Improvement of the Heisenberg and Fisher-information-based uncertainty relations for $D$-dimensional central potentials

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Abstract. The Heisenberg and Fisher-information-based uncertainty relations are improved for stationary states of single-particle systems in a $D$-dimensional central potential. The improvement increases with the squared orbital hyper-angular quantum number. The new uncertainty relations saturate for the isotropic harmonic oscillator wavefunction.

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1. Introduction

A most important role for the quantum-mechanical description of the internal structure of physical systems in $D$-dimensional spaces ([1]–[4] see also references herein) as well as for the development of the quantum information and computation ([5, 6] see also references herein) is played by uncertainty relations. There is not only the celebrated Heisenberg inequality [7, 8] given by

$$\langle r^2 \rangle \langle p^2 \rangle \geq \frac{D^2}{4},$$

and its moment generalizations [1], but also other similar relations based on more appropriate uncertainty quantities such as information-theoretic measures like, in a chronological way, the Fisher information [9, 10] and the Shannon [11, 12], Renyi [13, 14] and Tsallis [15, 16] entropies. The corresponding uncertainty relations, which are more stringent than the Heisenberg one, have been shown in [17, 18], [19]–[23], [1, 24] and [25] for the Fisher, Shannon, Renyi and Tsallis measures, respectively.

In this study, the attention is centred around the Heisenberg and the Fisher-information-based uncertainty relations. The Fisher information for a quantum-mechanical state of a single-particle system characterized by the probability density $\rho(\vec{r})$ in the $D$-dimensional position space is defined by

$$I_\rho \equiv \int_\mathbb{R} \rho(\vec{r}) [\nabla_D \ln \rho(\vec{r})]^2 d^D r,$$

where $\nabla_D$ denotes the $D$-dimensional gradient [26, 27]. The corresponding quantity for the momentum-space probability density $\gamma(\vec{p})$ will be denoted by $I_\gamma$.

Unlike the rest of the information-theoretic measures published in the quantum literature, the Fisher information has a local character due to the gradient operator. The higher this quantity, the more concentrated the density and the smaller the position uncertainty of the particle [10, 28]. This information quantity has been used for a wide variety of quantum-mechanical concepts and phenomena: to describe the kinetic [29, 30] and Weiszäcker [31, 32] energies, to characterize correlation properties of two-electron systems [33, 34] and to identify the most distinctive nonlinear spectroscopic phenomena (avoided crossings) of atomic systems in strong external fields [35]. Moreover, the Fisher information is the basic element of the principle of extreme physical information [10, 36], which has been used to derive various fundamental equations of quantum physics [10, 37].

The uncertainty relation associated with the Fisher information for general systems (i.e., $I_\rho I_\gamma \geq \text{constant}$) is not yet known despite the fact that it is the earliest found information measure [9]. Recently, two contributions to find the general Fisher uncertainty relation have been made. First, the inequality $I_\rho I_\gamma \geq 4$ has been proved for general monodimensional systems with even wavefunctions [38]. Moreover, some authors [17, 18] have found

$$I_\rho I_\gamma \geq 4D^2 \left[ 1 - \frac{(2l + D - 2)|m|^2}{2l(l + D - 2)} \right]^2$$

for stationary states of $D$-dimensional single-particle systems with a central potential $V_D(r)$ with the orbital and magnetic hyperangular quantum numbers $l$ and $m$, respectively.
Our aim, not yet been undertaken, is to improve the Heisenberg relation (1) for stationary $D$-dimensional central potentials and to refine the Fisher-information-based relation (2). The only related effort published in the literature, to the best of our knowledge, is the computation of the Heisenberg uncertainty product for various specific three-dimensional (3D) central potentials [39]. In section 2, the $D$-dimensional central force problem is briefly described and some concepts and notation are explicitly presented. Then, the aforementioned $D$-dimensional uncertainty relations are proved and examined in detail for some prototype systems in section 3. Finally, conclusions and some open problems are given. Atomic units are used throughout the paper.

