Parameter-free ansatz for inferring ground state wave functions of even potentials

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Abstract. Schrödinger's equation (SE) and the information-optimizing principle based on Fisher's information measure (FIM) are intimately linked, which entails the existence of a Legendre transform structure underlying the SE. In this comunication we show that the existence of such an structure allows, via the virial theorem, for the formulation of a parameter-free ground state's SE-ansatz for a rather large family of potentials. The parameter-free nature of the ansatz derives from the structural information it incorporates through its Legendre properties.

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1. Introduction

Few quantum-mechanical models admit of exact solutions. Approximations of diverse type constitute the hard-core of the armory at the disposal of the quantum-practitioner. Since the 60's, hypervirial theorems have been gainfully incorporated to the pertinent arsenal [1, 2]. We revisit here the subject in an information-theory context, via Fisher's information measure (FIM) with emphasis on i) its Legendre properties and ii) its relation with the virial theorem.

Remark that the notion of using a small set of relevant expectation values so as to describe the main properties of physical systems may be considered the leit-motiv of statistical mechanics [3]. Developments based upon Jaynes' maximum entropy principle constitute a pillar of our present understanding of the discipline [4]. This type of ideas has also been fruitfuly invoked for obtaining the probability distribution associated to pure quantum states via Shannon's entropy (see for instance, [5] and references therein). In such a spirit, Fisher information, the local counterpart of the global Shannon quantifier [6], first introduced for statistical estimation purposes [6]. has been shown to be quite useful for the variational characterization of quantal equations of motion [7]. In particular, it is well-known that a strong link exists between Fisher's information measure (FIM) I and Schrödinger's wave equation (SE) [8, 10, 9, 11, 12, 13, 14]. Such connection is based upon the fact that a constrained Fisher-minimization leads to a SE-like equation [6, 8, 10, 9, 11, 12, 13, 14]. In turn, this guarantees the existence of intriguing relationships between various quantum quantities reminiscent of the ones that characterize thermodynamics due to its Legendre-invariance structure [8, 10]. Interestingly enough, SE-consequences such as the Hellmann-Feynman and the Virial theorems can be re-interpreted in terms of thermodynamics' Legendre reciprocity relations [12, 11], a fact suggesting that a Legendre-transform structure underlies the non-relativistic Schrödinger equation. As a consequence, the possible energy-eigenvalues become constrained by such structure in a rather unsuspected way [11, 12, 13, 14], which allows one to obtain a first-order differential equation, unrelated to Schröedinger's equation [13, 14], that energy eigenvalues must necessarily satisfy. The predictive power of that equation was explored in [15], where the formalism was applied to the quantum anharmonic oscillator. Exploring further interesting properties of this "quantal-Legendre" structure will occupy us below. As a result, it will be seen that, as a direct consequence of the Legendre-symmetry that underlies the connection between Fisher's measure and Schröedinger's equation one immediately encounters an elegant expression for an ansatz, in terms of quadratures, of the ground state (gs) wave function of a rather wide category of potential functions.

2. Basic ideas

A special, and particularly useful FIM-expression (not the most general one) is to be quoted. Let x be a stochastic variable and $f(x) = \psi(x)^2$ the probability density function

(PDF) for this variable. Then I reads [6]

$$I = \int f(x) \left(\frac{\partial \ln f(x)}{\partial x} \right)^2 dx = 4 \int dx \, [\nabla \psi(x)]^2 \, ; \qquad f = \psi^2. \tag{1}$$

Focus attention now a system that is specified by a set of M physical parameters μ_k. We can write $\mu_k = \langle A_k \rangle$, with $A_k = A_k(x)$. The set of μ_k-values is to be regarded as our prior knowledge (available empirical information). Again, the probability distribution function (PDF) is called $f(x)$. Then,

$$\langle A_k \rangle \; = \; \int \; dx \; A_k(x) \; f(x), \qquad k = 1, \ldots, M. \tag{2}$$

