Fisher Information and Kinetic-energy Functionals: A Dequantization Approach

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Abstract

We strengthen the connection between Information Theory and quantum-mechanical systems using a recently developed dequantization procedure whereby quantum fluctuations latent in the quantum momentum are suppressed. The dequantization procedure results in a decomposition of the quantum kinetic energy as the sum of a classical term and a purely quantum term. The purely quantum term, which results from the quantum fluctuations, is essentially identical to the Fisher information. The classical term is complementary to the Fisher information and, in this sense, it plays a role analogous to that of the Shannon entropy. We demonstrate the kinetic energy decomposition for both stationary and nonstationary states and employ it to shed light on the nature of kinetic-energy functionals.

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I. INTRODUCTION

Over the past few years, Dehesa has been a pioneer in developing a connection between information theory and quantum-mechanical systems. This connection is potentially of significant practical value as it is related to density functional theory and, in particular, to the construction of kinetic-energy functionals. For one-electron systems with a central potential, such as the hydrogen atom, Dehesa obtained an analytic expression for the Fisher information in terms of the quantum numbers of the stationary states. Also over the past few years we have developed a dequantization procedure, first based on Witten deformation and subsequently based on a variational principle. This dequantization procedure results in a decomposition of the quantum kinetic energy as the sum of a classical term and a purely quantum term. We recently demonstrated the kinetic energy decomposition for hydrogenic orbitals.

In the present paper we examine connections between our work and that of Dehesa. We consider our kinetic energy decomposition for stationary states of the hydrogen atom and nonstationary states of a particle in a box and a free particle represented as a Gaussian wavepacket.

A. Fisher Information

The Fisher information, which is one of the cornerstones of information theory, was developed as a measure of spatial localization. For an $N$-electron system the Fisher information is given by

$$\mathcal{J} = \int \frac{\left| \nabla p(r) \right|^2}{p(r)} d^3 r,$$

where $p(r_1) = \int |\psi(r_1, \ldots, r_N)|^2 d^3 r_2 \ldots d^3 r_N$ is the one-electron (probability) density. The electron density, $\rho(r)$, is related to the one-electron (probability) density by $\rho(r) = N p(r)$. Thus the $\mathcal{J}$ is a functional of the electron density and is a local measure of the breadth of the electron density. The greater the localization of $\rho(r)$ the greater the value of the Fisher information. In contrast, the greater the delocalization of $\rho(r)$ the greater the value of the Shannon entropy. Thus the Fisher information and the Shannon entropy are complementary quantities and have been used in conjunction to analyze electron correlation and other atomic properties.
B. Density Functional Theory

Density functional theory (DFT) has developed into an extremely successful approach for the calculation of atomic and molecular properties. [4, 13, 19] In DFT, the electron density is the fundamental variable and properties such as the energy are obtained as a functional of \( \rho(r) \) rather than from the \( N \)-electron wavefunction, \( \psi(r_1, \ldots, r_N) \) thereby reducing a \( 3N \)-dimensional computation to a 3-dimensional one. The energy can be partitioned into kinetic and potential terms and a clear zeroth-order choice of functional for the potential energy is the classical expression

\[
-\frac{Ze^2}{r} \int \rho(r) \, d^3r + \frac{e^2}{2} \int \int \frac{\rho(r_1)\rho(r_2)}{r_{12}} \, d^3r_1 \, d^3r_2.
\]

However, for atomic and molecular systems, there is no correspondingly clear zeroth-order choice of functional for the kinetic energy.

A well-known kinetic-energy functional, formulated by Weizsäcker [28], is

\[
T_W = \frac{\hbar^2}{8m} \int \frac{|\nabla \rho(r)|^2}{\rho(r)} \, d^3r.
\]  

(2)

This expression is exact for the ground state of the hydrogen atom (a one-electron system) but not for the ground states of multi-electron atoms. Comparison of Eq. (1) and Eq. (2) shows that the information content of the Fisher information and the Weizsäcker term is the same and these quantities are essentially identical (with \( T_W = \frac{Nh^2}{8m} \mathcal{J} \)). In this paper we generally employ the Weizsäcker term as the connection to the kinetic energy is more direct.

