x)$ via the identification $\psi(x)^2 = f(x)$ (see comment below Eq. (32)) so that Eq. (29) adopts the Schrödinger wave equation (SWE) form

$$-\frac{1}{2}\nabla^2\psi - \sum_{k=1}^{M} \frac{\lambda_k}{8} A_k \psi = \frac{\alpha}{8}\psi, \tag{30}$$

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

$$U = U(x) = -\frac{1}{8}\sum_{k=1}^{M}\lambda_k A_k(x). \tag{31}$$

Then, in order to find the PDF one has to solve the above wave equation (WE), where the Lagrange multiplier $(\alpha/8)$ plays the role of an energy eigenvalue $E = \alpha/8$. The Lagrange parameters λ_k are fixed, of course, by recourse to the available prior information. Notice that the eigenenergy $\alpha/8$ automatically yields the value of the Lagrange multiplier associated to normalization (cf. Eq. (6) for the Shannon instance). The square of the solutions ψ yields the PDF

$$\psi(x)^2 = f(x), \tag{32}$$

and we point out that $\psi(x)$ is always real in the case of one-dimensional scenarios, or for the ground state of a real potential in N dimensions [36]. The reader may wonder whether the complex real Schrödinger equation can also be obtained with the same procedure. The answer is in the affirmative. One starts with a complex definition for I advanced by Frieden and Soffer [4,5] that uses a complex amplitude ψ^*, namely,

$$I = 4\int \mathrm{d}x \nabla\psi^* \nabla\psi. \tag{33}$$

For our present purposes, the real, standard I definition suffices. The connection between the solutions of Eq. (30) and thermodynamics has been established in Refs. [6,8]. Let us summarize the pertinent main details. The reciprocity relations (13) and their Fisher counterparts (to be found below) are an expression of the Legendre-invariant structure of thermodynamics and constitute its essential formal ingredient [37]. It is of the essence for our present purposes that they also hold for the Fisher treatment. Standard thermodynamics makes use of the derivatives of the entropy S with respect to both λ_i and $\langle A_i\rangle$ parameters (for instance, pressure and volume, respectively). Analogous properties of $\partial I/\partial\lambda_i$ and $\partial I/\partial\langle A_i\rangle$ are valid as well. Substituting (32) into Eq. (20), we find

$$I = 4\int \frac{\partial}{\partial x}\left(\psi_n \frac{\partial \psi_n}{\partial x}\right)\mathrm{d}x - 4\int \psi_n \frac{\partial^2}{\partial x^2}\psi_n \mathrm{d}x = -4\int \psi_n \frac{\partial^2}{\partial x^2}\psi_n \mathrm{d}x. \tag{34}$$

Then, via the SWE (30), we easily get

$$I = \int \psi_n \left(\alpha + \sum_{k=1}^{M}\lambda_k A_k\right)\psi_n \,\mathrm{d}x. \tag{35}$$

Now, through (i) the prior conditions (26) and (ii) the normalization condition (26), we arrive at

$$I(\langle A_1\rangle, \ldots, \langle A_M\rangle) = \alpha + \sum_{k=1}^{M}\lambda_k \langle A_k\rangle, \tag{36}$$

the Fisher counterpart of (8). Note that the Legendre transform of I is α; that is,

$$\alpha = I(\langle A_1\rangle, \ldots, \langle A_M\rangle) - \sum_{k=1}^{M}\lambda_k \langle A_k\rangle = \alpha(\lambda_1, \ldots, \lambda_M), \tag{37}$$

so

$$\frac{\partial\alpha}{\partial\lambda_i} = -\langle A_i\rangle. \tag{38}$$

Finally, according to (36),

$$\lambda_k = \frac{\partial I}{\partial\langle A_k\rangle}, \tag{39}$$

and, moreover,

$$\frac{\partial I}{\partial \lambda_i} = \sum_k^M \lambda_k \frac{\partial \langle A_k \rangle}{\partial \lambda_i}, \tag{40}$$

which is a generalized Fisher–Euler theorem that was previously proved in [6]. We see that the reciprocity relations (13) are also a feature of the Fisher treatment, which makes it reasonable to speak of a Fisher thermodynamics.

5. Fisher–Hellmann–Feynman connections

We are now in a position to establish a Fisher–Hellmann–Feynman link. According to the preceding section, let us consider a Schrödinger equation for a particle of unit mass,

$$-\frac{1}{2}\nabla^2\psi + U(x)\psi = E\psi. \tag{41}$$

If the eigenfunction $\psi(x)$ is real (which is always the case in one-dimensional scenarios, or for the ground state of a quantum system described by an N-dimensional configuration space and a real potential [36]), we can ascribe to (41) a Fisher measure

$$I = \int \mathrm{d}x f(x) \left\{ \frac{\partial}{\partial x} \ln[f(x)] \right\}; \quad f = \psi^2. \tag{42}$$