2. The $D$-dimensional problem for central potentials

The wavefunctions which describe the quantum-mechanical states of a particle in the $D$-dimensional central potential $V_D(\vec{r})$ have the form $\Psi_D(\vec{r}, t) = \psi_D(\vec{r}) \exp(-iE_D t)$, where $\{E_D, \psi_D(\vec{r})\}$ denote the physical eigensolutions of the Schrödinger equation

$$\left[ -\frac{i}{2} \vec{\nabla}_D^2 + V_D(\vec{r}) \right] \psi_D(\vec{r}) = E_D \psi_D(\vec{r}).$$

The symbol $\vec{r}$ is the $D$-dimensional position vector of the particle having the Cartesian $(x_1, x_2, \ldots, x_D)$ and the polar hyperspherical $(r, \theta_1, \theta_2, \ldots, \theta_D-1)$ coordinates respectively, where the hyperradius $r$ denotes the radial distance $r = (\sum_{i=1}^{N} x_i^2)^{1/2}$. The Laplacian operator $\vec{\nabla}_D^2 = \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2}$ can be expressed [18, 26, 27, 40] as

$$\Lambda_{D-1}^2 = \frac{1}{r^{D-1}} \frac{\partial}{\partial r} r^{D-1} \frac{\partial}{\partial r} - \frac{\Lambda_{D-1}^2}{r^2}, \quad (3)$$

$\Lambda_{D-1}$ being the $D$-dimensional generalization of the squared angular momentum operator, which only depends on the $D-1$ angular coordinates $\Omega_{D-1}$ of the $D$-dimensional sphere in the form

$$\Lambda_{D-1}^2 = -\sum_{i=1}^{D-1} \left( \frac{\sin \theta_i}{\prod_{j=1}^{i-1} \sin \theta_j} \right)^2 \frac{\partial^2}{\partial \theta_i^2} \left( \frac{\sin \theta_i}{\prod_{j=1}^{i-1} \sin \theta_j} \right)^2 \frac{\partial^2}{\partial \theta_i^2} \left( \frac{\sin \theta_i}{\prod_{j=1}^{i-1} \sin \theta_j} \right)^2 \frac{\partial^2}{\partial \theta_i^2}.$$  

(4)

This operator is known to fulfil [26, 27]

$$\Lambda_{D-1}^{l,\mu}(\Omega_{D-1}) = l(l + D - 2) \mathcal{Y}_{l,\mu}(\Omega_{D-1}), \quad (5)$$

where the $\mathcal{Y}$-symbol describes the hyperspherical harmonics characterized by the $D-1$ hyperangular quantum numbers $(l \equiv \mu_1, \mu_2, \mu_3, \ldots, \mu_{D-1} \equiv m) \equiv (l, \{\mu\})$, which are natural numbers with values $l = 0, 1, 2, \ldots$, and $l \equiv \mu_1 \geq \mu_2 \geq \ldots \geq \mu_{D-2} \geq |\mu_{D-1}| \equiv |m|$. These mathematical objects obey the orthonormalization condition

$$\int_{S_{D-1}} \delta D-1 \mathcal{Y}_{l,\mu}^* \mathcal{Y}_{l,\nu}(\Omega_{D-1}) = \delta[l, \mu] \delta[l', \mu'].$$  