II. BACKGROUND

One of the key aspects of quantum mechanics is that one cannot simultaneously ascribe well-defined (sharp) values for the position and momentum of a physical system. This characteristic of quantum mechanics is quantified by the position-momentum uncertainty principle. [10, 12] We note that qualitatively different position-momentum uncertainty relations based on the Fisher information have recently been proposed. [2, 3, 21, 23] Motivated by the position-momentum uncertainty principle, quantization procedures have been proposed in which the quantum regime is obtained from the classical regime by adding a stochastic term to the classical equations of motion. In particular, Nelson [17, 18] and earlier work of Fényes [5] and Weizel [27] has shown that the Schrödinger equation can be derived from Newtonian mechanics via the assumption that particles are subjected to Brownian motion.
with a real diffusion coefficient. The Brownian motion results in an osmotic momentum and adding this term to the classical momentum results in the quantum momentum.

**A. Dequantization**

We recently \[15\] proposed a dequantization procedure whereby the classical regime is obtained from the quantum regime by stripping these “quantum fluctuations” from the quantum momentum resulting in the classical momentum. In particular, we introduced a deformed momentum operator, which corresponds to generic fluctuations of the particle’s momentum. This leads to a deformed kinetic energy which possesses a unique minimum that is seen to be the classical kinetic energy. In this way, a variational procedure determines the particular deformation that has the effect of suppressing the quantum fluctuations, resulting in dequantization of the quantum-mechanical system.

**III. QUANTUM-CLASSICAL CORRESPONDENCE**

For an \(N\)-electron system, consider a local deformation \(P \to P_u\) of the quantum momentum operator \(P = -i\hbar\nabla\), with

\[
P_u\psi = (P - iu)\psi,
\]

where all quantities in bold face are \(3N\)-dimensional vectors and \(u\) is real.

Let

\[
T = \frac{1}{2m} \int (P\psi)^*(P\psi) d^{3N}r
\]

and

\[
T_u = \frac{1}{2m} \int (P_u\psi)^*(P_u\psi) d^{3N}r
\]

be the kinetic terms arising from \(P\) and \(P_u\), respectively.

We recently \[15\] showed that extremization of \(T_u\) with respect to \(u\)-variations leads to the critical \(u\) value

\[
u_c = -\frac{\hbar}{2} \frac{\nabla p_N}{p_N},
\]

where \(p_N(r_1, \ldots, r_N) = |\psi(r_1, \ldots, r_N)|^2\) is the \(N\)-electron (probability) density (with \(\int p_N d^3r_1 \cdots d^3r_N = 1\)). This critical \(u\) value of results in the \(N\)-electron classical momentum
operator

\[ P_{C,N}\psi = \left( P + \frac{i\hbar \nabla p_N}{2 p_N} \right) \psi. \]  

(7)

Thus our dequantization procedure automatically identifies the expression for \( u_c \) which when added to the quantum momentum results in the classical momentum. Here \( -u_c \) is identical to the osmotic momentum of Nelson \[17, 18\], and adding \( -u_c \) to the classical momentum results in the quantum momentum.

This value of \( u_c \) results in

\[ T_{u_c} = T - \frac{\hbar^2}{8m} \mathcal{J}_N = T - T_{W,N}, \]  

(8)

where \( \mathcal{J}_N \) is the \( N \)-electron Fisher information

\[ \mathcal{J}_N = \int \frac{(\nabla p_N)^2}{p_N} d^3N \mathbf{r} \]  

(9)

and \( T_{W,N} \) is the \( N \)-electron Weizsäcker term.