It can be shown (see [8, 9]) that the *physically relevant* PDF $f(x)$ minimizes FIM subject to the prior conditions and the normalization condition. Normalization entails $\int dx f(x) = 1$, and, consequently, our Fisher-based extremization problem becomes

$$\delta \left(I - \alpha \int \; dx \; f(x) - \sum_{k=1}^{M} \; \lambda_k \int \; dx \; A_k(x) \; f(x) \right) \; = \; 0, \tag{3}$$

with $(M+1)$ Lagrange multipliers λ_k $(\lambda_0 = \alpha)$. The reader is referred to Ref. [8] for the details of how to go from (3) to a Schrödinger's equation (SE) that yields the desired PDF in terms of the amplitude $\psi(x)$. This SE is of the form

$$\left[- \frac{1}{2} \, \frac{\partial^2}{\partial x^2} + U(x) \right] \psi \; = \; \frac{\alpha}{8} \, \psi, \qquad U(x) = \; - \frac{1}{8} \, \sum_{k=1}^{M} \lambda_k \; A_k(x), \tag{4}$$

and is to be interpreted as the (real) Schrödinger equation (SE) for a particle of unit mass $(\hbar = 1)$ moving in the effective, "information-related pseudo-potential" $U(x)$ [8] in which the normalization-Lagrange multiplier $(\alpha/8)$ plays the role of an energy eigenvalue. The λ_k are fixed by recourse to the available prior information. For one-dimensional scenarios, $\psi(x)$ is real [20] and

$$I = \int \psi^2 \left(\frac{\partial \ln \psi^2}{\partial x} \right)^2 dx \; = \; 4 \int \left(\frac{\partial \psi}{\partial x} \right)^2 dx \; = \; -4 \int \psi \frac{\partial^2}{\partial x^2} \psi \; dx \tag{5}$$

so from (4) one finds a simple and convenient $I-$expression

$$I \; = \; \alpha + \sum_{k=1}^{M} \; \lambda_k \, \langle A_k \rangle \, . \tag{6}$$

Legendre structure

The connection between the variational solutions f and thermodynamics was established in Refs. [8] and [10] in the guise of typical Legendre reciprocity relations. These constitute thermodynamics' essential formal ingredient [21] and were re-derived à la Fisher in [8] by recasting (6) in a fashion that emphasizes the role of the relevant independent variables,

$$I(\langle A_1 \rangle, \ldots, \langle A_M \rangle) \; = \; \alpha + \sum_{k=1}^{M} \; \lambda_k \langle A_k \rangle. \tag{7}$$

Obviously, the Legendre transform main goal is that of changing the identity of our relevant independent variables. As for the normalization multiplier α, that plays the role of an energy-eigenvalue in Eq. (4), we have

$$\alpha(\lambda_1, \ldots, \lambda_M) = I - \sum_{k=1}^{M} \lambda_k \langle A_k \rangle . \tag{8}$$

After these preliminaries we straightforwardly encounter the three reciprocity relations [8]

$$\frac{\partial \alpha}{\partial \lambda_k} = -\langle A_k \rangle \; ; \qquad \frac{\partial I}{\partial \langle A_k \rangle} = \lambda_k \; ; \qquad \frac{\partial I}{\partial \lambda_i} = \sum_{k}^{M} \lambda_k \frac{\partial \langle A_k \rangle}{\partial \lambda_i}, \tag{9}$$

the last one being a generalized Fisher-Euler theorem.

3. Fisher measure and quantum mechanical connection

Since the potential function $U(x)$ belongs to $\mathcal{L}_2$, it admits of a series expansion in the basis x, $x^2\, x^3$, *etc.* [22]. The $A_k(x)$ themselves belong to $\mathcal{L}_2$ as well, and can also be series-expanded in similar fashion. This enables us to base our future considerations on the assumption that the a priori knowledge refers to moments x^k of the independent variable, i.e., $\langle A_k \rangle = \langle x^k \rangle$, and that one possesses information about M of these moments $\langle x^k \rangle$. Our "information" potential U thus reads

$$U(x) = -\frac{1}{8} \sum_k \lambda_k \, x^k. \tag{10}$$

We will assume that the first M terms of the above series yield a satisfactory representation of $U(x)$. Consequently, the Lagrange multipliers are identified with U(x)'s series-expansion's coefficients.
In a Schrödinger-scenario the *virial theorem* states that [11]

$$\left\langle \frac{\partial^2}{\partial x^2} \right\rangle = - \left\langle x \, \frac{\partial}{\partial x} U(x) \right\rangle = \frac{1}{8} \sum_{k=1}^{M} k \, \lambda_k \, \langle x^k \rangle \, , \tag{11}$$

and thus, from (5) and (11) a useful, virial-related expression for Fisher's information measure can be arrived at [11]

$$I = - \sum_{k=1}^{M} \frac{k}{2} \lambda_k \, \langle x^k \rangle, \tag{12}$$

I is explicit function of the M physical parameters $\langle x^k \rangle$. Eq. (12) encodes the information provided by the virial theorem [12, 11].