(6)
With the ansatz
\[ \psi_{E,l,\{\mu\}}(\vec{r}) = R_{E_l}(r)Y_{l,\{\mu\}}(\Omega_{D-1}), \]
and keeping in mind (3)–(6), one obtains that the radial eigenfunction \( R_{E_l}(r) \) satisfies
\[
\left[ -\frac{1}{2} \frac{d^2}{dr^2} - \frac{D - 1}{2r} \frac{d}{dr} + \frac{l(l + D - 2)}{2r^2} + V_D(r) \right] R_{E_l}(r) = E_D R_{E_l}(r).
\]
As usual, to eliminate the first derivative, the reduced radial wavefunction
\[ u_{E_l}(r) = r^{(D-1)/2} R_{E_l}(r), \]
is used. Then, the previous equation reduces to a 1D Schrödinger equation in the coordinate \( r \):
\[
\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{L(L + 1)}{2r^2} + V_D(r) \right] u_{E_l}(r) = E_D u_{E_l}(r),
\]
where the grand orbital quantum number \( L \) is given by
\[ L = l + \frac{D - 3}{2}, \]
and \( l(l + D - 2) = L(L + 1) - (D - 1)(D - 3)/4 \). The physical solutions require that \( u_{E_l}(r) \to 0 \) when \( r \to 0 \) and \( r \to \infty \). Moreover, the normalization to unity of the wavefunction \( \Psi_D(\vec{r}, t) \) leads to the following property of the reduced radial eigenfunctions \( u_{E_l}(r) \):
\[
\int_0^\infty u_{E_l}^2(r) \, dr = 1,
\]
where the orthonormalization condition (6) of the hyperspherical harmonics has been taken into account. For completeness, let us underline that the reduced radial Schrödinger equation of any \( D \)-dimensional problem for central potentials, see (7), is the same as for \( D = 3 \) but with the orbital angular momentum given by \( L \) according to (8). This essentially indicates that there exists an isomorphism between the dimensionality \( D \) and the orbital quantum number \([41]\), so that \( D \to D + 2 \) is equivalent to \( l \to l + 1 \).

Finally, let us also point out that the kinetic energy \( \langle T \rangle \) is
\[
\langle T \rangle = \frac{1}{2} \int_0^\infty \left[ -u_{E_l}(r)u''_{E_l}(r) + \frac{L(L + 1)}{r^2}u^2_{E_l}(r) \right] \, dr.
\]
Then, since \( \langle T \rangle = \langle \hat{p}^2 \rangle / 2 \), a simple integration by parts leads to
\[
\langle \hat{p}^2 \rangle = \int_0^\infty [u'_{E_l}(r)]^2 \, dr + L(L + 1) \langle r^{-2} \rangle,
\]
which is used in the next section. The symbol \( \langle f(r) \rangle \) denotes the expectation value
\[
\langle f(r) \rangle = \int_0^\infty f(r) u^2_{E_l}(r) \, dr.
\]
3. Heisenberg and Fisher-information-based uncertainty relations for central potentials

Here, for states with an orbital hyperangular quantum number corresponding to a \( D \)-dimensional single-particle system with any spherically-symmetric potential, we shall show that the Heisenberg-type uncertainty relation

\[
\langle r^2 \rangle \langle p^2 \rangle \geq \left( l + \frac{D}{2} \right)^2,
\]

is fulfilled, and the Fisher-information-based uncertainty relation (2) is improved by

\[
I_{r}I_{\gamma} \geq 16 \left[ 1 - \frac{2l + D - 2}{2l(l + D - 2)} |m| \right]^2 \left( l + \frac{D}{2} \right)^2.
\]

To obtain (12) we start from an inequality [42] related to the reduced radial Schrödinger equation (7), modified in the form

\[
\int_{0}^{\infty} \left( u_{El}^2 - \frac{L + 1}{r} u_{El} - \lambda r u_{El} \right)^2 dr \geq 0,
\]

with \( u_{El} \equiv u_{El}(r) \) and \( \lambda \) being an arbitrary parameter. Taking into account (9)–(11) and that

\[
\int_{0}^{\infty} ru_{El}(r)u_{El}^\prime(r) dr = -\frac{1}{2},
\]

this expression transforms into the quadratic inequation in \( \lambda \):

\[
\langle r^2 \rangle \lambda^2 + (2L + 3) \lambda + \langle p^2 \rangle \geq 0,
\]

whose discriminant is necessarily negative. This observation leads in a straightforward manner to

\[
\langle r^2 \rangle \langle p^2 \rangle \geq \left( L + \frac{3}{2} \right)^2,
\]

which yields the sought Heisenberg inequality (12) once we take into account (8) which defines the grand orbital quantum number \( L \).

Then, the use of expression [18]

\[
I_{r}I_{\gamma} \geq 16 \left[ 1 - \frac{2l + D - 2}{2l(l + D - 2)} |m| \right]^2 \langle r^2 \rangle \langle p^2 \rangle,
\]

which clearly manifests the uncertainty character of the product of the Fisher informations in position and momentum spaces, together with (12) naturally produces the relation (13).

