

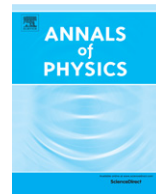


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Hellmann–Feynman connection for the relative Fisher information

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HIGHLIGHTS

- Legendre transform structure for the RFI is obtained with the Hellmann–Feynman theorem.
- Inference of the energy-eigenvalues of the SWE-like equation for the RFI is accomplished.
- Basis for reconstruction of the RFI framework from the FIM-case is established.
- Substantial qualitative and quantitative distinctions with prior studies are discussed.

ARTICLE INFO

Article history:

Received 9 December 2014

Accepted 16 April 2015

Available online 28 April 2015

Keywords:

Relative Fisher information
Hellmann–Feynman theorem
Reciprocity relations
Generalized RFI–Euler theorem
Legendre transform structure
Energy-eigenvalue inference

ABSTRACT

The (i) reciprocity relations for the relative Fisher information (RFI, hereafter) and (ii) a generalized RFI–Euler theorem are self-consistently derived from the Hellmann–Feynman theorem. These new reciprocity relations generalize the RFI–Euler theorem and constitute the basis for building up a mathematical Legendre transform structure (LTS, hereafter), akin to that of thermodynamics, that underlies the RFI scenario. This demonstrates the possibility of translating the entire mathematical structure of thermodynamics into a RFI-based theoretical framework. Virial theorems play a prominent role in this endeavor, as a Schrödinger-like equation can be associated to the RFI. Lagrange multipliers are determined invoking the RFI–LTS link and the quantum mechanical virial theorem. An appropriate ansatz allows for the inference of probability density functions (pdfs, hereafter) and energy-eigenvalues of the above mentioned Schrödinger-like equation. The energy-eigenvalues obtained here via inference are benchmarked against

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established theoretical and numerical results. A principled theoretical basis to reconstruct the RFI-framework from the FIM framework is established. Numerical examples for exemplary cases are provided.

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1. Introduction

The relative Fisher information (RFI, hereafter) is a measure of uncertainty that is the focus of much attention in statistical physics, estimation theory, and allied disciplines (see [1]). The RFI is defined by [2,3]

$$\mathfrak{F}[f|g] = \int_{\mathcal{X}^m} f(\mathbf{x}) \left| \nabla \ln \frac{f(\mathbf{x})}{g(\mathbf{x})} \right|^2 d\mathbf{x}, \tag{1}$$

where $|\bullet|^2$ is the square norm. Here, $g(\mathbf{x})$ is the *reference probability* which may be construed as encapsulating *prior knowledge*. Some of the various forms in which the RFI has been expressed have been cited in Refs. [4–11]. It is noteworthy to mention that a form of the RFI known as the ‘weighted Fisher information’ has been self-consistently derived on the basis of estimation theory in [12]. This also allowed the class of efficient pdfs $f(\mathbf{x})$ to be computed. These achieve minimizing the *weighted* mean-squared error of estimation.

The RFI may be legitimately construed as relating to the Fisher information measure (FIM, hereafter) akin to the manner in which the Kullback–Leibler divergence (K–Ld, hereafter) relates to the Shannon entropy [13]. Specifically, both the RFI and the K–Ld are not only measures of uncertainty, but also measures of discrepancy between two probability distributions. However, while the derivative term in the RFI tacitly implies its “localization” or “fine-grained” attributes, the K–Ld is, comparatively, “coarse-grained”. Ref. [1] demonstrated that the mathematical structure of thermodynamics seamlessly translates into an RFI context, within the framework of a time independent model. This was accomplished via the derivation of a generalized RFI–Euler theorem (of the form specified in [14]) and of the concomitant Legendre transform structure (LTS, hereafter) for the RFI. The basis for this LTS-derivation is a one dimensional time independent Schrödinger-like equation. One speaks of the Schrödinger-like link for the RFI (S–RFI link, hereafter). This S–RFI link is obtained by specifying the *reference probability* $g(x)$ in (1) for the one dimensional case (e.g. [4])

$$g(x) = e^{-V(x)}; \quad \int e^{-V(x)} dx = 1, \tag{2}$$

known as the *Gibbs form*, where $V(x)$ is an a-priori specified *convex* physical potential, such that $V_{xx}(x) > 0$. By Eqs. (1) and (2)

$$\mathfrak{F}[f|e^{-V(x)}] = \int f(x) |\nabla (\ln f(x) + V(x))|^2 dx. \tag{3}$$

Note that the so-called Gibbs form in (2) is perfectly acceptable within the context of this study, since equilibrium probabilities in quantum mechanics (QM, hereafter) are described by an exponential form. Setting $f(x) = \psi^2(x)$ and performing a variational extremization of (3) with respect to $\psi(x)$, subject to constraints, yields [1]

$$-\frac{1}{2} \frac{d^2 \psi(x)}{dx^2} - U_{RFI}(x) \psi(x) = \frac{\lambda_0}{8} \psi(x),$$

where

$$U_{RFI}(x) = \frac{1}{8} \left[\sum_{i=1}^M \lambda_i A_i(x) - V_x^2(x) + 2V_{xx}(x) \right], \tag{4}$$

is a pseudo-potential. Here, $\psi(x)$ is a real quantity (as always in a one dimensional setting [15]), $V_x(x) = \frac{dV(x)}{dx}$, and $V_{xx}(x) = \frac{d^2V(x)}{dx^2}$. The λ_i are M Lagrange multipliers associated to the expectation of the empirical observables $\langle A_i(x) \rangle = \int A_i(x) \psi^2(x) dx$, and λ_0 is the Lagrange multiplier for the normalization condition $\int \psi^2(x) dx = 1$. Ref. [1] also derived a procedure to infer the energy-eigenvalues of the S-RFI link, via solution of a linear partial differential equation (PDE)

$$\lambda_0 = \sum_{i=1}^M (1+k) \lambda_i \frac{\partial \lambda_0}{\partial \lambda_i}, \quad (5)$$

derived solely with recourse to the LTS of the RFI and the QM virial theorem.

The Hellmann–Feynman theorem (HFT, hereafter) [16,17] plays a central role in the application of QM. It demonstrates the relationship between perturbations in an operator in inner product spaces and the concomitant perturbations in the operators eigenvalue. The HFT states that a nondegenerate eigenvalue $E(\lambda)$ of a parameter-dependent Hermitian operator $H(\lambda)$, with associated (normalized) eigenvector $\psi(\lambda)$, relate as

$$\frac{\partial E_i}{\partial \lambda} = \langle \psi_i(\lambda) | \frac{\partial H}{\partial \lambda} | \psi_i(\lambda) \rangle. \quad (6)$$

Earlier works established a relation between the HFT and the LTS of FIM [18,19]. Refs. [18,19] make substantial use of the LTS of the FIM derived in [20]. In the case of FIM-based treatments, the empirical observables $A_i(x)$ are the only source of prior knowledge.

In RFI variational extremizations (4), both the empirical observables $A_i(x)$ and the convex physical potential $V(x)$ constitute prior knowledge. Thus, studies within the RFI framework will substantially differ, in a qualitative sense, from those obtained for the FIM scenario. Specifically, as it is evidenced by (4), values of $\psi(x)$ are determined by both the derivative terms of the physical potential $V(x)$ and the empirical contribution in (4), i.e. the $A_i(x)$.

Before proceeding further, it is of paramount importance to clarify certain terminologies and definitions. In this paper, the RFI is the primary measure of uncertainty. Likewise, the term FIM framework is used to describe treatments for which the FIM is the primary measure of uncertainty (see Refs. [18,19]). The expression for the RFI can be expressed in terms of a FIM and expectations of derivative terms of the physical potential $V(x)$, which comprise the reference probability $g(x)$ in (1)–(3). However, the pdf in (3) and (11) is the one which extremizes the RFI and not the FIM.

