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Fisher information and quantum systems with position-dependent effective mass

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Abstract

We show that effective masses in nonrelativistic quantum mechanics arise in a natural fashion from the Frieden and Soffer's Principle of Extremal Information (EPI) when the mean values of operators involving the momentum $\hat{p}$ and exhibiting the form $\hat{p}\, f(\hat{x})\, \hat{p}$ are included as constraints. A position-dependent effective mass, which is currently used in the literature as a simple model for diverse phenomena in quantum physics, appears after extremalizing Fisher's information measure with the above constraints. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Frieden and Soffer have recently shown that many important differential equations of Physics can be obtained from a general variational principle, the extreme physical information (EPI), which fixes both the Lagrangian and the physical constants of each scenario [1,2]. The Information here is that the version of the one originally introduced in 1925 by Fisher [3–5] (to be denoted as FIM) that applies for translation families, i.e., refers to a measure of the inverse uncertainty in determining *a position parameter* by a maximum likelihood estimation [6]. Applications of Fisher information to diverse problems in theoretical physics have received great impulse through the pioneering

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work of Frieden, Soffer, Silver, Abe, Nikolov, Reginatto, and others [1,2,6–19], who have unveiled many of its physically relevant properties and clarified its relation to Shannon's logarithmic information measure.

Frieden and coworkers have shown that fundamental equations of Physics can be traced back to FIM-related extremizing procedures, while Silver has introduced an interesting inference approach that, via a clever connection between Shannon's information measure and Fisher's one, allows for the conclusion that a judicious sort of "interpolation" between them yields deep and illuminating insights into the structure of quantum statistical mechanics. Reginatto [16,17] has shown that Madelung's [20,21] hydrodynamical formulation of both the time dependent Schrödinger equation and the Pauli equation can be derived using the principle of extremum Fisher information. It is worth mentioning that E. Schrödinger's first attempt to derive his celebrated equation from an appropriate Lagrangian was based on the extremalization of a functional that, in retrospect, can be seen to be essentially Fisher Information, although there seems to be no record that he was aware of Fisher's tenets at the time [22].

Given a probability distribution $\rho(x)$, $x \in \mathscr{R}$, Fisher's information measure (for translation families), expressed as an expectation value over ρ, adopts the appearance

$$I = \left\langle \left(\frac{1}{\rho} \frac{\mathrm{d}\rho}{\mathrm{d}x} \right)^2 \right\rangle . \tag{1}$$

The fact that a systematic procedure that involves an I-extremization principle with respect to a probability density $\rho(x)$ gives rise to the most important differential equations of Physics is discussed at length in Refs. [1,2]. There the authors have presented the EPI in terms of a Fisher information transfer process involving an agent akin to the celebrated Maxwell demon [1,2].

In the particular Schrödinger's equation instance, if for simplicity's sake we restrict our attention here to the one-dimensional case of a particle of mass m that moves in a potential well $V(x)$, we deal, for bound states, just with real wave functions and can write

$$\psi^2(x) = \rho(x) . \tag{2}$$

Now, if one assumes the knowledge of a set of, say, the expectation values of N commuting operators $\hat{O}_j(x)$, $j = 1, \ldots, N$ [6], a constrained extremization of (1) that respects the assumedly known values

$$\langle \hat{O}_1(x) \rangle, \ldots, \langle \hat{O}_N(x) \rangle , \tag{3}$$

leads to a Schrödinger-like equation in which the potential well acquires the form

$$V(x) = -\sum_{j=1}^{N} \gamma_j \hat{O}_j , \tag{4}$$

where the γ's are Lagrange's multipliers that arise in the FIM extremizing process [6].

What happens if, additionally, one a priori knows the expectation values of observables that involve the momentum operator $\hat{p}$? Such a situation has not been thus far addressed, as far as we know. Up to now all applications of the Frieden–Soffer variational principle to quantum mechanics were based on the assumption that the only available information is given by the expectation values of functions of the coordinate operator $\hat{x}$ alone. However, from a physical point of view, the mean value of observables involving the momentum operator $\hat{p}$ are as legitimate input information as are the functions of $\hat{x}$. There is no fundamental reason for restricting the discussion of the principle of extreme information to such a limited kind of prior information. We show here that interesting consequences can be traced to the foreknowledge of these additional pieces of information. We discuss their role in detailed fashion in the next section. Some applications are discussed in Section 3, and, finally, conclusions are drawn in Section 4.

