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Article

Information Theory Consequences of the Scale-Invariance of Schröedinger's Equation

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Abstract: In this communication we show that Fisher's information measure emerges as a direct consequence of the scale-invariance of Schröedinger's equation. Interesting, well-known additional results are re-obtained as well, for whose derivation **only** (and this is the novelty) the scale invariance property is needed, without further ado.

Keywords: scaling invariance; Fisher Information; MaxEnt; reciprocity relations

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1. Introduction

Information is carried, stored, retrieved and processed by physical devices of various kinds (or by living organisms). The substratum for any means of handling information is then, of course, physical. Thus, physics and information possess a rich interface and, indeed, the goal of the physical endeavor can be described as that of modelling and predicting natural phenomena by recourse to relevant information (concerning systems of interest). Accordingly, it is reasonable to expect that

- the laws of physics should be a reflection of the methods for manipulating information (the Wheeler paradigm, see [1] and references therein) and/or
- the laws of physics could be used to manipulate information (see [2] and references therein).

In this communication we will present an example of the second instance that starts with the scaling properties of Schrödinger's equation and ends up with most celebrated local measure of information. Details of our travelling route are given in Subsection 2.4.

2. Background Notions

2.1. *The Hellmann-Feynman Rheorem*

We start our considerations by reminding the reader of a celebrated quantum theorem, the Hellmann-Feynman one, that relates (i) the derivative of the total energy E with respect to a Hamiltonian (H) parameter b to (ii) the expectation value of the derivative of the Hamiltonian with respect to that same parameter.

$$\frac{dE}{db} = \frac{d\langle H\rangle}{db} \tag{1}$$

Its most common application is in the calculation of forces in molecules (with the parameters being the positions of the nuclei) where it states that once the spatial distribution of the electrons has been determined by solving the Schrödinger equation, all the forces in the system can be calculated using concepts of classical electrostatics. The theorem has been proven independently by many authors, including Guettinger (1932), Pauli (1933), Hellmann (1937), and Feynman (1939) [3–5].

2.2. *Scaling*

Scale invariance (SI) refers to objects or laws that remain invariant if scales of length, energy, *etc*., are multiplied by a common factor, a process called dilatation. Probability distributions of random processes may display SI. In classical field theory SI most commonly applies to the invariance of a whole theory under dilatations while in quantum field theory SI is usually interpreted in terms of particle physics. In a SI-invariant theory the strength of particle interactions does not depend on the energy of the particles involved. In statistical mechanics SI is a feature of phase transitions. Near a phase transition or critical point fluctuations appear at all length scales, forcing one to look for an explicitly SI theory to describe things. These theories are SI statistical field theories, being formally very similar to scale-invariant quantum field ones [6].

2.3. *The Hamiltonian H*

Consider a time-independent Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \tag{2}$$

and its associated Schröedinger wave equation (SWE),

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\psi(x) = E\psi(x) \tag{3}$$

The potential function $U(x)$ belongs to $\mathcal{L}_2$ and thus admit of a series expansion in x, $x^2\, x^3$, *etc.* [7–9]. This enables us to base our future considerations on the assumption that the potential can be written as

$$U(x) = \sum_{k=1}^{M} a_k\, x^k \tag{4}$$

and we will assume that *the first M terms of the above series yield a satisfactory representation of* $U(x)$. The concomitant "coupling constants"

$$\{a_1, \ldots, a_M\} \tag{5}$$

will play a dominant role in our considerations.

2.4. Our Program

The scheme below illustrates the path to be followed in this paper.

$$\boxed{\begin{array}{c}
(1)\ Derive\ the\ scaling\ rule\ (SR)\ for Schroedinger's\ equation \\
under\ length-changes\ \xi \\
(2)\ Manipulate\ the\ SR\ and\ get \\
a\ partial\ differential\ equation\ (PDE)\ for\ \langle H\rangle \\
in\ terms\ of\ \frac{\partial\langle H\rangle}{\partial a_k};\ k=1,\ldots,M \\
(3)\ This\ establishes\ that\ \langle H\rangle\ is\ a\ function\ only\ of\ the\ coupling\ constants\ (CC) \\
(4)\ Construct\ the\ Legendre\ transform\ (LT) \\
of\ \langle H\rangle\ so\ as\ to\ change\ independent\ variables \\
from\ the\ M\ CC\ to\ \langle x^k\rangle;\ k=1,\ldots,M \\
(5) Discover\ that\ the\ concomitant\ LT\ is\ -K = -\langle \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\rangle \\
(6)\ K = Average\ kinetic\ energy\ \ LT:\ \langle H\rangle \overset{LT}{\leftrightarrow} -K \\
(7)\ Study\ associated\ reciprocity\ relations \\
(8) Encounter\ significant\ information\ theory\ results.
\end{array}}$$