If the wavefunction is written as \( \psi = \sqrt{p_N} e^{i S_N / \hbar} \) where \( S_N(\mathbf{r}_1, \ldots, \mathbf{r}_N) \) is the \( N \)-electron phase then a straightforward calculation shows that the action of \( P_{C,N} \) on \( \psi \) is given by

\[ P_{C,N}\psi = \nabla S_N \psi, \]  

(10)

so that, from Eq. (5),

\[ T_{u_c} = \frac{1}{2m} \int p_N |\nabla S_N|^2 d^3N \mathbf{r}. \]  

(11)

This quantity is the mean kinetic energy of a classical ensemble, described by the density \( p_N \) and momentum \( \nabla S_N \) \[8, 11\] and we therefore refer to \( T_{u_c} \) as the \( N \)-electron classical kinetic energy \( T_{C,N} \).

IV. RESULTS AND DISCUSSION

From Eq. (8), the \( N \)-electron kinetic energy can be expressed as

\[ T_N = T_{C,N} + T_{W,N}. \]  

(12)

This is the sum of the \( N \)-electron classical kinetic energy and the \( N \)-electron Weizsäcker term which is purely quantum and results from the quantum fluctuations. We showed \[9\] previously that the \( N \)-electron Weizsäcker term can be decomposed as \( T_W \) (a one-electron
term) and a purely quantum kinetic correlation term, $T_{Q}^{corr}$. Furthermore we showed that $T_W$ results from the local quantum fluctuations while $T_{Q}^{corr}$ results from the nonlocal quantum fluctuations. Then, assuming that the $N$-electron classical kinetic energy can be decomposed as $T_C$ (a one-electron term) and a classical kinetic correlation term, $T_{C}^{corr}$, we can write

$$T_N = T_C + T_{C}^{corr} + T_W + T_{Q}^{corr}.$$  \hspace{1cm} (13)

A. Noninteracting kinetic energy

In the orbital approximation, kinetic correlation is neglected. Omitting these terms in Eq. (13), we obtain the noninteracting kinetic energy as

$$T_s = T_C + T_W.$$  \hspace{1cm} (14)

There are two limiting cases for which this expression can be obtained analytically. For the ground state of the hydrogen atom (an $N = 1$ system), the electron phase is zero, so $T_C = 0$. Therefore, $T_s = T_W$ which is the correct result for this limit. For the uniform electron gas (an $N = \infty$ system) $\rho$ is uniform so $T_W = 0$. Therefore $T_s = T_C$ which can be calculated by adding up the kinetic energies of one-electron orbitals approximated as local plane waves. This results in the Thomas-Fermi term \[6, 26, 29\] which is the correct result for this limit.

B. One-particle systems

For a one-particle system the noninteracting kinetic energy is simply the kinetic energy and Eq. (14) becomes $T = T_C + T_W$. We note that the integrands of $T_C$ and $T_W$ ($T_C$ and $T_W$) are never negative and correspondingly, $T_C$ and $T_W$ are never negative. Thus both $T_C$ and $T_W$ are lower bounds to the kinetic energy. In the next two subsections we explicitly show that our expression for the kinetic energy is correct for both stationary and nonstationary states. Furthermore:

$$T = T_C + T_W.$$  \hspace{1cm} (15)

That is, the integrand of $T$ is equal to the sum of the integrands of $T_C$ and $T_W$. This is the case for all values of the position at each value of the time.
C. Stationary states

The hydrogenic orbitals, \( \psi(n, l, m) \), are dependent on the principal quantum number \( n \), the angular momentum quantum number \( l \) and the magnetic quantum number \( m \) but the total energy is dependent only on \( n \) and is (in atomic units) \( E = -1/2n^2 \). Then, from the virial expression for Coulombic systems, the kinetic energy is \( T = -E = 1/2n^2 \). For \( n = 1 \), the classical kinetic energy is zero.