2. The constrained Fisher information extremization

Consider now the set of operators

$$\hat{C}_i = \frac{1}{2m}\hat{p}\, f_i(\hat{x})\,\hat{p}, \quad i = 1,\ldots,M\,, \tag{5}$$

and assume we add, to the set $\hat{O}_j$ $(j = 1,\ldots,N)$ discussed in the preceding section (cf. (3)), the foreknowledge of the set of expectation values $\langle \hat{C}_i \rangle$ (associated multipliers β_i). The associated variational problem involves the Lagrangian $\mathscr{L}$

$$\mathscr{L} = \frac{\hbar^2}{2m}\int \mathrm{d}x \left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right)^2 - \sum_{j=1}^{N} \gamma_j \int \mathrm{d}x\, \psi^2 \hat{O}_j(x)$$

$$-\frac{\hbar^2}{2m}\sum_{i=1}^{M} \beta_i \int \mathrm{d}x\, f_i(x)\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right)^2 - E\int \mathrm{d}x\, \psi^2\,. \tag{6}$$

The first term is the Fisher information measure for translation families while the second and third ones impose appropriate constraints via the Lagrange multipliers γ_j and β_i (a partial integration step is needed in the case of the β-integrals). The last term represents the normalization condition, with Lagrange multiplier E. Extremizing (6) with these constraints leads now to

$$-\frac{\hbar^2}{2m^*(x)}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\hbar^2}{2m^*(x)}\right)\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} + V\psi = E\psi\,, \tag{7}$$

which can be regarded as a Schrödinger's equation *only* if we are willing to consider *a position-dependent effective mass* $m^*(x)$, which constitutes indeed a well known and useful model for the description of many physical problems.

In particular, the effective mass approximation is an important tool for the determination of electronic properties in semiconductors [23] and quantum dots [24]. The concept of effective mass is also relevant in connection with the popular energy density functional (EDF) treatment of the quantum many body problem [25]. In the EDF approach the non-local terms of the associated potential can be expressed in terms of a position-dependent effective mass $m^*(x)$. The ensuing formalism is extensively used in nuclei [25], quantum liquids [26], ^{3}He clusters [27], and metal clusters [28].

The effective mass in (7) adopts the appearance

$$\frac{\hbar^2}{2m^*(x)} = \frac{\hbar^2}{2m}\left(1 - \sum_{i=1}^{M} \beta_i f_i(x)\right) , \tag{8}$$

while, as stated above,

$$V = -\sum_{j=1}^{N} \gamma_j \hat{O}_j . \tag{9}$$

By recourse to the standard transformation [25],

$$\psi = \sqrt{\frac{m^*(x)}{m}}\, u(x) , \tag{10}$$

one is in a position to write down a Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u(x)}{\mathrm{d}x^2} + V(x,E)u(x) = Eu(x) , \tag{11}$$

that involves a *local* equivalent potential $V(x,E)$,

$$V(x,E) = \frac{m^*(x)}{m}\left[V(x) - \frac{(Q')^2}{4Q} + \frac{1}{2}Q''\right] + \left(1 - \frac{m^*(x)}{m}\right)E , \tag{12}$$

where the primes indicate derivatives with respect to x and

$$Q = \frac{\hbar^2}{2m^*(x)} . \tag{13}$$

Some comments concerning our particular choice (5) for the observables C_i are in order before proceeding with the applications of the above formalism. Operators of the form $\hat{p} f_i(\hat{x})\hat{p}$ are among the simplest hermitic operators quadratic in p. Alternative choices like

$$\tilde{C}_i = \hat{p}^2 f_i(\hat{x}) + f_i(\hat{x})\hat{p}^2 \tag{14}$$

are also possible, leading to a Schrödinger equation with effective mass exhibiting essentially the same form (7). Our particular choice (5) for the momentum-dependent constraints has, however, an appealing formal property. When no prior knowledge of expectation values of operators depending only on $\hat{x}$ is available, Schrödinger equations with no potential energy terms are obtained. Operators linear in $\hat{p}$ do not lead to a Schrödinger equation with an effective mass. A kinetic energy term with a vector potential-like contribution is obtained instead (this can be appreciated more clearly in a three dimensional setting). On the other hand, constraints associated with observables involving cubic or larger powers of the momentum would originate eigenvalue differential equations with higher than second spatial derivatives.