3. The Schrödinger-Scaling Rule

3.1. Preliminaries

Set the scaling parameter $\xi \equiv a$. It is known that, under the scaling transformation $x \to ax$ $(a > 0)$, H goes over to a unitarily equivalent Hamiltonian $\bar{H}$ (see Appendix A for details)

$$H(x, a_1, \cdots, a_M) \quad \overset{x\to ax}{\longrightarrow} \quad a^{-2}\bar{H}(x, \bar{a}_1, \cdots, \bar{a}_M)\,, \qquad \bar{a}_k = a^{k+2} a_k \tag{6}$$

so that the $H-$eigenvalues E satisfy the scaling relation

$$a^2 E(a_1, \cdots, a_M) = \bar{E}(\bar{a}_1, \cdots, \bar{a}_M), \qquad \bar{a}_k = a^{k+2} a_k \tag{7}$$

3.2. Manipulating the Scaling Rule

At this stage we begin presenting our results. Differentiating Relation (7) with respect to the $a-$parameter one obtains

$$\frac{\partial}{\partial a}\left[a^2 E(a_1, \cdots, a_M)\right] = \frac{\partial}{\partial a}\left[\bar{E}(\bar{a}_1, \cdots, \bar{a}_M)\right] \tag{8}$$

i.e.,

$$2aE = \sum_{k=1}^{M} \frac{\partial \bar{E}}{\partial \bar{a}_k} \frac{\partial \bar{a}_k}{\partial a} \tag{9}$$

Note that

$$\frac{\partial \bar{a}_k}{\partial a} = \frac{\partial}{\partial a}\left(a^{k+2} a_k\right) \; = \; (k+2)\, a^{k+1} a_k \; = \; (k+2)\, a^{-1}\, \bar{a}_k \tag{10}$$

so that

$$2aE \; = \; a^{-1} \sum_{k=1}^{M} \; (k+2) \; \bar{a}_k \, \frac{\partial \bar{E}}{\partial \bar{a}_k} \tag{11}$$

or,

$$a^2 \; E \; = \; \sum_{k=1}^{M} \; \left(\frac{k}{2} + 1\right) \; \bar{a}_k \, \frac{\partial \bar{E}}{\partial \bar{\lambda}_k} \tag{12}$$

Now, Equation (7) states that

$$a^2 \; E \; = \; \bar{E} \qquad , \qquad \bar{a}_k \equiv a^{k+2} a_k$$

implying that the following linear partial differential equation (PDE) is obeyed:

$$E \; = \; \sum_{k=1}^{M} \left(\frac{k}{2} + 1\right) \; a_k \, \frac{\partial E}{\partial a_k} \tag{13}$$

an important relation that was reported in [10], that deals with the WKB approach to the SWE. Equation (13) is in that reference depicted as a relationship that rules the scaling behavior of SWE-energy-eigenvalues with respect to the parameters a_k of the Hamiltonian.

3.3. Interpreting Equation (13)

In [11] the present authors went way beyond the above interpretation of such PDE, provided an entirely different demonstration for Equation (13), and took it as a "prescription", a linear PDE that energy eigenvalues must necessarily comply with. A careful mathematical study of this PDE was undertaken in [11]. Its complete solution was given in the form

$$E(a_1, ..., a_M) = \; \sum_{k=1}^{M} \; D_k \; |a_k|^{2/(2+k)} \tag{14}$$

where the D_ks are positive real constants (integration constants). It was also shown that the E-domain is $D_E = \{(a_1, \cdots, a_M)/a_k \in \Re\} = \Re^M$. One sees that Equation (14) states that for $a_k > 0$, E is a monotonically increasing function of the a_k, and for all $a_k \in D_E$, E is a concave function. The authors were able to demonstrate in [11] that the general solution for the $E-$PDE does exist and its uniqueness was ascertained via an analysis of the associated Cauchy problem.