We previously [9] presented results for \( n = 2 \) which is the first nontrivial case and here we present results for \( n = 3 \). The classical kinetic energy is zero for \( \psi(3, 0, 0), \psi(3, 1, 0) \) and \( \psi(3, 1, 0) \) and, from direct calculation, \( T_W = 1/18 \) which is equal to \( T \). However, the classical kinetic energy is nonzero for \( \psi(3, 1, 1) \) and \( \psi(3, 1, -1) \) and, from direct calculation, \( T_C = 1/54 \) and \( T_W = 1/27 \) and \( T_C + T_W = 1/18 \) which is equal to \( T \). Radial distributions (integrated over the angular variables) of the integrands for \( T_C, T_W \) and \( T \) for this case are shown in Fig. 1(a).

The radial distribution for \( T_C \) is dependent on \( n, l \) and \( |m| \) but the classical kinetic energy is dependent only on \( n \) and \( |m| \) and \( T_C = \frac{|m|}{n}T = |m|/2n^3 \). Correspondingly, \( T_W = \frac{n-|m|}{n}T = (n-|m|)/2n^3 \) and we note that this expression could be deduced from the analytic expression for the Fisher information obtained by Dehesa. [21] We also note that whereas \( T_C \) can equal zero, \( T_W \) cannot since, for a normalizable state, \( \rho \) cannot be uniformly constant and therefore \( \nabla \rho \) cannot be identically zero. The fact that the purely quantum term cannot equal zero is in complete accord with the position-momentum uncertainty principle. From the above expressions, \( T_C \) and \( T_W \) are constant for \( n \) and \( |m| \) fixed and this is illustrated in Fig. 1(b) which shows the radial distributions for \( T_C, T_W \) and \( T \) for \( n = 3, l = 2 \) and \( |m| = 1 \). Although the radial distribution for \( T_C \) and \( T_W \) are clearly different from those of Fig. 1(a) they again integrate to 1/54 and 1/27 respectively and \( T_C + T_W = 1/18 \). For \( n \) and \( l \) fixed, \( T_C \) increases from 0 to \( l/2n^3 \) while \( T_W \) decreases from \( 1/2n^2 \) to \((n - l)/2n^3 \) as \( |m| \) increases from 0 to \( l \) and this is illustrated in Fig. 1(c) which shows the radial distributions for \( T_C, T_W \) and \( T \) for \( n = 3, l = 2 \) and \( |m| = 2 \). In this case the radial distributions for \( T_C \) and \( T_W \) integrate to 1/27 and 1/54 respectively and we again have \( T_C + T_W = 1/18 \). The results for these stationary states support our expression for the kinetic energy. Furthermore, it is clear from Fig. 1 that the integrand of \( T \) is equal to the sum of the integrands of \( T_C \) and \( T_W \) for all values of the position.
FIG. 1: Radial distributions (integrated over the angular variables) of $T_C$ (dashed curve), $T_W$ (dotted curve) and $T$ (solid curve) for hydrogenic orbitals with $n = 3$ and (a) $l = 1, |m| = 1$; (b) $l = 2, |m|$; (c) $l = 2, |m| = 2$. The horizontal axis is in atomic units.

D. Nonstationary states

We first consider a one-dimensional particle in a box (pib) state that is initially $\phi(x) = 2^{-1/2}(\psi_1(x) + \psi_2(x))$ where $\psi_1(x)$ and $\psi_2(x)$ are the first two pib eigenfunctions. The pib eigenfunctions are, of course, stationary states and, for both $\psi_1(x)$ and $\psi_2(x)$, $T_C = 0$ and $T = T_W$. However, $\phi(x)$ is a nonstationary state and whereas $T_C = 0$ for $t = 0$, this is generally not the case for later times. This is clear from Fig. 2 which shows the probability distribution (upper panel) and integrands for $T_C$, $T_W$ and $T$ (lower panel). Note that at $t = 0.075$ there is a relatively flat shoulder on the right side of the probability distribution and that in this region, $T_W$ is small whereas $T_C$ is large. At $t = 0.150$ there is a relatively flat shoulder on the left side of the probability distribution for which this is also the case.