The goals of this paper are

- (i) to establish that the reciprocity relations and the generalized RFI–Euler theorem which are central to the LTS of the RFI [1] may be derived from first-principles from the HFT (Section 3), by specializing *virial theorems* [21] to the information-theoretic domain,
- (ii) to establish with the aid of the HFT, a principled basis to describe the interplay between the probability amplitude $\psi(x)$, the derivatives of the *a-priori* specified convex physical potential $V(x)$, and the empirical observables $A_i(x)$. This is accomplished in Section 4 by inference of an ansatz for the pdf,
- (iii) to demonstrate the inference of the energy-eigenvalues of the S-RFI link, by recourse only to the QM virial theorem and the reciprocity relations. This is achieved by subjecting (5) to the reciprocity relation (8) in Section 2, thereby demonstrating the practical utility of (5) in actual inference settings. The said task is accomplished in Section 5 by inference of pdf's whose profile is dictated by the ansatz introduced in Section 4,
- (iv) to exemplify the distinct nature of the pdf profiles inferred from empirical observables within the RFI framework vis-à-vis equivalent Fisher-based ones. This is accomplished in Section 5. Notably, Section 5 establishes the fact that solutions of the variational extremization of the FIM constitute a subset of solutions within the RFI framework. Specifically, it is established that the Lagrange multipliers λ_k associated with the constraints in variational extremizations performed in both the RFI and the FIM frameworks are identical. This is attributed to the *Gibbs form* employed in Eqs. (2) and (3). Section 5 also demonstrates that the energy-eigenvalues for the cases of the harmonic oscillator potential and the quartic anharmonic oscillator potential, inferred from empirical observations, show remarkable consistency with established studies [22,23],

- (v) a theoretical basis to reconstruct the pdf of the RFI framework from that of the FIM-case is established. *This reconstruction demonstrates the efficacy of the relation (13) in inference scenarios.* The fact that the Lagrange multipliers associated with the constraints in the RFI-framework and the FIM-framework are equal—a feature of the *Gibbs form* employed in (2) and (3), is shown to ameliorate the process of reconstruction.

Numerical examples for exemplary cases are provided. To the best of the authors' knowledge, these objectives have never hitherto been accomplished.

2. Theoretical preliminaries

The RFI-Legendre transform structure links the RFI-measure, the normalization Lagrange multiplier λ_0 , the prior information contained in a set of expectation values, and the Lagrange multipliers related to them. Throughout this paper, unless specifically specified otherwise, expectations are denoted by $\langle \bullet \rangle_{\psi_{RFI}^2(x)}$ and are evaluated with respect to the pdf $f_{RFI}(x) = \psi_{RFI}^2(x)$ which extremizes the RFI subject to constraints. (cf. Eq. (4)). It is therefore desirable to define the RFI as $\mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}]$, instead of $\mathfrak{S} [\psi(x) | e^{-V(x)/2}]$ (as is the case in [1]). The pertinent relationships from [1] remain unaffected, and are re-stated as

$$\lambda_0(\lambda_1, \dots, \lambda_M) = \mathfrak{S} \left(\langle A_1(x) \rangle_{\psi_{RFI}^2}, \dots, \langle A_M(x) \rangle_{\psi_{RFI}^2} \right) - \sum_{i=1}^M \lambda_i \langle A_i(x) \rangle_{\psi_{RFI}^2}, \tag{7}$$

plus the reciprocity relations and the generalized RFI–Euler theorem, i.e.,

$$\frac{\partial \lambda_0}{\partial \lambda_i} = - \langle A_i(x) \rangle_{\psi_{RFI}^2}, \tag{8}$$

$$\frac{\partial \mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}]}{\partial \langle A_j(x) \rangle_{\psi_{RFI}^2}} = \lambda_j, \tag{9}$$

and

$$\frac{\partial \mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}]}{\partial \lambda_i} = \sum_{j=1}^M \lambda_j \frac{\partial \langle A_j(x) \rangle_{\psi_{RFI}^2}}{\partial \lambda_i}, \tag{10}$$

respectively. The RFI obeys the following relations [1]

$$\mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}] = I[\psi_{RFI}^2] - 2 \langle V_{xx}(x) \rangle_{\psi_{RFI}^2} + \langle V_x^2(x) \rangle_{\psi_{RFI}^2} \tag{11}$$

and

$$\mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}] = \lambda_0 + \sum_{i=1}^M \lambda_i \langle A_i(x) \rangle_{\psi_{RFI}^2}, \tag{12}$$

where $I[\psi_{RFI}^2]$ is the FIM defined in terms of the amplitude ψ_{RFI} . *Note that this amplitude and its associated probability distribution function (pdf) $f_{RFI}(x) = \psi_{RFI}^2(x)$, extremize the RFI subject to constraints. It is critical to note that this $I[\psi_{RFI}^2]$ does not correspond to the FIM scenario, that can be re-obtained by setting $V(x) = 0$ resulting in $I[\psi_{FIM}^2]$.*

A necessary condition for the derivation of (5) is that the following relation

$$4 \left\langle x \frac{d\tilde{U}_{RFI}^{Physical}(x)}{dx} \right\rangle_{\psi_{RFI}^2} = 2 \langle V_{xx}(x) \rangle_{\psi_{RFI}^2} - \langle V_x^2(x) \rangle_{\psi_{RFI}^2}, \tag{13}$$

be satisfied. Here, $\tilde{U}_{RFI}^{Physical}(x)$ is defined by (15) in Section 3. Appendix provides an interpretation of (13). Eq. (13) is generally satisfied in the case of many prominent QM potentials, such as the anharmonic quartic, and sextic potentials [24,25], when expressed in polynomial-form $V(x) = \sum_j c_j x^j$.

3. Hellmann–Feynman–RFI connections

Multiplying (4) by 2 and re-arranging terms yields

$$-\frac{d^2 \psi_{RFI}(x)}{dx^2} + \tilde{U}_{RFI}(x) \psi_{RFI}(x) = \frac{\lambda_0}{4} \psi_{RFI}(x), \tag{14}$$

where the RFI pseudo-potential (14) is re-defined as

$$\tilde{U}_{RFI}(x) = \underbrace{-\frac{1}{4} \left[\sum_{i=1}^M \lambda_i A_i(x) \right]}_{\tilde{U}_{RFI}^{Data}(x)} \underbrace{-\frac{1}{4} [2V_{xx}(x) - V_x^2(x)]}_{\tilde{U}_{RFI}^{Physical}(x)}. \tag{15}$$

Note that (14) adopts the form of the usual time independent Schrödinger equation, having energy eigenvalue E , for $\frac{\hbar^2}{2m} = 1$ and $\frac{\lambda_0}{4} = E$. The quantum mechanical virial theorem states that [15]

$$-\int \psi_{RFI}(x) \frac{d^2 \psi_{RFI}(x)}{dx^2} dx = \left\langle x \frac{d\tilde{U}_{RFI}(x)}{dx} \right\rangle_{\psi_{RFI}^2}, \tag{16}$$

where $\langle \bullet \rangle_{\psi_{RFI}^2}$ denotes expectations evaluated with respect to $f_{RFI}(x) = \psi_{RFI}^2(x)$. Following through with the derivation and invoking (13) and (15), yields

$$\lambda_0 + \sum_{i=1}^M \lambda_i \langle A_i(x) \rangle_{\psi_{RFI}^2} = - \sum_{i=1}^M \lambda_i \left\langle x \frac{dA_i(x)}{dx} \right\rangle_{\psi_{RFI}^2}. \tag{17}$$

Here, (17) is exactly Eq. (41) in [1]. Note that $\tilde{U}_{RFI}^{Physical}(x)$ is not inferred from the empirical observables. Thus, even in the absence of them, $\tilde{U}_{RFI}^{Physical}(x) \neq 0$ is an a-priori specified analytical expression derived from a known physical potential. Further, the a-priori specified QM potential $V(x)$ is taken to be generic in this section. Since the $A_i(x)$ can always be expressed as power-series, one can write, without loss of generality invoking (15),

$$\tilde{U}_{RFI}^{Data}(x) = -\frac{1}{4} \sum_k \lambda_k A_k(x) = \sum_k a_k x^k; \quad a_k = -\frac{\lambda_k}{4}. \tag{18}$$