In the following section we show that both the Lagrange multipliers γ_j and β_i can be selfconsistently determined according to the methodology detailed in Refs. [29,30].

Good results are obtained. The addition of information concerning operators (5) is seen to improve on the quality of inferred wave functions obtained with the sole knowledge of the operators $\hat{O}_j$. One also infers the effective mass.

3. Applications

3.1. Morse potential

We tackle, as a first example, the Morse potential, used in modelling the interaction of diatomic molecules [31,32]

$$V(x) = A(1 - e^{-x})^2 \tag{15}$$

with $A = 40$. We assume the foreknowledge of the expectation values $\langle \hat{x}^m \rangle$, $m = 1, \ldots, 4$ and $\langle \hat{C}_i \rangle$, $i = 1, 2$, with $f_1 = \exp(-x^2)$ and $f_2 = x \exp(-x^2)$. The results are depicted in Fig. 1. The effective mass that results from the foreknowledge of the $\langle \hat{C}_i \rangle$ is also displayed in Fig. 2. Assuming one particle per level and $\mathcal{N} = 5$ occupied levels, the inferred density obtained with the informational supplement represented by the expectation values of the operators $\hat{C}_i$ improves upon the density obtained assuming only the foreknowledge of x^m-mean values. A similar assertion applies in the case of inferred x^m-moments (see Table 1).

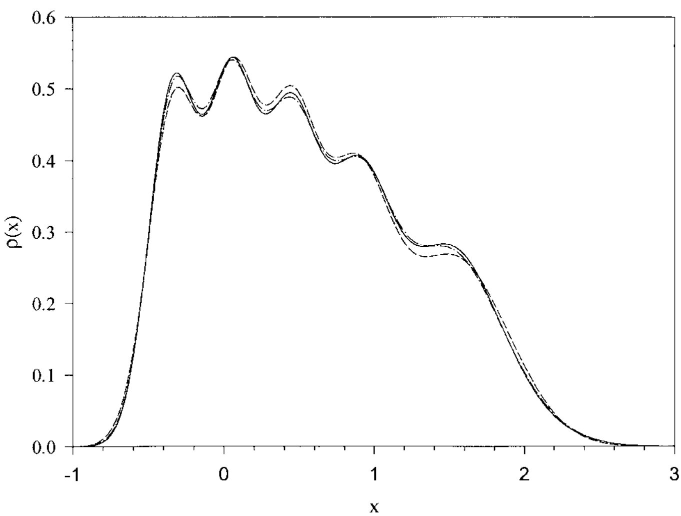

Fig. 1. Morse potential with five occupied states (see text for details). Comparison between the exact density (continuous line) and two inferred ones by assuming (i) only the knowledge of x-space expectation values (dashed line) and (ii) also the knowledge of p-expectation values (dot–dashed line).

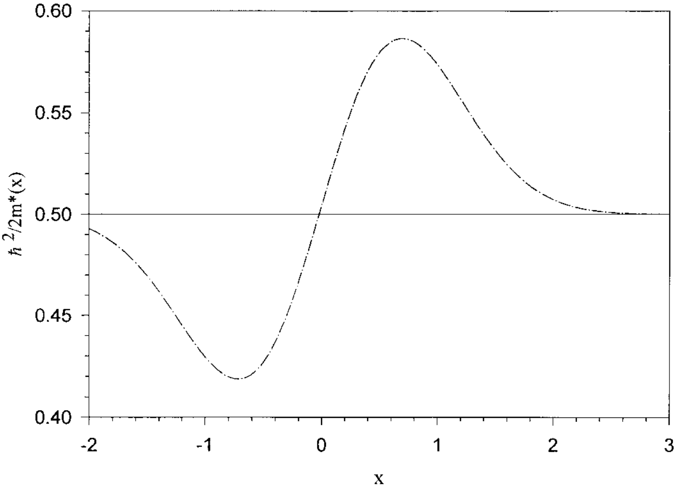

Fig. 2. Inferred effective mass for the Morse potential obtained by assuming the knowledge of the expectation values of two p-space operators (dot–dashed line) as compared to the bare mass (continuous line).