Interestingly enough, the reciprocity relations (RR) (9) can be re-derived on a strictly pure quantum mechanical basis [11], starting from the quantum Virial theorem [which leads to Eq. (12)] plus information provided by the quantum Hellmann-Feynman theorem. This fact strongly suggests that a Legendre structure underlays the one-dimensional Schröedinger equation [11]. Thus, with $\langle A_k \rangle = \langle x^k \rangle$, our "new" reciprocity relations are given by

$$\frac{\partial \alpha}{\partial \lambda_k} = -\langle x^k \rangle \; ; \qquad \frac{\partial I}{\partial \langle x^k \rangle} = \lambda_k \; ; \qquad \frac{\partial I}{\partial \lambda_i} = \sum_k^M \lambda_k \frac{\partial \langle x^k \rangle}{\partial \lambda_i}, \tag{13}$$

FIM expresses a relation between the independent variables or control variables (the prior information) and I. Such information is encoded into the functional form $I = I(\langle x^1 \rangle, ..., \langle x^M \rangle)$. For later convenience, we will also denote such a relation or encoding-process as $\{I, \langle x^k \rangle\}$. We see that the Legendre transform FIM-structure involves both eigenvalues of the "information-Hamiltonian" and Lagrange multipliers. Information is encoded in I via these Lagrange multipliers, i.e., $\alpha = \alpha(\lambda_1, ...\lambda_M)$, together with a bijection $\{I, \langle x^k \rangle\} \quad \longleftrightarrow \quad \{\alpha, \lambda_k\}$.

In a $\left\{I, \langle x^k \rangle\right\}$ - scenario, the λ_k are functions dependent on the $\langle x^k \rangle$-values. As shown in [12], substituting the RR given by (13) in (12) one is led to a *linear, partial differential equations (PDE)* for I,

$$\lambda_k = \frac{\partial I}{\partial \langle x^k \rangle} \qquad \longrightarrow \qquad I = -\sum_{k=1}^M \frac{k}{2} \langle x^k \rangle \frac{\partial I}{\partial \langle x^k \rangle} \,. \tag{14}$$

and a complete solution is given by

$$I(\langle x^1 \rangle, ..., \langle x^M \rangle) = \sum_{k=1}^M C_k \; \left| \langle x^k \rangle \right|^{-2/k} , \tag{15}$$

where C_k are positive real numbers (integration constants). The I - domain is $D_I = \left\{(\langle x^1 \rangle, ..., \langle x^M \rangle) / \langle x^k \rangle \; \in \; \Re_o \right\}$. Eq. (15) states that 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 [6], I is a convex function. We may obtain λ_k from the reciprocity relations (13). For $\langle x^k \rangle \; > \; 0$ one gets,

$$\lambda_k = \frac{\partial I}{\partial \langle x^k \rangle} = -\frac{2}{k} C_k \; \langle x^k \rangle^{-\,(2+k)/k} < 0 \,. \tag{16}$$

and then, using (6), we obtain the α - normalization Lagrange multiplier. For a discussion on how to obtain the reference quantities C_k see [15].

The general solution for the I - PDE does exist and its uniqueness has been demonstrated via an analysis of the associated Cauchy problem [12]. Thus, Eq. (15) implies what seems to be a kind of "universal" prescription, a linear PDE that any variationally (with constraints) obtained FIM must necessarily comply with.

4. Present results

4.1. Inferring the PDF for even potentials

For even informational potentials good SWE-ansatz can be formulated via probability distribution functions (PDF) that satisfy the virial theorem. The potentials are of the form

$$U(x) = -\frac{1}{8}\sum_{k=1}^{M} \lambda_{2k}\; x^{2k}, \tag{17}$$

and the ansatz can be straightforwardly derived from (1) and (11). This constitutes our main present result. The procedure is as follows. Begin with the Fisher measure I, "virially" expressed as

$$I \;=\; -\,4\left\langle \frac{\partial^2}{\partial x^2} \right\rangle = 4\left\langle x\,\frac{\partial}{\partial x} U(x) \right\rangle \quad\longrightarrow\quad I \;=\; -\left\langle \sum_{k=1}^{M} k\,\lambda_{2k}\; x^{2k} \right\rangle \tag{18}$$

which, in the Fisher-scenario, can obviouly be written as

$$\int dx\; f(x)\left(\frac{\partial \ln f(x)}{\partial x}\right)^2 \;=\; -\int dx\; f(x)\,\sum_{k=1}^{M} k\,\lambda_{2k}\; x^{2k}\;, \tag{19}$$

or

$$\int dx\; f(x)\left[\left(\frac{\partial \ln f(x)}{\partial x}\right)^2 \;+\; \sum_{k=1}^{M} k\,\lambda_{2k}\; x^{2k}\right] \;=\; 0. \tag{20}$$