The practical utility of (18), modified in Section 4, will be seen in Section 5, wherein the coefficients of the QM potentials obtained via inference from experimental measurements are seamlessly related to the concomitant Lagrange multipliers. Setting for simplicity $A_k(x) = x^k$, and substituting into (17), one finds

$$\lambda_0 = - \sum_{k=1}^M (k+1) \lambda_k \langle A_k(x) \rangle_{\psi_{RFI}^2}. \tag{19}$$

As is demonstrated in Section 5, (19) proves invaluable in inferring first the values of λ_0 , and then the energy-eigenvalue E , without recourse to solving (4) or (14). It is readily verifiable that (19) is a consequence of (5), subjected to the reciprocity relation (8). Substituting now (19) into (12) yields

$$\Im[\psi_{RFI}^2(x) | e^{-V(x)}] = - \sum_{k=1}^M k \lambda_k \langle A_k(x) \rangle_{\psi_{RFI}^2}. \tag{20}$$

We have from (14)

$$H_{RFI} \psi_{RFI}(x) = \frac{\lambda_0}{4} \psi_{RFI}(x) = E \psi_{RFI}(x), \tag{21}$$

where the information-theoretic Hamiltonian is defined by $H_{RFI} = \left[-\frac{d^2}{dx^2} + \tilde{U}_{RFI}(x) \right]$, and the energy eigenvalue relates to the normalization Lagrange multiplier as $E = \frac{\lambda_0}{4}$. Application of the HFT to (21) yields the reciprocity relation (8)

$$\frac{\partial}{\partial \lambda_k} \left(\frac{\lambda_0}{4} \right) = \langle \psi_{RFI} | -\frac{A_k(x)}{4} | \psi_{RFI} \rangle \Rightarrow \frac{\partial \lambda_0}{\partial \lambda_k} = - \langle A_k(x) \rangle_{\psi_{RFI}^2} . \tag{22}$$

Now, operating on (19) leads to

$$\frac{\partial \lambda_0}{\partial \lambda_k} = - (j + 1) \langle A_k(x) \rangle - (k + 1) \sum_{k=1}^M \lambda_k \frac{\partial \langle A_k(x) \rangle_{\psi_{RFI}^2}}{\partial \lambda_j} . \tag{23}$$

Eqs. (22) and (23) together produce

$$j \langle A_j(x) \rangle_{\psi_{RFI}^2} = - (k + 1) \sum_{k=1}^M \lambda_k \frac{\partial \langle A_k(x) \rangle_{\psi_{RFI}^2}}{\partial \lambda_j} , \tag{24}$$

and taking derivatives of (20) one encounters

$$\frac{\partial \mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}]}{\partial \lambda_j} = -j \langle A_j(x) \rangle_{\psi_{RFI}^2} - k \sum_{k=1}^M \lambda_k \frac{\partial \langle A_k(x) \rangle_{\psi_{RFI}^2}}{\partial \lambda_j} . \tag{25}$$

Finally, substituting (24) into (25) yields the generalized RFI–Euler theorem (10)

$$\frac{\partial \mathfrak{S} [\psi_{RFI}^2(x) | e^{-V(x)}]}{\partial \lambda_j} = \sum_{k=1}^M \lambda_k \frac{\partial \langle A_k(x) \rangle_{\psi_{RFI}^2}}{\partial \lambda_j} . \tag{26}$$

On the other hand, taking derivatives of (7) with respect to λ_j , and comparing the ensuing result with (25), immediately leads to the reciprocity relation (9)

$$\frac{\partial \mathfrak{S} (\langle A_1(x) \rangle_{\psi_{RFI}^2} , \dots , \langle A_M(x) \rangle_{\psi_{RFI}^2})}{\partial \langle A_j(x) \rangle_{\psi_{RFI}^2}} = \lambda_j . \tag{27}$$

Thus, the reciprocity relations (8) and (9) and the generalized RFI–Euler theorem (10) are shown to be self-consistently derived from the HFT. An important result follows from substituting (27) into (20). One arrives at a linear, partial differential equation (PDE) for the RFI

$$\mathfrak{S} = - \sum_{k=1}^M k \langle A_k(x) \rangle_{\psi_{RFI}^2} \frac{\partial \mathfrak{S}}{\partial \langle A_k(x) \rangle_{\psi_{RFI}^2}} . \tag{28}$$

Here, (28) is a qualitative extension of the result obtained in [25]. Investigations into the physical implications of (28) is the task of future works. The solution of (28) is

$$\mathfrak{S} (\langle A_1(x) \rangle_{\psi_{RFI}^2} , \dots , \langle A_M(x) \rangle_{\psi_{RFI}^2}) = \sum_{k=1}^M C_k \langle A_k(x) \rangle_{\psi_{RFI}^2}^{-\frac{1}{k}} , \tag{29}$$

where $C_k > 0$ is a constant of integration. Note that $\langle A_k(x) \rangle_{\psi_{RFI}^2} = \langle x^k \rangle_{\psi_{RFI}^2}$.

4. Ansatz

Multiplying the LHS of (14) by four yields the FIM in amplitude form, subjected to a single integration-by-parts. Thus, redefining (14) in terms of the pdf $f_{RFI}(x) = \psi_{RFI}^2(x)$ one finds

$$\int f_{RFI}(x) \left(\frac{d \ln f_{RFI}(x)}{dx} \right)^2 dx = 4 \int f_{RFI}(x) \left(x \frac{d \tilde{U}_{RFI}(x)}{dx} \right) dx. \tag{30}$$

Eqs. (30) and (15) together yield

$$\int f_{RFI}(x) \left[\left(\frac{d \ln f_{RFI}(x)}{dx} \right)^2 - 4x \frac{d \tilde{U}_{RFI}^{Data}(x)}{dx} - 4x \frac{d \tilde{U}_{RFI}^{Physical}(x)}{dx} \right] dx = 0. \tag{31}$$

In another vein, (15) and (18) are expeditiously cast to give the empirical pseudo-potential contributions in (31) a useful form

$$4x \frac{d \tilde{U}_{RFI}^{Data}(x)}{dx} = - \sum_k k \lambda_k x^k, \tag{32}$$

while the contributions of the physical pseudo-potential in (31) are obtained from (15) in the fashion

$$4x \frac{d \tilde{U}_{RFI}^{Physical}(x)}{dx} = x \frac{dV_x^2(x)}{dx} - 2x \frac{dV_{xx}(x)}{dx}. \tag{33}$$

Now, substituting (32) and (33) into (31) yields

$$\int f_{RFI}(x) \left[\left(\frac{d \ln f_{RFI}(x)}{dx} \right)^2 + \sum_k k \lambda_k x^k - x \frac{dV_x^2(x)}{dx} + 2x \frac{dV_{xx}(x)}{dx} \right] dx = 0. \tag{34}$$

In (34), $f_{RFI}(x) = \psi_{RFI}^2(x)$ where $\psi_{RFI}(x)$ is obtained via solution of (4). Eq. (4) is most generally satisfied by Hermite–Gauss polynomials, which are orthogonal to the Gaussian (exponential) distribution. To study the leading-order contributions, specializing the solution of (34) to exponential forms requires that the terms in [•] satisfy

$$f_{RFI}(x) = N \exp \left\{ \pm \int \sqrt{- \sum_k k \lambda_k x^k + x \frac{dV_x^2(x)}{dx} - 2x \frac{dV_{xx}(x)}{dx}} \right\}. \tag{35}$$