Table 1
Morse potential. Inferred moments corresponding to $\mathcal{N} = 5$ occupied states. The values $\langle x^m/\mathcal{N}\rangle$ listed under (I1) correspond to predictions made without taking into account momentum space information. Those under (I2) do take into account that information. For the sake of comparison, the (exact) quantal results are also displayed

	Quantal	I1	I2
$\langle x^5\rangle$	3.328	3.310	3.324
$\langle x^6\rangle$	6.178	6.082	6.154
$\langle x^7\rangle$	11.98	11.58	11.87
$\langle x^8\rangle$	24.16	22.78	23.74
$\langle x^9\rangle$	50.53	46.03	49.01
$\langle x^{10}\rangle$	109.3	95.27	104.1

3.2. Harmonic oscillator

Let us face now a different situation, one in which an effective mass is involved from the very beginning in the description of the system under study. Consider then an harmonic oscillator potential with a position-dependent effective mass of the form

$$\frac{m^*(x)}{m} = \frac{\alpha + x^2}{1 + x^2} \,. \tag{16}$$

We assume the foreknowledge of the expectation values of $\hat{x}^2$ and of some operators $\hat{C}_i$. As shown in Fig. 3, adding only $\langle\hat{C}_1\rangle$ (with $f_1 = \exp(-x^2)$) to the knowledge of $\langle\hat{x}^2\rangle$ one obtains a quite reasonable fit of the density for a system with $\mathcal{N} = 5$ occupied levels. Note that the (exact) quantal results are obtained by numerically solving (11). Assuming the knowledge of $\langle\hat{C}_i\rangle$, $i = 1,\ldots,4$, with $f_1 = \exp(-0.1x^2)$,

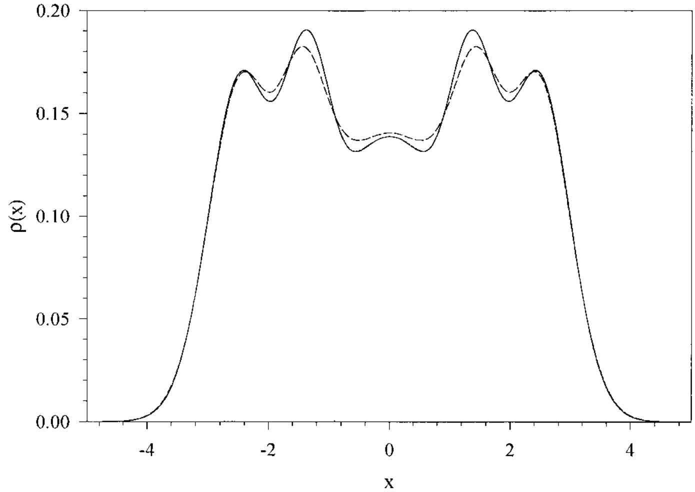

Fig. 3. Harmonic oscillator potential with a position-dependent effective mass given by Eq. (16) ($\alpha = 0.25$). The exact density (continuous line) is compared to two inferred ones by assuming the knowledge of (i) $\langle \hat{C}_1 \rangle$ (dashed line) and (ii) $\langle \hat{C}_1 \rangle, \ldots, \langle \hat{C}_4 \rangle$ (dot–dashed line).

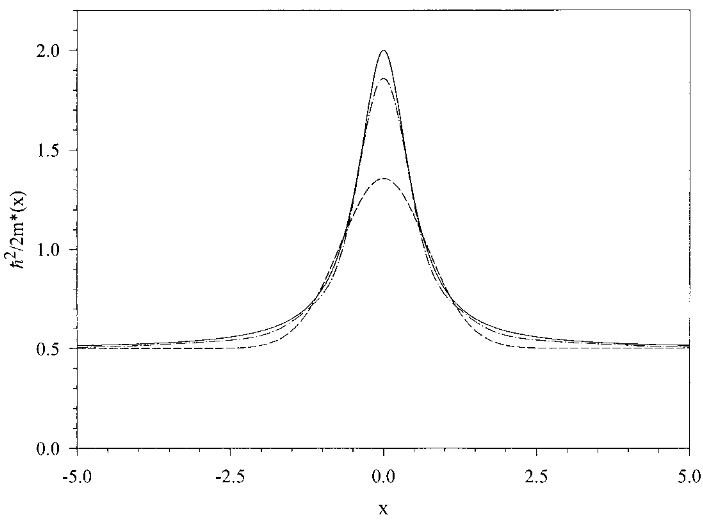

Fig. 4. Inferred effective masses for the potential of Fig. 3 are compared to the exact one (see the text and the caption of Fig. 3 for more details).