Appeal to the Hellmann-Feynman theorem is now needed here with reference to Cauchy-uniqueness. For our present case, the Lipschitz condition can be seen to be verified always since the Hellmann-Feynman theorem [3–5] guarantees that

$$\frac{\partial E}{\partial a_k} = \left\langle x^k \right\rangle < \infty \tag{15}$$

4. A Question of Independent Variables. The Legendre Transform

According to *our* viewpoint, Equation (13) expresses a relation between (i) the independent variables or control variables (the $U(x)-$expansion coefficients a_k) and (ii) a dependent energy-value E. Such information is encoded into the functional form of $E = E(a_1, ..., a_M)$. For later convenience, we will also denote such a relation or encoding as $\{E, a_k\}$. Now, from the SWE (3), in which $U(x)$ is given by (4), one has

$$\left\langle -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_{k=1}^{M} a_k\, x^k \right\rangle = \langle H \rangle \qquad \longrightarrow \qquad K + \sum_{k=1}^{M} a_k\, \langle x^k \rangle = \langle H \rangle \tag{16}$$

where the $K-$function stands for the expectation value of the kinetic energy,

$$K = \left\langle -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \right\rangle \tag{17}$$

We arrive here to the crucial stage of our current developments: a change of independent variables from the a_k to the $\langle x^k \rangle$, which can always be provided by a suitable Legendre transform [12]. We thus envisage an $M-$terms Legendre transform [12,13] of $L = -K$, and write

$$\begin{aligned} L(\langle x^1 \rangle, \cdots, \langle x^M \rangle) = \textstyle\sum_{k=1}^{M} a_k \langle x^k \rangle - \langle H \rangle = \\ = \langle U \rangle - \langle H \rangle = -K \quad \longrightarrow \quad K = \langle H \rangle - \textstyle\sum_{k=1}^{M} a_k \langle x^k \rangle \end{aligned} \tag{18}$$

where the associated reciprocity relation, essential for this kind of transform, reads [13]

$$\langle x^k \rangle \equiv \frac{\partial \langle H \rangle}{\partial a_k} \tag{19}$$

We realize here that the Legendre transform of $L = -K$ is the expectation value of the Hamiltonian $\langle H \rangle$

$$\langle H \rangle (a_1, \cdots, a_M) = \sum_{k=1}^{M} a_k\, \langle x^k \rangle - L \qquad \longrightarrow \quad \langle H \rangle = K + \sum_{k=1}^{M} a_k\, \langle x^k \rangle \tag{20}$$

with a reciprocity relation given by,

$$a_k \equiv \frac{\partial L}{\partial \langle x^k \rangle} = -\frac{\partial K}{\partial \langle x^k \rangle} \tag{21}$$

We see that the Legendre transform displays the information encoded in $\langle H\rangle$, via M $\langle x^k\rangle-$parameters, in $L = -K(\langle x^1\rangle, ...\langle x^M\rangle)$

$$\{\langle H\rangle, a_k\} \quad \overset{LT}{\longleftrightarrow} \quad \{K, \langle x^k\rangle\}$$

where the relations between the two sets of associated, independent variables are given by the relations (19) and (21).

5. Virial Theorem Derived from $\langle H\rangle$ and K

Although the relationship *virial-scaling* is well known (see the excellent monograph of Fernandez and Castro [14]), *the novel ingredient here is Equation (13)*. Let us now return to it

$$E \;=\; \sum_{k=1}^{M}\left(\frac{k}{2}+1\right)\, a_k\,\frac{\partial E}{\partial a_k} \tag{22}$$

and recast it, for $E = \langle H\rangle_\psi$, in the fashion

$$\langle H\rangle_\psi \;=\; \sum_{k=1}^{M}\left(\frac{k}{2}+1\right)\, a_k\,\frac{\partial \langle H\rangle_\psi}{\partial a_k} \tag{23}$$

The Relations (23) and (19) together lead us to regard the later in the fashion

$$\frac{\partial\langle H\rangle_\psi}{\partial a_k} = \langle x^k\rangle_\psi \qquad \longrightarrow \qquad \langle H\rangle_\psi \;=\; \sum_{k=1}^{M}\frac{k+2}{2}\, a_k\,\langle x^k\rangle_\psi \tag{24}$$

Substituting now (24) into (18), the $K-$function can be written as

$$K \;=\; \sum_{k=1}^{M}\frac{k}{2}\, a_k\,\langle x^k\rangle_\psi \tag{25}$$

which can be written as

$$K \;=\; \left\langle \sum_{k=1}^{M}\frac{k}{2}\, a_k\, x^k\right\rangle_\psi \;=\; \frac{1}{2}\left\langle x\,\frac{\partial}{\partial x}U(x)\right\rangle_\psi \tag{26}$$

where $U(x)$ is given by (4). Comparing (17) and (26) we can assert that

$$\left\langle -\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2}\right\rangle_\psi \;=\; \left\langle x\,\frac{\partial}{\partial x}U(x)\right\rangle_\psi$$

which is the celebrated Virial theorem [7–9]. For a different information-theory derivation, in which the Legendre structure is itself derived starting from the HF and Virial theorems, see [15].