The arbitrary constant of integration in (35) is absorbed into the normalization factor: $N = \int_{-\infty}^{\infty} f(x) dx = 1$, which ensures that the pdf vanishes at $\pm\infty$. Note that the normalization factor may also be construed as being the *partition function*. Note that the more general solution for $f(x)$ in the form of Hermite–Gauss polynomials is the task of future work (see Section 7). This is recast with the aid of (18) and (35) as

$$f_{RFI}(x) = N \exp \left\{ \pm \int \sqrt{\sum_k 4ka_k x^k + x \frac{dV_x^2(x)}{dx} - 2x \frac{dV_{xx}(x)}{dx}} \right\}, \tag{36}$$

where a_k are the coefficients of the QM physical potential, inferred through empirical observations. In accordance with prior studies (e.g. [24,25]) which describe commonly encountered QM potentials such as the anharmonic quartic, and sextic potentials in terms of polynomials, the a-priori specified physical QM potential in (33)–(36) be expressed as the particular solution

$$V(x) = \sum_j c_j x^j. \tag{37}$$

Here, c_j is a known constant given in the form of the a-priori specified physical QM potential. The sign in the exponential is chosen, contingent to (i) the nature of $V(x)$ (together with its derivative terms)

and (ii) the QM potential, in such a manner that $f_{RFI}(x)$ as $x \rightarrow \pm\infty$ is physical. Note that in (35) taking the negative value in the exponential is tenable since $\left(\frac{d \ln f_{RFI}(x)}{dx}\right)^2 = \left(\frac{d(-\ln f_{RFI}(x))}{dx}\right)^2$. For the sake of comparisons of the pdf profiles between the RFI and FIM scenarios, it is important to specify the Fisher-equivalent of (32) [18,19] by setting $V(x) = 0$. This produces the following ansatz for the pdf

$$f_{FIM}(x) = N \exp \left\{ \pm \int \sqrt{-\sum_k k \lambda_k^{FIM} x^k} dx \right\} = N \exp \left\{ \pm \int \sqrt{\sum_k 4ka_k x^k} dx \right\}. \tag{38}$$

5. Analysis and numerical simulations

The theoretical results in the previous sections are now employed to establish the qualitative distinction between RFI-based variational extremizations vis-à-vis equivalent Fisher-based ones. This is accomplished via the ansatz derived in Section 4, specialized to pseudo-potentials corresponding to QM potentials. One of the most salient results of this paper is to demonstrate the inference of the energy-eigenvalues of the S-RFI link, without recourse to solving (4). The treatment for this procedure is provided in this section wherein the necessary mathematical and procedural “machinery” to accomplish the above task are established, commencing with a candidate physical QM potential of the form [23]

$$\tilde{V}^{inf}(x) = \omega^2 x^2 + \varepsilon x^k; \quad k = 4, 6, \dots, \tag{39}$$

inferred from the empirical observables $\langle x^k \rangle$; $k = 2, 4, \dots$. Here, ε is the anharmonicity constant. Generically, (39) may be cast in the form

$$\tilde{V}^{inf}(x) = \sum_k a_k x^k; \quad k = 2, 4, \dots, \tag{40}$$

where a_k are coefficients related to the concomitant Lagrange multipliers through (18).

An observation of much significance arises here: while the energy-eigenvalues and the concomitant pdf profiles pertaining to the RFI framework noticeably differ from their FIM counterparts, the Lagrange multipliers for the constraint terms, corresponding to the experimental observables, are readily demonstrated to be the same for both the RFI and the FIM scenarios. The cause for this somewhat surprising finding is traced to the Gibbs form utilized in (2) and (3) of this paper. Specifically, on account of the Gibbs form in (2) and (3), the S-RFI link (4), (14), and (15) have the Lagrange multipliers corresponding to the inference process completely separated and delineated from the a-priori specified knowledge denoted by the derivatives of the physical QM potential $V(x)$. Note that within the RFI framework, the empirical observables are explicitly defined as $\langle x^k \rangle_{\psi_{RFI}^2}$. Likewise, in the FIM-case the empirical observables are defined as $\langle x^k \rangle_{\psi_{FIM}^2}$.

This section treats the cases of both perturbed and non-perturbed QM potentials, inferred from empirical observables, viz. the harmonic oscillator (HO, hereafter) potential and the quartic anharmonic oscillator (QAHO, hereafter) potential, respectively. For all cases herein, the a-priori specified physical QM potential is taken to be the simple HO potential

$$V(x) = \omega^2 x^2. \tag{41}$$

In this paper, all computations are performed using MATHEMATICA®.

5.1. Procedure for the inference process

- (i) Given empirical observables $\langle x^k \rangle_{\psi_{RFI,FIM}^2}$, a candidate (inferred) QM potential of the form given by (40) is specified. Note that the pdf expressed in the form of amplitudes ψ_{RFI}^2 and ψ_{FIM}^2 which defines the expectations of the empirical observables depends solely upon whether the RFI or the FIM frameworks are being studied, and does not influence the choice of the inferred QM potential.

(ii) Invoking (14) and (15), yields the S–RFI link

$$\left[-\frac{d^2}{dx^2} - \sum_k a_k x^k + \tilde{U}_{RFI}^{Physical}(x) \right] \psi_{RFI}(x) = E \psi_{RFI}(x). \tag{42}$$

(iii) From (18), the Lagrange multipliers λ_k are related to the coefficients a_k via (40).

(iv) The physical contributions in (35) are obtained by seeking consistency between (37) and (41), which requires

$$c_2 = \omega^2; \quad V_x^2(x) = 4\omega^4 x^2; \quad 2V_{xx}(x) = 4\omega^2; \quad j = 2. \tag{43}$$

Thus,

$$x \frac{dV_x^2(x)}{dx} = 8\omega^4 x^2 \quad \text{and} \quad 2x \frac{dV_{xx}(x)}{dx} = 0. \tag{44}$$

(v) The inferred pdf is then obtained from (35), which are employed to obtain the moments in (19) thereby the λ_0 value. From Section 3, the energy-eigenvalue is $E = \frac{\lambda_0}{4}$. Thus, inference of the energy-eigenvalues is accomplished without solving the Schrödinger-like link for the RFI.

(vi) To benchmark the inference process with published results expressed either in terms of the Schrödinger wave equation (SWE, hereafter) [23] or its information theoretic counterpart derived in FIM-based studies [22], it is imperative that $V(x) = 0$ be specified in the RFI results presented in this paper. This is accomplished for the case of the HO and the QAHO potentials in Section 5.2.

(vii) Setting $V(x) = 0$ in (42) yields the Schrödinger-like equation for the FIM-framework.

$$\left[-\frac{d^2}{dx^2} - \sum_k a_k x^k \right] \psi_{FIM}(x) = E_{FIM} \psi_{FIM}(x). \tag{45}$$

5.2. Test cases

5.2.1. Non-perturbed case $\varepsilon = 0$

Let the empirical measurements be $\langle x^2 \rangle_{\psi_{RFI, FIM}^2}$, depending upon whether the RFI or the FIM frameworks are being studied. Thus, an empirically inferred QM candidate potential is the HO of the form

$$\tilde{V}^{Inf}(x) = \omega^2 x^2. \tag{46}$$

The a-priori specified QM physical potential is also taken to be of the form described by (41). Note that the distinction between the RFI and FIM frameworks is obvious, even in the simple cases of the HO solution.

Invoking (18) yields

$$\lambda_2 = -4\omega^2. \tag{47}$$

The inferred pdf is thus obtained from (35) with the aid of (44) and (47) as

$$f_{RFI}(x) = N \exp \left\{ -\int \sqrt{8\omega^2 x^2 (1 + \omega^2)} dx \right\} = N \exp \left\{ -\sqrt{(2\omega^2 (1 + \omega^2))} x^2 \right\}, \tag{48}$$

where N is a normalization factor. Setting $\omega^2 = 0.5$ yields

$$\int_{-\infty}^{\infty} f(x) dx = 1 \Rightarrow N = 0.624378. \tag{49}$$

For $k = 2$ and $\omega^2 = 0.5$, the normalization Lagrange multiplier is explicitly obtained from (19), with the aid of (47) and (48), as $\lambda_0 \approx 2.44596$. From Section 3, $E = \frac{\lambda_0}{4} \approx 0.611489$. Note that, from (42) and (15), it is evident that E is not the energy-eigenvalue for the harmonic oscillator potential.