Now, let us assume that the potential function U can be series expanded in the form

$$U(x) = \sum_k a_k x^k = -\frac{1}{8}\sum_k \lambda_k x^k, \quad (A_k = x^k), \tag{43}$$

where the second equality refers to Eq. (30). We then make the identifications

$$\alpha = 8E; \quad \text{and} \quad \lambda_k = -8a_k, \tag{44}$$

so that (cf. Eq. (38))

$$\frac{\partial(8E)}{\partial(-8a_i)} = -\langle x^i \rangle. \tag{45}$$

It follows now from Eqs. (39)–(45) that the coefficients a_k satisfy the relations

$$\frac{\partial I}{\partial \langle x^k \rangle} = \lambda_k = -8a_k, \tag{46}$$

and

$$\frac{\partial E}{\partial a_k} = \langle x^k \rangle. \tag{47}$$

The last equation above is an instance of the Hellmann–Feynman theorem if the a_k are regarded as parameters of the Hamiltonian. Noticing that E in (47) is the particular Lagrange multiplier guaranteeing normalization of the probability distribution that yields an extremum for I, such an equation turns out to constitute a nice, and as far as we know new, relation between Fisher's measure, expectation values, and the coefficients of the potential's series expansion. We have encountered that the coefficients a_k in the $U(x)$-expansion behave, in a fashion, like the temperature T or the pressure p, typical "Lagrande multipliers" in statistical thermodynamics, our main (and non-trivial) finding here. Of course, we could have, instead of (43), a more general expansion in terms of arbitrary functions $f_k(x)$ of the form

$$U(x) = \sum_k a_k f_k(x), \tag{48}$$

with reciprocity relations of the type (46) that would now involve the $\langle f_k(x)\rangle$ instead of the $\langle x^k\rangle$. What happens if no expectation values are known a priori? Then, according to (36), one has

$$I = \alpha = 8E, \tag{49}$$

which entails that the HF theorem gets expressed directly in I-terms. If the energy depends upon some parameter ξ then so does the FIM, and we have

$$(1/8)\frac{\mathrm{d}I(\xi)}{\mathrm{d}\xi} = \frac{\mathrm{d}E}{\mathrm{d}\xi}, \tag{50}$$

which substitutes for the HFT, in the sense that I plays the role assigned to H in the theorem, a new I-property, as far as we know.

6. Examples

We illustrate now in simple examples how the Hellmann–Feynman strictures apply in a Fisher context. We set $\hbar = m = 1$.

6.1. Quantum square well

Consider a free particle moving along the x-axis between infinitely high walls at $x = \pm a$. The eigenstates are, for example,

$$\psi_n = a^{-1/2}\cos(n\pi x/2a); \quad n \text{ odd integer}. \tag{51}$$

Our parameter here is, of course, a. The eigenenergies read

$$E_n = \pi^2 n^2/(8a^2). \tag{52}$$

Since no mean value is known, one wonders whether relation (50) will hold. Here, the Fisher measure is

$$I = 4\int_{-a}^{a}\mathrm{d}x(\psi_n')^2 = \pi^2 n^2/a^2, \tag{53}$$

so relation (50) indeed holds.

6.2. Ground state of the harmonic oscillator

We have, with $\lambda_2 = -8a_2$ and $a_2 = \omega^2/2$,

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + a_2x^2\right)\psi = \frac{\alpha}{8}\psi. \tag{54}$$

The Gaussian wave function,

$$\psi(x) = \left(2\pi\sigma^2\right)^{-1/4}\exp\left(-\frac{x^2}{4\sigma^2}\right), \tag{55}$$

is a solution of the above Schrödinger equation [38] with α, λ_2 linked in the fashion

$$n\langle x^2\rangle = \sigma^2 \qquad \alpha = \frac{2}{\sigma^2}, \qquad \lambda_2 = -\frac{1}{\sigma^4}, \qquad a_2 = \frac{1}{8\sigma^4}, \tag{56}$$

entailing

$$\psi(x) = (\omega/\pi)^{1/4}\exp\left(-\frac{\omega x^2}{2}\right). \tag{57}$$

The pertinent $I(f)$ turns out to be

$$I = I_{\mathrm{HO}} = \int \mathrm{d}x f(x) \left\{ \frac{\partial}{\partial x} \ln[f(x)] \right\}^2 = \sigma^{-2} = 2\omega \Rightarrow (\mathrm{d}I_{\mathrm{HO}}/d\langle x^2\rangle) = -8a_2 = \lambda_2, \tag{58}$$

as it should (first reciprocity relation). We also have

$$\begin{aligned} &\alpha = 4\omega, \qquad \lambda_2 = -4\omega^2 \qquad E = \alpha/8 = \omega/2 = \sqrt{8a_2}/4, \\ &(\mathrm{d}E/\mathrm{d}a_2) = (1/\sqrt{8a_2}) = \sigma^2 = \langle x^2\rangle, \end{aligned} \tag{59}$$

and we reobtain the second reciprocity relation as an instance of the Hellmann–Feynman theorem. It is perhaps instructive to spell out the canonical form $I = \alpha + \lambda_2\langle x^2\rangle$, which can be cast here in the fashion

$$I = 2\omega = 4\omega + [-4\omega^2][1/2\omega] = 4\omega[1 - 1/2]. \tag{60}$$

6.3. Harmonic oscillator in a uniform field

Our unit-mass particle moving in the harmonic oscillator (HO) potential is now assumed additionally (i) to have electrical charge q and (ii) to be subjected to a uniform electric field ϵ in the x-direction. We have