$f_2 = \exp(-x^2)$, $f_3 = \exp(-2x^2)$ and $f_4 = \exp(-3x^2)$, the inferred density and the (exact) quantal one coincide within the figure's scale. The inferred effective mass generated by the informational supplement represented by the $\langle \hat{C} \rangle$ is also displayed. The agreement with the mass given by (16) improves as the amount of suppletory information grows (see Fig. 4).

Table 2
Harmonic oscillator potential with a position-dependent effective mass given by Eq. (16) ($\alpha = 0.25$). Inferred moments $\langle x^m/\mathcal{N}\rangle$ for $\mathcal{N} = 5$ occupied states obtained using input information concerning both $\hat{x}2$ and $\hat{C}_1$ are listed under (I1). The predictions made using input information concerning $\hat{x}2$ and $\hat{C}_1,\dots,\hat{C}_4$ are listed under (12). For the sake of comparison, the (exact) quantal results are also displayed

	Quantal	I1	I2
$\langle x^4\rangle$	22.643	22.737	22.648
$\langle x^6\rangle$	182.90	184.65	183.04
$\langle x^8\rangle$	1706.1	1736.2	1709.1
$\langle x^{10}\rangle$	17766.0	18271.0	17825.0

The inferred moments $\langle x^m\rangle$ are compared to the exact quantal results in Table 2. The results are of a rather good quality.

3.3. Infinite square well

As an example of an steep potential we consider now the infinite square well

$$V(x) = \begin{cases} 0 & \text{if } -1 \leqslant x \leqslant 1 \\ \infty & \text{otherwise} \end{cases} \tag{17}$$

with a position-dependent effective mass of the form

$$\frac{m^*(x)}{m} = \frac{1}{1+\exp(-10x^2)} . \tag{18}$$

We assume the foreknowledge of the expectation values of the operators $\hat{C}_n$, with $f_n = \exp(-nx^2)$ and $n = 2, 3, 5$, and 7. Two different combinations are used, namely, $\langle\hat{C}_2\rangle$ and $\langle\hat{C}_5\rangle$, on the one hand, and $\langle\hat{C}_2\rangle$, $\langle\hat{C}_3\rangle$, $\langle\hat{C}_5\rangle$, and $\langle\hat{C}_7\rangle$, on the other. The ensuing results corresponding to the inferred densities and the inferred masses for a system with $\mathcal{N} = 5$ occupied levels are depicted in Figs. 5 and 6. In Table 3 the predictive power of the approach is tested with reference to some moments. Good agreement is obtained.

Table 3
Infinite square well with a position-dependent effective mass given by Eq. (18). Inferred moments $\langle x^m/\mathcal{N}\rangle$ for $\mathcal{N} = 5$ occupied states obtained using input information related to $\hat{C}_2$ and $\hat{C}_5$ are listed under (I1). Those evaluated using input information related to $\hat{C}_2$, $\hat{C}_3$, $\hat{C}_5$, and $\hat{C}_7$ are listed under (I2). For the sake of comparison, the (exact) quantal results are also displayed

	Quantal	I1	I2
$\langle x^2\rangle$	0.30428	0.30380	0.30427
$\langle x^4\rangle$	0.15507	0.15450	0.15506
$\langle x^6\rangle$	0.09293	0.09227	0.09293
$\langle x^8\rangle$	0.06060	0.05994	0.06059
$\langle x^{10}\rangle$	0.04171	0.04110	0.04171