Specifically, it corresponds instead to a different potential, namely, a superposition of the empirical HO contributions and the derivative terms of the a-priori specified QM potential (41), which in this study is also the HO potential.

To benchmark the inference process, comparison between the second term on the LHS of (45) with (46) clearly shows $a_k = \omega^2$ for $k = 2$. Invoking (18) yields

$$\lambda_2^{FIM} = -4\omega^2. \tag{50}$$

This is identical to (47). Carrying through with the analysis in a manner exactly similar to that given above, the inferred pdf from the FIM framework is obtained with the aid of (38) for $\omega^2 = 0.5$ as

$$f_{FIM}(x) = N \exp\{-x^2\}, \tag{51}$$

which exhibits the correct HO-form, where the normalization factor N is

$$\int_{-\infty}^{\infty} f_{FIM}(x) dx = 1 \Rightarrow N = \frac{1}{\sqrt{\pi}}, \tag{52}$$

which is the exact theoretical result as given in [22].

Along the lines of [22], the inferred energy-eigenvalue is theoretically obtained by specifying

$$\langle x^2 \rangle_{\psi_{FIM}^2} = \frac{9}{64\omega^4}. \tag{53}$$

Setting $V(x) = 0$, $k = 2$, and $C_2 = 1$ in (29) yields

$$I[\psi_{FIM}^2] = \langle x^2 \rangle_{\psi_{FIM}^2}^{-\frac{1}{2}}. \tag{54}$$

Setting $V(x) = 0$ in the reciprocity relation (9) and substituting (54) into the resulting expression gives for $k = 2$

$$\lambda_2^{FIM} = -\frac{1}{2} \langle x^2 \rangle_{\psi_{FIM}^2}^{-\frac{3}{2}} = -4\omega^2. \tag{55}$$

Setting $V(x) = 0$ and $k = 2$ into (12), the FIM-case is obtained as

$$\lambda_0^{FIM} = I[\psi_{FIM}^2] - \lambda_2^{FIM} \langle x^2 \rangle_{\psi_{FIM}^2} = \frac{3}{2} \langle x^2 \rangle_{\psi_{FIM}^2}^{-\frac{1}{2}}. \tag{56}$$

Substituting (54) and (55) into (56), invoking (53), and setting $\omega^2 = 0.5$ into the resultant yields $\lambda_0^{FIM} = 2.0$. From Section 3, the inferred energy-eigenvalue $E = \frac{1}{2}$ is the desired result. Note that unlike the analysis in [22], (54) does not saturate the Cramer–Rao bound [27]. This issue will be discussed in Section 5.3.

5.2.2. Perturbed case $\epsilon \neq 0$

Let the empirical measurements be $\langle x^2 \rangle_{\psi_{RFI,FIM}^2}$ and $\langle x^4 \rangle_{\psi_{RFI,FIM}^2}$. Thus, an empirically inferred QM candidate potential is the QAHO of the form [23]

$$\tilde{V}^{Inf}(x) = \omega^2 x^2 + \epsilon x^4, \tag{57}$$

where ϵ is the anharmonicity constant. The a-priori specified QM physical potential is again taken to be of the form described by (40). Note that the pdf expressed in the form of amplitudes ψ_{RFI}^2 and ψ_{FIM}^2 which defines the expectations of the empirical observables depends solely upon whether the RFI or the FIM frameworks are being studied, and does not influence the choice of the inferred QM potential (57). Comparison between the second term on the LHS of (42) with (57) clearly shows $a_2 = \omega^2$ together with $a_4 = \epsilon$. Invoking now (18) yields

$$\lambda_2 = -4\omega^2, \quad \text{and,} \quad \lambda_4 = -4\epsilon. \tag{58}$$

Since the a-priori specified QM potential is the simple HO, the physical portion of the ansatz for the inferred pdf (35) is identical to (43) and (44). The inferred pdf is thus obtained from (37) with the aid of (44) and (58) as

$$\begin{aligned}
 f_{RFI}(x) &= N \exp \left\{ - \int \sqrt{8\omega^2(1 + 2\omega^2)x^2 + 16\epsilon x^4} dx \right\} \\
 &= N \exp \left\{ - \frac{\sqrt{2} [x^2 (\omega^2 + 2\omega^4 + 2\epsilon x^2)]^{\frac{3}{2}}}{3\epsilon x^3} \right\} \\
 &= N \exp \left\{ - \frac{\sqrt{2}}{3\epsilon} [\omega^2 + 2\omega^4 + 2\epsilon x^2]^{\frac{3}{2}} \right\}, \tag{59}
 \end{aligned}$$

where N is a normalization factor.

This paper seeks to benchmark the inferred energy-eigenvalues of the QAHO with established numerical solutions for the SWE within the limit $V(x) = 0$. Ref. [23] employs the following scaling relation as its basis

$$a^2 E_n^k (\omega_{SWE}^2, \epsilon_{SWE}) \approx E_n^k (\omega_{SWE}^2 a^4, \epsilon_{SWE} a^{k+2}), \tag{60}$$

where n is the quantum number (which is zero for this study), and $a > 0$. For the QAHO, $k = 4$. Thus, for $\omega_{SWE}^2 = \epsilon_{SWE} = 1$, let $a^2 = 0.5$, and thus $\omega^2 = \omega_{SWE}^2 a^4 = 0.25$ and $\epsilon = \epsilon_{SWE} a^6 = 0.125$.

From (19) for $k = 2, 4$, the normalization Lagrange multiplier is explicitly stated in terms of its moments as

$$\lambda_0 = 3.0 \langle x^2 \rangle_{\psi_{RFI}^2} + 2.5 \langle x^4 \rangle_{\psi_{RFI}^2}. \tag{61}$$

Owing to the highly oscillatory nature of the integrals over the entire range $[-\infty, \infty]$, convergence cannot be guaranteed in general. Thus, the moments in (61) are numerically evaluated in $[-2.0, 2.0]$ yielding $N = 1.35953$, $\lambda_0 \approx 2.54677$ and $E \approx 0.636693$. Again, remark that, from (42) and (15), E is not the QMHO potential energy-eigenvalue, but that for a potential which is a superposition of the HO contributions and the a-priori specified QM potential (41).

For benchmarking purposes, we carry through with an analysis analogous to the that for the HO-case in Section 5.2.1. Accordingly, setting $V(x) = 0$ yields

$$\lambda_2^{FIM} = -4\omega^2, \quad \text{and,} \quad \lambda_4^{FIM} = -4\epsilon. \tag{62}$$

The inferred pdf for the case of the quartic anharmonic oscillator in the FIM framework obtained with the aid of (38) is thus

$$f_{FIM}(x) = N \exp \left\{ - \frac{\sqrt{2}}{3\epsilon} [\omega^2 + 2\epsilon x^2]^{\frac{3}{2}} \right\}, \tag{63}$$

where N is a normalization factor.

For the case of $\omega^2 = 0.25$, $\epsilon = 0.125$, the energy-eigenvalue obtained from (19), (60)–(63) is $E \approx 0.72176$. The energy-eigenvalue from [23] scaled by $a^2 = 0.5$ for the quantum number $n = 0$ and $\omega^2 = 1.0$, $\epsilon = 1.0$ is $E^{SWE} \approx 0.696176$. Note that the equivalent expressions for the QAHO case in the FIM-study [22] yield a value of the energy-eigenvalue $E \approx 0.320024$ for $\omega^2 = 0.25$, $\epsilon = 0.125$, which represents a highly inaccurate inference. Further, the case of $\omega^2 = 0.5$, $\epsilon = 0.353553$ yields the energy-eigenvalue obtained from (19), (60)–(63) as $E \approx 1.0936$. The corresponding energy-eigenvalue from [23] scaled by $a^2 = 0.707107$ for the quantum number $n = 0$ and $\omega^2 = 1.0$, $\epsilon = 1.0$ is $E^{SWE} \approx 0.984541$. The QAHO energy-eigenvalue obtained from the inference model in this paper displays an excellent degree of consistency with the scaled energy-eigenvalues for the SWE [23], for a wide range of coefficient values of the inferred QM potential.