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + a_1 x + a_2 x^2 \right) \psi = E\psi, \tag{61}$$

with $a_1 = -q\epsilon$ and $a_2 = \omega^2/2$. In general, we may then add a term $-\omega^2\xi x$ to the HO term, which results in a polarization energy $\omega^2\xi^2/2$ [38],

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}u^2} + \frac{1}{2}\omega^2 u^2 \right) \psi = \bar{E}\psi, \tag{62}$$

where

$$u = x - \xi, \quad \xi = \frac{q\epsilon}{\omega^2}, \qquad \bar{E} = E + \frac{1}{2}\omega^2\xi^2. \tag{63}$$

A slightly modified version of (57) now represents the exact ground state,

$$\psi(x) = (\omega/\pi)^{1/4} \exp\left(-\frac{\omega(x-\xi)^2}{2} \right), \tag{64}$$

for which the Fisher measure turns out to be

$$I = 2\omega. \tag{65}$$

Also,

$$\begin{aligned} &\langle (x-\xi)\rangle = 0 \longrightarrow \langle x\rangle = \xi, \\ &\langle (x-\xi)^2\rangle = \frac{1}{2\omega} \longrightarrow \langle x^2\rangle = \frac{1}{2\omega} + \xi^2. \end{aligned}$$

Then, with $\lambda_1 = -8a_1 = 8q\epsilon$ and $\lambda_2 = -8a_2 = -4\omega^2$, we obtain

$$\begin{aligned} \alpha &= I - \lambda_1\langle x\rangle - \lambda_2\langle x^2\rangle = 2\omega - 8q\epsilon\xi + 4\omega^2\left(\frac{1}{2\omega} + \xi^2\right) \\ &= 4\omega - 8q\epsilon\xi + 4\omega^2\xi^2 4\omega - 4\omega^2\xi^2, \end{aligned}$$

so that the mandatory division by 8 (cf. (49)) yields the polarization energy mentioned above,

$$\alpha = 4\omega - 4\omega^2\xi^2 \longrightarrow E = \frac{\omega}{2} - \frac{1}{2}\omega^2\xi^2,$$

and the reciprocity relations hold.

7. Conclusions

In this communication, we have shown

- how to associate a (real) Schrödinger equation to a Fisher information measure, and
- how to link the Hellmann–Feynman theorem to the Jaynes reciprocity relations of information theory (cf. Eq. (13)), for potential functions that can be series expanded. Here, the pertinent expansion coefficients are to be regarded as Lagrange multipliers for the Fisher expression (36).

The Hellmann–Feynman theorem is seen to be just one special reciprocity relation. In order to find this result, restriction to real wave functions was necessary. This is not so drastic as one might, at first sight, think. If ψ is an eigenfunction, so is $\psi*$, and, because of linearity, their sum $\psi+\psi*$, which is real, is also an eigenfunction. Moreover, a quantum system's eigenfunctions can always be taken as real for one-dimensional scenarios, or for the ground state of systems with an N-dimensional configuration space and a real potential function [36].

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Appendix. Sketch of the proof of the Hellmann–Feynman theorem

Let ψ' stand for $(\partial\psi/\partial b)$, and remember that (1) $H|\psi_i(b)\rangle = E_i|\psi_i(b)\rangle$ and (2) $\langle\psi_i(b)|\psi_i(b)\rangle = 1 \Rightarrow (\mathrm{d}/\mathrm{d}b)\langle\psi_i(b)|\psi_i(b)\rangle = 0$. Then,

$$\begin{aligned}\frac{\partial E_i(b)}{\partial b} &= \langle\psi_i'(b)|H|\psi_i(b)\rangle + \langle\psi_i(b)|H|\psi_i'(b)\rangle + \langle\psi_i(b)|\frac{\partial H}{\partial b}|\psi_i(b)\rangle \\ &= \langle\psi_i'(b)|E_i(b)|\psi_i(b)\rangle + \langle\psi_i(b)|E_i(b)|\psi_i'(b)\rangle + \langle\psi_i(b)|\frac{\partial H}{\partial b}|\psi_i(b)\rangle \\ &= E_i(b)(\mathrm{d}/\mathrm{d}b)\langle\psi_i(b)|\psi_i(b)\rangle + \langle\psi_i(b)|\frac{\partial H}{\partial b}|\psi_i(b)\rangle \\ &= 0 + \langle\psi_i(b)|\frac{\partial H}{\partial b}|\psi_i(b)\rangle, \end{aligned} \tag{66}$$

where, obviously, the differentiability of E_i, H and ψ_i with respect to b was assumed. The HFT, and others derived from it, has been used in many areas of physics, and specially in solid state and molecular physics after the pioneering work of Feynman [31].

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