6. Legendre Transform Leads to a PDE for K

The Legendre transform we have just considered allows for interesting consequences. From (25), taking into account (21), we can obtain the partial differential equation that governs the $K-$function,

$$a_k = -\frac{\partial K}{\partial\langle x^k\rangle_\psi} \qquad \longrightarrow \qquad K \;=\; -\sum_{k=1}^{M}\frac{k}{2}\langle x^k\rangle_\psi\,\frac{\partial K}{\partial\langle x^k\rangle_\psi} \tag{27}$$

A complete solution for K-DPE (27) is given by [11],

$$K = \sum_{k=1}^{M} C_k \, |\langle x^k \rangle_\psi|^{-\,2/k} \tag{28}$$

where the C_ks are positive real constants (integration constants). The K-domain is $D_K = \left\{(\langle x^1\rangle_\psi, \cdots, \langle x^M\rangle_\psi)/\langle x^k\rangle_\psi \in \Re_o\right\}$. Also, Equation (28) states that for $\langle x^k\rangle_\psi > 0$, K is a monotonically decreasing function of the $\langle x^k\rangle_\psi$, and as one expect from the Legendre transform of $\langle H\rangle$, we end up with a convex function ($L = -K$ result a concave function). The general solution for K-PDE exists. Uniqueness is, again, proved from an analysis of the associated Cauchy problem [11]. Thus, Equation (27) can be interpreted as a "universal" prescription, a linear PDE that $K-$function must necessarily comply with. For notational simplicity we drop here from the subscript (ψ).

7. A New Form for the Uncertainty Principle

The precise statement of the position-momentum uncertainty principe (UP) reads [9]

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2} \qquad \textit{or} \qquad (\Delta x)^2(\Delta p)^2 \geq \frac{\hbar^2}{4} \tag{29}$$

where

$$(\Delta x)^2 = \left\langle (x - \langle x\rangle)^2 \right\rangle = \langle x^2\rangle - \langle x\rangle^2 \tag{30}$$

$$(\Delta p)^2 = \left\langle (p - \langle p\rangle)^2 \right\rangle = \langle p^2\rangle - \langle p\rangle^2 \tag{31}$$

In a one-dimensional configuration-space, where ψ is always a real wave function [7],

$$\langle p\rangle = \langle -i\hbar \frac{\partial}{\partial x}\rangle = -i\hbar \int \psi \frac{\partial}{\partial x}\psi \, dx = -i\frac{\hbar}{2}\int \frac{\partial}{\partial x}\psi^2 \, dx = 0 \tag{32}$$

Substituting (32) in (31) and using (17) we have,

$$(\Delta p)^2 = \langle p^2\rangle = \left\langle -\hbar^2 \frac{\partial^2}{\partial x^2} \right\rangle = 2m\,K \tag{33}$$

If this relation is substituted into (29) we arrive to,

$$K\,(\Delta x)^2 \geq \frac{\hbar^2}{8m} \tag{34}$$

possibly providing new garments to the UP.

8. From Quantum Mechanics to a Fisher Measure

8.1. *Preliminaries on Fisher's Information Measure (FIM)*

The bridge linking between Information Theory and Thermodynamics—Statistical Mechanics—was erected by Jaynes half a century ago [16]. It is supported by a variational approach that entails extremization of Shannon's information measure subject to the constraints posed by the *a priori* knowledge one may possess concerning the system of interest. The entire edifice of statistical mechanics can be constructed if one chooses Boltzmann's constant as the informational unit and identifies Shannon's information measure S with the thermodynamic entropy. The concomitant methodology is referred to as the *Maximum Entropy Principle (MaxEnt)* [16]. In the 1990s a similar program was successfully developed that replaces Shannon's information measure S by Fisher's one (FIM) I [17]

$$I \;=\; \int dx\; f\, \left(\frac{\partial \ln f}{\partial x}\right)^2 ;\;\; \text{f being a normalized probability density} \tag{35}$$

not the most general FIM-form, but the one most employed in physical applications [17,18]. Since $f-$derivatives enter I's definition, FIM is a local measure. Shannon's instead, is global [19].