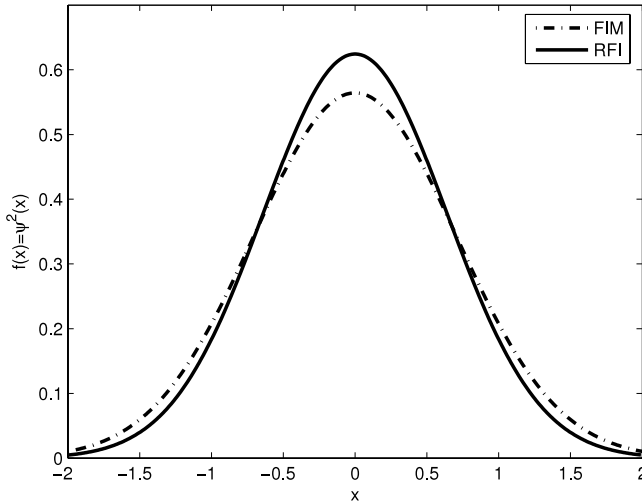


Fig. 1. Inferred pdf profiles for the harmonic oscillator obtained from the RFI framework (solid line) and the FIM framework (dash-dots) evaluated from Eqs. (35) and (38), respectively. Here, $\omega^2 = 0.5$.

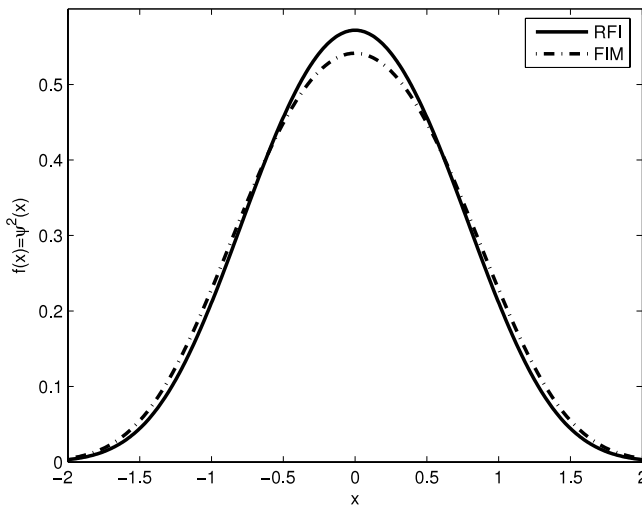


Fig. 2. Inferred pdf profiles for the quartic anharmonic oscillator obtained from the RFI framework (solid line) and the FIM framework (dash-dots) evaluated from Eqs. (35) and (38), respectively. Here, $\omega^2 = 0.25$ and $\varepsilon = 0.125$.

5.3. Comments and numerical simulations

The peculiar circumstance that makes identical the Lagrange multipliers for both the RFI and the FIM frameworks is a consequence of the *Gibbs form* adopted in (2) and (3). In Section 5.2.1, the energy-eigenvalue for the HO potential inferred from empirical observables shows excellent consistency with theoretical results within the limit $V(x) = 0$ [22,23]. This precision of the inference process described in this paper carries over to the case of the QAHO potential in Section 5.2.2 within the limit $V(x) = 0$, when compared with scaled energy-eigenvalues that are numerically obtained [23]. Figs. 1 and 2 depict the inferred pdfs for the RFI and FIM frameworks for the HO and the QAHO, respectively. In both cases, it is readily observed that the inferred pdfs obtained from the RFI framework are more sharply peaked than their FIM and SWE counterparts.

It is important to note that for expressions in this paper to reduce to those in prior FIM-studies [18,19,22,26] in the limit $V(x) = 0$, the constant in (19) and (20) $k \rightarrow \frac{k}{2}$. This discrepancy arises on account of the manner in which the empirical pseudo-potential $\tilde{U}_{RFI}^{Data}(x)$ and the physical pseudo-potential $\tilde{U}_{RFI}^{Physical}(x)$ are defined in (14) and (15). Likewise, for (29) to reduce to its FIM-counterpart as defined in previous studies (e.g. [20,22]), in the limit $V(x) = 0$, the power in (29) in this paper becomes $-\frac{1}{k} \rightarrow -\frac{2}{k}$. It is for this reason that the FIM in (54) does not saturate the Cramer–Rao bound [27] in a manner similar to its counterpart in [22]. Additionally, this discrepancy (in the limit $V(x) = 0$) between the expressions in this paper and those in previous FIM studies results in differences in the values of the normalization Lagrange multiplier and, consequently, the inferred energy-eigenvalues.

6. Reconstruction of the RFI-framework

This section establishes the theoretical basis to reconstruct the RFI-framework from the FIM-case given: (i) the values of the energy-eigenvalues of the FIM model, (ii) the empirical observations $\langle x^k \rangle_{\psi_{FIM}^2}$ (and thus the coefficients of the inferred QM potential), and (iii) the form of the a-priori specified QM potential. This is accomplished with the aid of (13) and the fact that the Lagrange multipliers λ_k associated with the constraint terms are identical for both the RFI and the FIM frameworks, a peculiarity which is traced to the Gibbs form employed in (2) and (3). Note that, owing to the transitions between the FIM and the RFI frameworks in this section all quantities (e.g. Lagrange multipliers, expectation values, amplitudes, and pdf's), are explicitly associated with the measure of uncertainty that they are associated with.

For example, the expectations $\langle \bullet \rangle_{\psi_{RFI}^2}$ and $\langle \bullet \rangle_{\psi_{FIM}^2}$ are evaluated with respect to $f_{RFI}(x)$ and $f_{FIM}(x)$, the pdf's which extremize the RFI and the FIM, respectively. With the aid of (18), and setting $E^{FIM} = \frac{\lambda_0^{FIM}}{4}$, one has from (45)

$$-\frac{d^2 \psi_{FIM}(x)}{dx^2} - \frac{1}{4} \sum_k \lambda_k A_k(x) \psi_{FIM}(x) = \frac{\lambda_0^{FIM}}{4} \psi_{FIM}(x). \tag{64}$$

Multiplying (64) by $4\psi_{FIM}(x)$ and integrating yields, on invoking the virial theorem (30) and setting $V(x) = 0$,

$$I[\psi_{FIM}^2] = \lambda_0^{FIM} + \sum_k \lambda_k \langle x_k \rangle_{\psi_{FIM}^2}. \tag{65}$$

Note that (65) has taken advantage of the fact discussed in Section 5, that the *Gibbs form* employed in (2) and (3) permits setting $\lambda_k^{RFI} = \lambda_k^{FIM} = \lambda_k$. Expressing (65) in terms of pdf's, leads to

$$\int f_{FIM}(x) \left[\left(\frac{d \ln f_{FIM}(x)}{dx} \right)^2 - \lambda_0^{FIM} - \sum_k \lambda_k x^k \right] dx = 0. \tag{66}$$

Eq. (66) is satisfied by specifying $f_{FIM}(x)$ as an exponential form resulting in

$$f_{FIM}(x) = \exp \left\{ - \int \sqrt{\lambda_0^{FIM} + \sum_k \lambda_k x^k} dx \right\}. \tag{67}$$