We now consider a free particle represented as a one-dimensional Gaussian wavepacket
that is initially $\phi(x) = \pi^{-1/4}e^{-x^2/2}$. Again, $T_C = 0$ for $t = 0$ but it is clear from Fig. 3, which shows the probability distribution (upper panel) and integrands for $T_C$, $T_W$ and $T$ (lower panel), that, as the Gaussian wavepacket spreads, $T_C$ increases while $T_W$ decreases and that as $t \to \infty$, $T_C \to T$ while $T_W \to 0$. Note that as $t$ increases and the probability distribution becomes flatter, $T_W$ becomes smaller whereas $T_C$ becomes larger. Thus as the particle becomes delocalized there is a transition from purely quantum kinetic energy to classical kinetic energy.

The results for these nonstationary states support our expression for the kinetic energy. Furthermore, it is clear from Figs. 2 and 3 that the integrand of $T$ is equal to the sum of the integrands of $T_C$ and $T_W$ for all values of the position at each value of the time.

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**FIG. 2:** One-dimensional pib state that is initially $\phi(x) = 2^{-1/2}(\psi_1(x) + \psi_2(x))$ where $\psi_1(x)$ and $\psi_2(x)$ are the first two pib eigenfunctions. Distributions shown at $t = 0.000$; $t = 0.075$; $t = 0.150$: Probability distribution (upper panel); Distributions of $T_C$ (dashed curve), $T_W$ (dotted curve) and $T$ (solid curve). (lower panel)
V. CONCLUSIONS

In Nelson’s quantization procedure an osmotic momentum term is added to the classical momentum resulting in the quantum momentum. This osmotic momentum term represents the quantum fluctuations that are an essential part of quantum mechanics in accord with the position-momentum uncertainty principle. In our dequantization procedure this osmotic momentum term is removed from the quantum momentum resulting in the classical momentum. We obtain the osmotic momentum term via a variational approach in which the deformed quantum kinetic energy is minimized with respect to variations of the deformation parameter. The critical value of the deformation parameter which minimizes the deformed kinetic energy is directly related to the osmotic momentum term.

The result of our dequantization procedure is the decomposition of the kinetic energy into the classical kinetic energy and the purely quantum kinetic energy. The purely quantum kinetic energy is the Weizsäcker term which is essentially identical to the Fisher information. The purely quantum kinetic energy is thereby a direct functional of the electron density and is a critical component of the kinetic-energy functional (and this is well-known). However, the classical kinetic energy is also a critical component of the kinetic-energy functional. Unfortunately, the classical kinetic energy is explicitly dependent on the phase of the wavefunction and is manifestly not a direct functional of the electron density. Devising a functional of the electron density that indirectly but accurately approximates classical kinetic energy
is a major challenge for the development of quantitative kinetic-energy functionals.

It is well-known that the Weizsäcker term, $T_W$, which is greater than or equal to zero, is a lower bound to the kinetic energy, $T$. We have shown that the classical kinetic energy, $T_C$, which is also greater than or equal to zero, is also a lower bound to the kinetic energy and $T = T_W + T_C$. Furthermore, we have shown that the integrands of the Weizsäcker term and the classical kinetic energy (which are both greater than or equal to zero) are each lower bounds to the integrand of the kinetic energy and $T = T_W + T_C$. Examples have been given for which this is the case at each value of the position and, for nonstationary states, for which this is also the case at each value of the time. It is well-established that the Fisher information and the Shannon entropy are complementary quantities. We have shown that the Weizsäcker term (which is essentially identical to the Fisher information) and the classical kinetic energy are complementary quantities and, in this sense, the classical kinetic energy is analogous to the Shannon entropy.

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