We devise an ansatz f_A that by construction verifies (20). We merely require fulfillment of

$$\left(\frac{\partial \ln f_A(x)}{\partial x}\right)^2 \;+\; \sum_{k=1}^{M} k\,\lambda_{2k}\; x^{2k} \;=\; 0. \tag{21}$$

Clearly, we inmediatly obtain,

$$\left(\frac{\partial \ln f_A(x)}{\partial x}\right)^2 \;=\; -\sum_{k=1}^{M} k\,\lambda_{2k}\; x^{2k}\;, \tag{22}$$

that leads to

$$f_A(x) \;=\; exp\left\{-\int dx\,\sqrt{-\sum_{k=1}^{M} k\,\lambda_{2k}\; x^{2k}}\right\}\;, \tag{23}$$

where the minus sign in the exponential argument was chosen so as to enforce the condition that $f(x) \overset{x\to\pm\infty}{\longrightarrow} 0$. Eq. (23) provides us with a nice, rather general and virially motivated ansatz. Is it good enough for dealing with the SWE?. We look for an answer below.

4.2. Harmonic oscillator (HO)

It is obligatory to start our investigation with reference to the harmonic oscillator. One assumes that the prior Fisher-information is given by

$$\langle x^2\rangle \;=\; \frac{1}{2\omega}\;. \tag{24}$$

The pertinent FIM can now be obtained by using (15),

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

which saturates the Cramer-Rao bound [6] when $C_2 = 1$,

$$I \, \langle x^2 \rangle \;=\; C_2 \;=\; 1 \qquad \Longrightarrow \qquad I \;=\; \langle x^2 \rangle^{-1} \, . \tag{25}$$

The pertinent Lagrange multiplier can be obtained by recourse to the reciprocity relations (9) and (25),

$$\lambda_2 \;=\; \frac{\partial I}{\partial \langle x^2 \rangle} \;=\; - \, \langle x^2 \rangle^{-2} \, . \tag{26}$$

The prior-knowledge (24) is encoded into the FIM (25), and the Lagrange multiplier λ_2 (26),

$$I \;=\; \langle x^2 \rangle^{\,-1} = \; 2\omega \, ; \qquad \lambda_2 \;=\; - \, \langle x^2 \rangle^{\,-2} \;=\; - \, 4\omega^2 \, . \tag{27}$$

and the $\alpha-$value is gotten from (8),

$$\alpha \;=\; I - \;\lambda_2 \, \langle x^2 \rangle = \; 4 \, \omega. \tag{28}$$

Our ansatz-PDF can be extracted from (23) as follows

$$f(x) \;=\; exp \left\{ - \int dx \, \sqrt{\, 4\omega^2 \, x^2} \right\} \;=\; N \, exp \left\{ - \, \omega x^2 \right\} \, , \tag{29}$$

with,

$$\int \, f(x) \, dx = \; 1 \qquad \longrightarrow \qquad N \;=\; \left(\frac{\omega}{\pi} \right)^{1/2} \, , \tag{30}$$

the exact result.

5. Ground state eigenfunction of the general, even-anharmonic oscillator

We outline here the methodology for constructing the ground state ansatz for an anharmonic oscillator of the form (we shall herefrom omit the subscript A)

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \sum a_{2k} x^{2k} \right] \psi(x) \;=\; E\psi(x) \tag{31}$$

According to [13, 14], we can ascribe to (34) a Fisher measure and effect then the following identifications:

$$\alpha = 8E \, , \qquad \lambda_{2k} = -8 \; a_{2k} \, , \qquad f(x) = \psi^2(x). \tag{32}$$

Accordingly, we get our ansatz by substituting into (23) the quantities given by (32).

$$\psi(x) \;=\; exp \left\{ -\frac{1}{2} \int dx \, \sqrt{ \sum_{k=1}^{M} \, 8 \; k \, a_{2k} \; x^{2k} } \right\} \, , \tag{33}$$

As an illustration of the procedure, we deal below with the quartic anharmonic oscillator.

5.1. Quartic anharmonic oscillator

The Schrödinger equation for a particle of unit mass in a quartic anharmonic potential reads,

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}\,\omega^2\,x^2\,+\frac{1}{2}\,\lambda\,x^4\right]\psi \;=\; E\,\psi, \tag{34}$$

where λ is the anharmonicity constant. Expression (33) takes the form

$$\psi(x) \;=\; exp\left\{-\frac{1}{2}\int\;\sqrt{4\,\omega^2\,x^2+8\,\lambda\,x^4}\;dx\right\}.$$

Now, from an elemental integration, we obtain the desired eigenfunction

$$\psi(x) = \;N\;exp\left\{\frac{\omega^3}{6\lambda}\left[1-\;\left(1+\frac{2\lambda}{\omega^2}\,x^2\right)^{3/2}\right]\;\right\}\;, \tag{35}$$

where N is the normalization constant.