Invoking (17) for the FIM-framework, it is readily observed that (67) is a manifestation of (38). Comparison of (66) and (34) for $V(x) = 0$ yields

$$\sum_k k \lambda_k x^k = -\lambda_0^{FIM} - \sum_k \lambda_k x^k. \tag{68}$$

Note that even in the case $V(x) \neq 0$, the term $\sum_k k \lambda_k x^k$ corresponds to the empirical pseudopotential in (15) and is independent of the a-priori specified QM potential. Specifying in (66)

$$\lambda_0^{RFI} = \lambda_0^{FIM} + x \frac{dV_x^2(x)}{dx} - 2x \frac{dV_{xx}(x)}{dx}, \tag{69}$$

results in the transition from $f_{FIM}(x) \rightarrow f_{RFI}(x)$ and subsequently the transition from the $FIM \rightarrow RFI$ frameworks, yielding

$$\int f_{RFI}(x) \left[\left(\frac{d \ln f_{RFI}(x)}{dx} \right)^2 - \lambda_0^{RFI} - \sum_k \lambda_k x^k \right] = 0. \tag{70}$$

For exponential forms of $f_{RFI}(x)$, the solution of (70) is

$$f_{RFI}(x) = \exp \left\{ - \int \sqrt{\lambda_0^{RFI} + \sum_k \lambda_k x^k} dx \right\}. \tag{71}$$

Multiplying (69) by $f_{RFI}(x)$ and integrating, and, invoking (33) and (13), results in

$$\begin{aligned} \lambda_0^{FIM} &= \lambda_0^{RFI} - \left\langle x \frac{dV_x^2(x)}{dx} \right\rangle_{\psi_{RFI}^2} + 2 \left\langle x \frac{dV_{xx}(x)}{dx} \right\rangle_{\psi_{RFI}^2} \\ &\stackrel{(33)}{=} \lambda_0^{RFI} - 4 \left\langle \frac{d\tilde{U}_{RFI}^{Physical}(x)}{dx} \right\rangle_{\psi_{RFI}^2} \stackrel{(13)}{=} \lambda_0^{RFI} - 2 \langle V_{xx}(x) \rangle_{\psi_{RFI}^2} + \langle V_x^2(x) \rangle_{\psi_{RFI}^2}. \end{aligned} \tag{72}$$

Similarly, multiplying (69) by $f_{FIM}(x)$ and integrating, and, invoking (33) and (13), results in

$$\begin{aligned} \lambda_0^{RFI} &= \lambda_0^{FIM} + \left\langle x \frac{dV_x^2(x)}{dx} \right\rangle_{\psi_{FIM}^2} - 2 \left\langle x \frac{dV_{xx}(x)}{dx} \right\rangle_{\psi_{FIM}^2} \\ &\stackrel{(33)}{=} \lambda_0^{FIM} + 4 \left\langle \frac{d\tilde{U}_{RFI}^{Physical}(x)}{dx} \right\rangle_{\psi_{FIM}^2} \stackrel{(13)}{=} \lambda_0^{FIM} + 2 \langle V_{xx}(x) \rangle_{\psi_{FIM}^2} - \langle V_x^2(x) \rangle_{\psi_{FIM}^2}. \end{aligned} \tag{73}$$

Simultaneously subtracting and adding (13) from (65) yields

$$\begin{aligned} I[\psi^2] - 2 \langle V_{xx}(x) \rangle_{\psi^2} + \langle V_x^2(x) \rangle_{\psi^2} \\ + \lambda_0^{FIM} + 2 \langle V_{xx}(x) \rangle_{\psi^2} - \langle V_x^2(x) \rangle_{\psi^2} + \sum_k \lambda_k \langle x^k \rangle_{\psi^2} = 0. \end{aligned} \tag{74}$$

Note that in (74), the nature of the probability with which the expectation in the term $\sum_k \lambda_k \langle x^k \rangle_{\psi^2}$ is evaluated is *deliberately unspecified*. Further, it is *deliberately unspecified* as to whether ψ extremizes the RFI or the FIM. From (11), the first three terms in the LHS of (74) constitute the RFI $\mathfrak{S}[\psi_{RFI}^2 | e^{-V(x)}]$ if $I[\psi^2] = I[\psi_{RFI}^2]$ and $\langle \bullet \rangle = \langle \bullet \rangle_{\psi_{RFI}^2}$. From (72), it is evident that next three terms in the LHS of (74) comprise λ_0^{RFI} , and the expectations are specified as: $\langle V_{xx}(x) \rangle_{\psi_{RFI}^2}$ and $\langle V_x^2(x) \rangle_{\psi_{RFI}^2}$. Specifying $\sum_k \lambda_k \langle x^k \rangle = \sum_k \lambda_k \langle x^k \rangle_{\psi_{RFI}^2}$, (12) is recovered. *The introduction of the expectations of the derivatives of the physical potential via (72) facilitates the transition from the $FIM \rightarrow RFI$ frameworks. Note that (12) constitutes one of the most fundamental relations governing the RFI framework. Thus, (65) in conjunction with (11) and (72) allows for the reconstruction of the RFI framework from the FIM framework.*

In a similar vein, substituting (11) into (12) and suitably manipulating the pertinent terms results in

$$\begin{aligned} \mathfrak{S}[\psi_{RFI}^2 | e^{-V(x)}] - \langle V_x^2(x) \rangle_{\psi_{RFI}^2} + 2 \langle V_{xx}(x) \rangle_{\psi_{RFI}^2} \\ = \lambda_0^{RFI} - \langle V_x^2(x) \rangle_{\psi_{RFI}^2} + 2 \langle V_{xx}(x) \rangle_{\psi_{RFI}^2} + \sum_k \lambda_k \langle x^k \rangle. \end{aligned} \tag{75}$$

Again, note that in (75) the nature of the probability with which the expectation in the term $\sum_k \lambda_k \langle x^k \rangle$ is evaluated is *deliberately unspecified*. From (11), the LHS of (75) is $I[\psi^2]$, where again it is *deliberately unspecified* as to whether ψ extremizes the RFI or the FIM. However, from (72) it is evident that first three terms in the RHS of (75) comprise λ_0^{FIM} . Specifically, there is no explicit dependence upon the a-priori specified physical QM potential, whose derivative terms have been absorbed into λ_0^{FIM} . Thus, specifying $I[\psi^2] = I[\psi_{FIM}^2]$ and $\sum_k \lambda_k \langle x^k \rangle = \sum_k \lambda_k \langle x^k \rangle_{\psi_{FIM}^2}$, (65) is recovered. Thus, (72) in conjunction with (11) and (12) offers an alternate to setting $V(x) = 0$ in achieving a transition from the RFI \rightarrow FIM frameworks.

The workings of the above reconstruction procedure are now exemplified with the aid of a simple example. The inference of the energy-eigenvalues without recourse to the S–RFI link (4) and (14) constitutes one of the primary objectives of this paper. This is described in Section 5.2. Section 5.2.1 demonstrated excellent consistency between the theoretical results for the inference process presented in this paper with published works [22], for the case of the HO potential for $\omega^2 = 0.5$. This was accomplished by setting the a-priori specified physical QM potential $V(x) = 0$, thereby converting the RFI-framework presented herein into an FIM-framework. The energy-eigenvalue and the normalization Lagrange multiplier for the FIM-case presented in Section 5.2.1 for the inferred HO potential are $E^{FIM} = 0.5$ and $\lambda_0^{FIM} = 2.0$, respectively.

For the case of the a-priori specified QM potential (that is again the HO expression (41)), invoking (73) and (44) results in

$$\lambda_0^{RFI} = 2.0 + 8\omega^4 \langle x^2 \rangle_{\psi_{FIM}^2} . \tag{76}$$

With the aid of (53), $\lambda_0^{RFI} = 3.125$ and $E = \frac{\lambda_0^{RFI}}{4} = 0.78125$. In contrast to the *approximate* inferred values of λ_0^{RFI} and E presented in Section 5.2.1 (obtained from (19), (48), and (49)), the values presented in this section represent an inference of the RFI energy-eigenvalues that uses *exact* theoretical results for the FIM-case. Reasons for the discrepancy between the inferred energy-eigenvalues presented in this section for the RFI framework, and those of the type presented in Section 5.2.1, are the objective of on-going work, as are obtaining high precision numerical solutions of the SWE (instead of theoretical results for the FIM-case) for more complex inferred QM potentials.