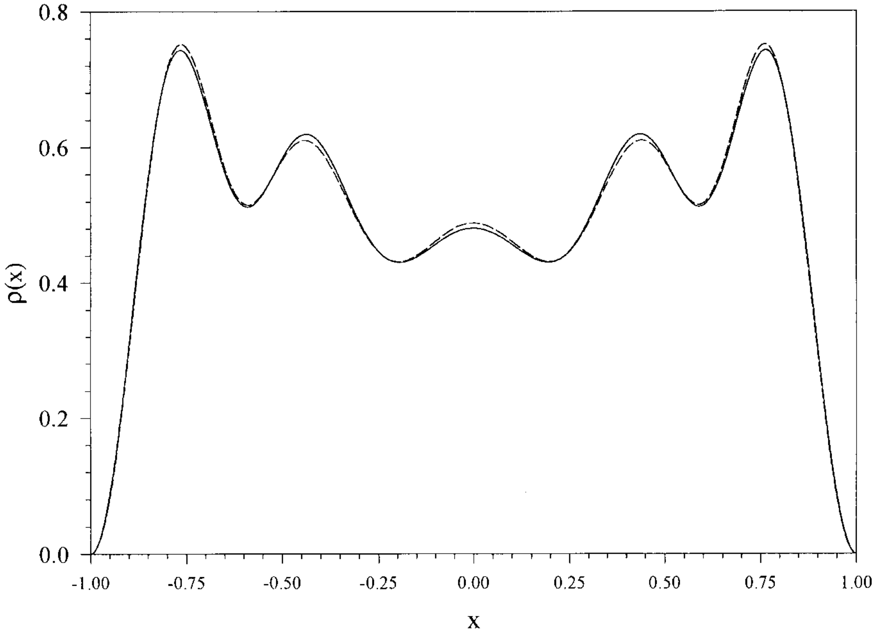

Fig. 5. Infinite square well with a position-dependent effective mass given by Eq. (18). The exact density (continuous line) is compared to two inferred ones by assuming the knowledge of (i) $\langle \hat{C}_2 \rangle$ and $\langle \hat{C}_5 \rangle$ (dashed line) and (ii) $\langle \hat{C}_2 \rangle$, $\langle \hat{C}_3 \rangle$, $\langle \hat{C}_5 \rangle$, and $\langle \hat{C}_7 \rangle$ (dot–dashed line).

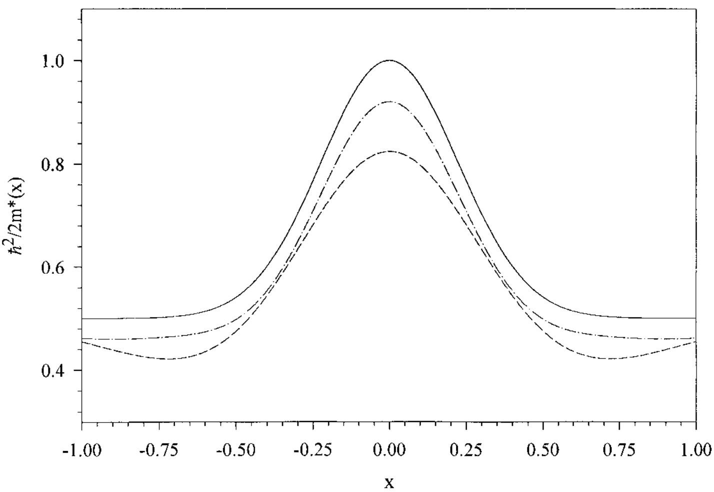

Fig. 6. Inferred effective masses for the potential of Fig. 5 are compared to the exact one (see the text and the caption of Fig. 5 for more details).

The (exact) quantal density (obtained by solving (11)) and the inferred one practically coincide if enough information is available. The inferred effective mass generated by the informational supplement represented by the $\langle \hat{C} \rangle$ is also displayed. The corresponding fit improves as one increases the information supply.

4. Conclusions

We have shown that assuming the knowledge of the expectation values of some operators involving the momentum, a constrained extremalization of the Fisher information measure leads to a Schrödinger equation that involves an effective mass.

By recourse to an appropriate transformation, this Schrödinger equation with effective mass can be recast as an ordinary one (i.e., with constant mass), but endowed with a local (albeit energy dependent) equivalent potential [33]. The energy dependence of the local equivalent potential (see Eq. (12)) actually entails nonlocal contributions to the system's potential energy. Invoking the Frieden–Soffer variational principle, one could advance the idea that including operators of the form $\hat{p}\, f(\hat{x})\, \hat{p}$ among the relevant constraints is tantamount to introducing nonlocal effects.

The results reported here may be regarded, perhaps, as yet another hint pointing towards Wheeler's view that an informational content underlies all things physical [34,35].

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