When $\lambda \to 0$ one re-obtains the Gaussian form,

$$\lim_{\lambda\to 0}\psi(x) \;=\; \psi_{HO} \;=\; N\;exp\left(-\,\omega x^2\right)\;, \tag{36}$$

and, when $\omega \to 0$ the pure anharmonic oscillator eigenfunction is given by,

$$\lim_{\omega\to 0}\psi(x) = \;\psi_{PAO} \;=\; N\;exp\left(-\,\frac{\sqrt{2\lambda}}{3}\;|x|^3\right)\;, \tag{37}$$

Once we have at our dispossal the anzsatz gs-eigengenfunction, we obtain the corresponding eigenvalues following one of the two procedures.

Schröedinger procedure:

$$E \approx \langle\psi|H|\psi\rangle = \int\;dx\;\psi(x)\left[-\,\frac{1}{2}\,\frac{\partial^2}{\partial x^2}+\;\frac{1}{2}\,\omega^2\,x^2\;+\frac{1}{2}\,\lambda\,x^4\right]\psi(x)\;=$$

$$=\int\;dx\;\psi(x)\left[\frac{\omega}{2}\left(1+\frac{2\lambda}{\omega^2}\,x^2\right)^{1/2}+\frac{\lambda}{\omega}\,x^2\;\left(1+\frac{2\lambda}{\omega^2}\,x^2\right)^{-1/2}-\frac{\lambda}{2}\,x^4\right]\psi(x)\;. \tag{38}$$

Fisher procedure:

From (6) and (12), with $\lambda_2 = -4\omega^2$, $\lambda_4 = -4\lambda$, we have

$$\alpha \;=I-\sum_{k=1}^{M}\,\lambda_k\left\langle x^k\right\rangle \;=\; -\sum_{k=1}^{M}\left(\frac{k}{2}+1\right)\lambda_k\,\langle x^k\rangle \;=\; 8\,\omega^2\,\langle x^2\rangle+12\,\lambda\,\langle x^4\rangle, \tag{39}$$

Evaluating the moments with the anzsatz function, we have

$$\langle x^p\rangle_A \;\approx\; \int dx\;x^p\;f(x) \;=\; \int dx\;x^p\;\psi^2(x) \tag{40}$$

and, accordingly,

$$E = \frac{\alpha}{8}\;\approx\;\omega^2\,\langle x^2\rangle_A+\frac{3}{2}\,\lambda\,\langle x^4\rangle_A\;, \tag{41}$$

We determine E *without passing first through a Schrödinger equation*, which is a nice aspect of the present approach. The question for the suitability of our ansatz is answered by looking at the Table below.

Table:
SE-ground-state eigenvalues (34) for $\omega = 1$ and several values of the anharmonicity-constant λ.

The values of the second column correspond to those one finds in the literature, obtained via a numerical approach to the SE. *These* results, in turn, are nicely reproduced by some interesting theoretical approaches that, however, need to introduce and adjust some empirical constants [19]. Our ansatz-values, in the third column, are obtained by a parameter-free procedure. The fourth column displays the associated Cramer-Rao bound, which is almost saturated in all instances.

λ	E_{num}	E	$I\ \langle x^2 \rangle$
0.0001	0.50003749	0.50003749	1.000000015
0.001	0.50037435	0.50037444	1.000001477
0.01	0.50368684	0.50369509	1.000129847
0.1	0.53264275	0.53305374	1.000129847
1	0.69617582	0.70188134	1.046344179
10	1.22458704	1.25080186	1.099588057
100	2.49970877	2.57093830	1.123451126
1000	5.31989436	5.48276171	1.130099216

6. Conclusions

The link Schröedinger equation - Fisher measure has been employed so as to infer, via the pertinent reciprocity relations, a parameter-free ground state ansatz wave function for a rather ample family of even potentials, of the form

$$U(x) = \sum a_{2k} x^{2k}, \tag{42}$$

in terms of the coefficients a_{2k}. Its parameter-free character notwithstanding, our ansatz provides good results, as evidenced by the examples here examined. It incorporates only the knowledge of the virial theorem, via the Legendre-symmetry that underlies the connection between Fisher's measure and Schröedinger equation. One may again speak here of the power of symmetry considerations. in devising physical treatments.

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