7. Summary and conclusions

The derivation of the reciprocity relations for the RFI have been self-consistently established in this paper using the Hellmann–Feynman theorem. The inference of an ansatz for pdf’s possessing an exponential form for the RFI framework has been obtained solely on the basis of the S–RFI link and the QM virial theorem. The qualitative distinctions between the RFI and the FIM frameworks have been established. The energy-eigenvalues of (4) have been self-consistently inferred solely on the basis of the ansatz (derived in Section 4). This has been demonstrated in Section 5 for the case of both the harmonic oscillator and the quartic anharmonic oscillator potentials. Such an inference has been made possible by solely utilizing the Legendre transform structure of the RFI, and the fundamental properties of the QM virial theorem embedded in Eq. (19) in Section 3.

Apart from the analysis and numerical simulations described in Section 5, one of the most poignant examples of the distinction between RFI and FIM variational extremizations is stated in Section 3. Specifically, the RFI framework yields a solution even of there are no empirical observables. Thus, the Quantum square well example provided in Ref. [18] cannot hold true in the RFI framework, since the physical pseudo-potential of (4) and (14) is non-vanishing. Further, a most noteworthy observation, highlighted in Section 5, is that the Gibbs form adopted in (2) and (3) renders the Lagrange multipliers associated with the empirical observables identical for both the RFI and the FIM frameworks.

There is a pronounced difference between the methodology employed in this paper to infer energy-eigenvalues and pdf’s, and that employed in previous FIM studies [18,22]. While relations analogous to the one between the Lagrange multipliers and the coefficients of the QM potential inferred from empirical observables (18) have been derived in [18,22], Ref. [18] makes no attempt to infer the

energy-eigenvalues and obtain the pdf profiles. In contrast, this paper presents results for the inferred pdf's for *both* the RFI and the FIM frameworks, and accomplishes inferring the energy-eigenvalues for the RFI framework for inferred QM potentials of *both* the harmonic oscillator and the quartic anharmonic oscillator models. Next, in the case of [22] there are pronounced distinctions between the methodology employed therein and that followed in this paper.

Specifically: (i) for the case of the harmonic oscillator (HO, hereafter) potential inferred from empirical observables, [22] first assumes $\langle x^2 \rangle_{\psi_{FIM}^2}$ and then further *specifies* that the FIM saturates the Cramer–Rao bound. In contrast, no such specifications are possible in this paper because of the differences between (19), (20), and (29) herein and their counterparts in previous FIM-studies. Specifically, these differences stem from the fact that the Schrödinger-like link for the RFI (14) in the limit $V(x) = 0$ is of the more fundamental form of the Schrödinger wave equation (SWE, hereafter) in [23], instead of the “scaled” version in [22], (ii) for the case of the quartic anharmonic oscillator (QAHO, hereafter), the results of the inferred energy-eigenvalues in [22] cannot be benchmarked with the more fundamental ones in [23] without recourse to *restrictive* and ad-hoc “adjustments”. In contrast, the procedure employed in this study prescribes no such “adjustments” for benchmarking the inferred energy-eigenvalues for both the RFI and the FIM frameworks. Instead, a fundamental scaling relation (60) underlying the basis for the work presented in [23] is employed, and (iii) while [26] does not present numerical results for the nature of the inferred pdf profiles, this paper presents such cases for *both* the RFI *and* the FIM frameworks, for *both* inferred harmonic oscillator *and* quartic anharmonic oscillator potentials. Finally, it is important to note that in the QAHO case, the energy-eigenvalues obtained via the inference procedure demonstrated in this paper show greater consistency with the numerical results in [23] than those described in [22].

The work presented herein is the generalization of prior studies within the FIM framework [18,19,22,26] to the case of the RFI framework. The results presented herein establishes the basis for a comprehensive comparison between the RFI and the FIM frameworks using established theoretical and/or numerical results for HO and QAHO models [22,23]. Further, Sections 4 and 5 of this paper establish the qualitative distinction between the RFI and FIM frameworks based on an inferred ansatz of exponential form. Finally, Section 6 of this paper establishes the theoretical framework for reconstructing RFI pdf's from the FIM pdf's obtained from inference, employing the ansatz derived in Section 4. In addition to establishing the transition between the *FIM* \rightarrow *RFI* frameworks, the analysis prescribes a method to achieve a transition from the *RFI* \rightarrow *FIM* frameworks without recourse to setting the a-priori specified potential $V(x) = 0$.

The work presented in this paper may be readily extended to more complex empirical and physical pseudo-potentials. Specifically, such an endeavor would entail the evaluation of a number of Lagrange multipliers. In this case, a potentially attractive and credible ansatz for the inferred pdf is

$$f_{RFI}(x) = \exp \left\{ - \int \sqrt{ - \sum_{k=1}^M k \lambda_k x^k + x \frac{dV_x^2(x)}{dx} - 2x \frac{dV_{xx}(x)}{dx} } \right\} H_n(x), \quad (77)$$

where $H_n(x)$ are Hermite–Gauss polynomials. A candidate approach to accomplish this task is the extension of the framework presented in this paper via a suitable adaptation of the information-theoretic optimization scheme described in [29,28]. The game-theoretic aspects of [29,28] have their origins in [30]. The process of inference constitutes the basis of machine learning [31].

The process of obtaining the energy-eigenvalues in Section 5 and the transitions between the *RFI* \Leftrightarrow *FIM* frameworks in Section 6 lend immense credence to the prospect of formulating a comprehensive inference framework for compressed sensing [32]. These studies are the task of ongoing works.

Acknowledgments

Gratitude is expressed towards the reviewers for their invaluable comments. RCV gratefully acknowledges support from NSFC-CS & NI contract 111017-01-2013.

Appendix. Interpretation of Eq. (13)

A necessary condition for the RFI derivations is the following relation (cf. Eq. (13)):

$$4 \left\langle x \frac{d\tilde{U}_{RFI}^{Physical}(x)}{dx} \right\rangle_{\psi_{RFI}^2} = 2 \langle V_{xx}(x) \rangle_{\psi_{RFI}^2} - \langle V_x^2(x) \rangle_{\psi_{RFI}^2}. \quad (A.1)$$

The RFI pseudo-potential was re-defined in (15) as

$$\tilde{U}_{RFI}(x) = -\frac{1}{4} \underbrace{\left[\sum_{i=1}^M \lambda_i A_i(x) \right]}_{\tilde{U}_{RFI}^{Data}(x)} - \frac{1}{4} \underbrace{\left[2V_{xx}(x) - V_x^2(x) \right]}_{\tilde{U}_{RFI}^{Physical}(x)}. \quad (A.2)$$

(A.1) and (A.2) imply that

$$x \frac{d\tilde{U}_{RFI}^{Physical}(x)}{dx} = -\tilde{U}_{RFI}^{Physical}(x). \quad (A.3)$$

This entails

$$\int x \frac{d\tilde{U}_{RFI}^{Physical}(x)}{dx} dx = - \int \tilde{U}_{RFI}^{Physical}(x) dx. \quad (A.4)$$

Subjecting the LHS of (A.4) to a single integration-by-parts yields

$$x \tilde{U}_{RFI}^{Physical}(x) \Big|_{B.C.} - \int \tilde{U}_{RFI}^{Physical}(x) dx = - \int \tilde{U}_{RFI}^{Physical}(x) dx. \quad (A.5)$$

For vanishing $\tilde{U}_{RFI}^{Physical}(x)$ at the boundaries in (A.5), (A.3) is true for any $\tilde{U}_{RFI}^{Physical}(x)$.

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