Let us now discuss the new inequalities (12) and (13). Firstly, we observe that for \( s \) states both of them reduce to the general known ones (1) and (2), respectively; so, no improvement is achieved. However, the enhancement is notorious for states with \( l > 0 \) growing as \( l^2 \).
Secondly, both inequalities saturate, i.e. the equality is achieved, for nodeless isotropic harmonic oscillator wavefunctions (e.g. the ground state) as shown below. Indeed, for the oscillator potential $V(r) = \omega^2 r^2/2$ (mass = 1) one has [18]

$$\omega \langle r^2 \rangle = \omega^{-1} \langle p^2 \rangle = \eta + \frac{3}{2} = 2n_r + L + \frac{3}{2} = 2n_r + l + \frac{D}{2},$$

and

$$\omega^{-1} I_\rho = \omega I_\gamma = 16 \left( \eta - |m| + \frac{3}{2} \right)^2 = 16 \left( 2n_r + l - |m| + \frac{D}{2} \right)^2,$$

with the grand principal quantum number $\eta = n + (D - 3)/2 = 2n_r + L, l = 0, 1, 2, \ldots$, and $n_r = 0, 1, 2, \ldots$, being the number of nodes of the wavefunction. So, the Heisenberg and Fisher-information-based uncertainty products for the oscillator case are

$$\langle r^2 \rangle \langle p^2 \rangle = \left( 2n_r + l + \frac{D}{2} \right)^2$$

and

$$I_\rho I_\gamma = 16 \left( \eta - |m| + \frac{3}{2} \right)^2 = 16 \left( 2n_r + l - |m| + \frac{D}{2} \right)^2,$$

respectively, which are equal to the new lower bounds (12) and (13) for $n_r = 0$; otherwise they have a larger value growing with $n_r^2$.

Thirdly, for hydrogen atom $V(r) = -1/r$, one has [18]

$$\langle r^2 \rangle = \frac{1}{2} \eta^2 [5\eta^2 - 3L(L + 1) + 1], \quad \langle p^2 \rangle = \frac{1}{\eta^2},$$

and

$$I_\rho = \frac{4}{\eta^3} (\eta - |m|), \quad I_\gamma = 2\eta^2 [5\eta^2 - 3L(L + 1) - [8\eta - 3(2L + 1)]|m| + 1],$$

where $\eta = n + (D - 3)/2, n = 1, 2, 3, \ldots$ and $l = 0, 1, \ldots, n - 1$. Then the uncertainty products are

$$\langle r^2 \rangle \langle p^2 \rangle = \frac{1}{2} [5\eta^2 - 3L(L + 1) + 1],$$

for the Heisenberg case, and

$$I_\rho I_\gamma = \frac{8}{\eta} (\eta - |m|) [5\eta^2 - 3L(L + 1) - [8\eta - 3(2L + 1)]|m| + 1]$$

for the Fisher-information-based case. Notice that since $n \geq l + 1$, then $\eta \geq L + 1$, the values of the two uncertainty products are larger than the corresponding lower bounds given by (12) and (13), respectively.

Finally, the Heisenberg uncertainty product has the same value for the states of $D$-dimensional systems with hyperangular momentum $l + 1$ and for the states of $(D + 2)$-dimensional systems with hyperangular momentum $l$, according to the isomorphism previously mentioned.
4. Conclusions and open problems

Starting from an inequality directly associated to the radial Schrödinger equation, we have found the Heisenberg uncertainty relation for time-independent $D$-dimensional central potentials, and we have refined the recently discovered Fisher-information-based uncertainty relation for such systems. These improvements follow a $l^2$-law, where $l$ is the orbital hyperangular quantum number of the particle. In particular, these inequalities have been studied for the harmonic oscillator and the Coulomb potentials obtaining that they saturate for the oscillator ground state.

These results suggest various important open problems: to find the uncertainty relations based on the Renyi and Tsallis information measures, and the Cramer–Rao uncertainty inequality for central potentials and, most importantly, to derive a Fisher-information-based uncertainty principle for general systems. It would be an uncertainty relation of the same category, in the quantum-mechanical literature, as the Heisenberg [7] and entropic (Shannon) [23] ones.

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