A new viewpoint was in this way provided within the so-called Wheeler's program of establishing an information theoretical foundation for the basic theories of physics [1,20]. Much effort has consequently been expended upon FIM-applications. See for instance [18,21], and references therein.

8.2. FIM Results from Quantum Mechanics' Scaling Rules

At this stage, we may realize that K-function is intimately linked to Fisher's information measure (FIM). From (17) we have

$$K \;=\; \left\langle -\,\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial x^2}\right\rangle \;=\; -\,\frac{\hbar^2}{2m}\int dx\,\psi\,\frac{\partial^2}{\partial x^2}\,\psi \;=\; \frac{\hbar^2}{2m}\int dx\,\left(\frac{\partial \psi}{\partial x}\right)^2 \tag{36}$$

Defining $f = \psi^2$, we can write,

$$K \;=\; \frac{\hbar^2}{8m}\int dx\; f\,\left(\frac{\partial \ln f}{\partial x}\right)^2 \tag{37}$$

Recalling from Equation (35) the FIM-definition of I

$$I \;=\; \int dx\; f\,\left(\frac{\partial \ln f}{\partial x}\right)^2 \tag{38}$$

we reach the conclusion that

$$K \;=\; \frac{\hbar^2}{8m}\; I \tag{39}$$

a fact we can read about in [17]. The uncertainty principle (34) expresses the Fisher-inequality $I(\Delta x)^2 \;\geq\; 1$, that expresses the well-known Cramer-Rao bound [18,22]. We appreciate the fact that f is taken to be of the form ψ^2, I emerges dressed as K. Also, the accompanying Cramer-Rao bound emerges in natural form from the UP.

9. Conclusions

In this communication we have considered the scaling transformation of the Schröedinger equation (SWE). From the partial differential equation that governs the behavior of the energy eigenvalues (8) one finds for the expectation value of $\langle H\rangle$ an explicit function that depends on the potential-series-expansion parameters. The study of this $\langle H\rangle$-function, via its Legendre transform, allows one to re-derive in new fashion several interesting and well-known quantal results.

The SWE allows us to identify the scaling, Legendre-transformed of $\langle H \rangle$ as the expectation value of the kinetic energy K. Finally, the Legendre structure leads one to find partial differential equation that governs the K-structure.

Finally, if the square of the $H-$eigenfunctions is interpreted as a probability density, both the Fisher measure I as well as the Cramer-Rao bound emerge in natural manner.

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Appendix A: The Hamiltonian Scaling Transform

We describe here the theory-changes under a scaling transformation. We start with

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_k a_k\, x^k\right]\psi \;=\; E\,\psi \tag{40}$$

Under the scaling transform $x \to ax$ we get

$$\left[-\frac{\hbar^2}{2ma^2}\frac{\partial^2}{\partial x^2} + \sum_k a_k\, a^k x^k\right]\bar{\psi}(x) \;=\; E\,\bar{\psi}(x) \tag{41}$$

where $\bar{\psi}$ is ψ's scaling transformed function. Multiplying now both terms of (41) by a^2 we obtain

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_k a_k\, a^{k+2} x^k\right]\bar{\psi}(x) \;=\; a^2\,E\,\bar{\psi}(x) \tag{42}$$

that we can cast as

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_k \bar{a}_k\, x^k\right]\bar{\psi}(x) \;=\; \bar{E}\,\bar{\psi}(x) \tag{43}$$

where

$$\bar{a}_k \;=\; a^{k+2} a_k\,, \qquad\qquad \bar{E} \;=\; a^2 E \tag{44}$$

The relation between the two eigenfunction is given by $\bar{\psi}(x) = N\psi(ax)$, with N obtained by requesting that both the original and the transformed wave functions be normalized to unity

$$1 \;=\; \int \bar{\psi}(x)^2\,dx = \int N^2\,\psi(ax)^2\,dx = \frac{N^2}{a}\int \psi(x)^2\,dx = \frac{N^2}{a} \quad\longrightarrow\quad N \;=\; \sqrt{a} \tag{45}$$