Generalized position-momentum uncertainty products: inclusion of moments with negative order. Application in atoms

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Abstract

Rigorous and universal relationships among radial expectation values of any D-dimensional quantum-mechanical system are obtained, using Rényi-like position-momentum inequalities in an information-theoretical framework. Although the results are expressed in terms of four moments (two in position space and two in the momentum one), especially interesting are the cases that provide expressions of uncertainty in terms of products $\langle r^a\rangle^{1/a}\langle p^b\rangle^{1/b}$, widely considered in the literature, including the famous Heisenberg relationship $\langle r^2\rangle\langle p^2\rangle \geq D^2/4$. Improved bounds for these products have recently been provided, but always restricted to positive orders $a, b > 0$. A novelty in this work are inequalities for negative orders. A study of the aforementioned relationships is carried out for atomic systems in their ground state. Some results are given in terms of relevant physical quantities, including the kinetic and electron-nucleus attraction energies, the diamagnetic susceptibility and the height of the peak of the Compton profile, among other.

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I. INTRODUCTION

The one-particle density $\rho(\vec{r})$ of many-fermion systems is an essential quantity for the introspection on their main physico-chemical properties [1]. The study of this density has attracted consequently the attention of many researchers, especially after the formulation of the Hohenber-Kohn theorem [2] concerning the existence of a universal density functional for the energy of these systems. The so-called 'frequency moments' of the density play a relevant role within such a Density Functional Theory framework [3, 4].

Much effort has been paid in order to get a similar formulation of this theory in the conjugated space, i.e. in terms of the momentum one-particle density $\gamma(\vec{p})$, with many succesful results [5–8].

Different studies based on the simultaneous use of quantities in the position and momentum spaces have been carried out. The aim in most of them it to provide uncertainty-like relationships. For instance, the well-known Heisenberg uncertainty principle [9–11] involves variances (defined by means of radial expectation values) in conjugate spaces. Since the formulation of the Heisenberg principle, many other uncertainty relations have been obtained, with a diversity of expectation values and/or density functionals. Especially relevant are the lower bounds to products of radial expectation values $\langle r^\alpha \rangle$ and $\langle p^\beta \rangle$ [12] emphasizing the particular case $\alpha = \beta = 2$. Bounds to the product of logarithmic uncertainties [12] and the sum of Shannon [13] and Rényi [14] entropies are also known. Although these relationships are usually applied in three-dimensional systems (i.e. with vectors of three components $\vec{r}$ and $\vec{p}$), all of them are valid for arbitrary dimensionality [15, 16].

This type of uncertainty relations are physically relevant, not only because of their importance in a theoretical quantum-mechanical framework [17–19], but also in the development of quantum information and computation [20, 21].

The aforementioned inequalities in terms of radial expectation values of positive order [12, 15] were obtained chaining the lower bound to the sum of Shannon entropies in conjugate spaces [13], and variational upper bounds to the entropy in each space. A recent improvement on those lower bounds to radial products has been achieved [22], using a similar inequality for the sum of Rényi entropies. The Rényi entropy [23] includes the Shannon one as a particular case. All previous inequalities for products of two moments (one in each conjugate space) are valid subject to the constraint of positivity for orders α and β. However, there are not

known bounds on uncertainty products involving radial expectation values of negative order, to the best of our knowledge. It is worthy to remark also that uncertainty products have been always defined in terms of exactly two factors.

The aim of this study is to present a generalized uncertainty inequality in terms of a number of radial expectation values up to four, whose validity extends to arbitrary dimensionality. Such inequality can handle radial expectation values of negative order, including the simplest products of two factors. Lower bounds provided here are of universal validity (i.e. for any D-dimensional quantum mechanical system). For illustration, we carry out a numerical study for selected inequalities of physical interest in atomic systems, and the results are interpreted based on revelant physical properties, such as e.g. atomic shell structure. Let us mention that some radial expectation values for atomic densities, in both position and momentum spaces, are physically relevant and/or experimentally accessible.

The paper is structured as follows: Section II is devoted to the definition of the one-particle densities from the wave function, as well as the main quantities we will deal with (radial expectation values, frequency moments, Shannon and Rényi entropies). The uncertainty relations associated to those quantities are provided also. In Section III, a universal lower bound to uncertainty-like products of radial expectation values is obtained. Its expression has validity for arbitrary quantum systems of any dimensionality. Particular cases of physical interest are discussed in detail in Section IV, first by providing rigorous inequalities and then performing a numerical study for atomic one-particle densities. Some concluding remarks are finally given in Section V.

II. FREQUENCY MOMENTS AND RÉNYI ENTROPIES OF QUANTUM SYSTEMS

Let us a consider the one-particle density of a D-dimensional N-fermion system, defined by

$$\rho(\vec{r}) = \int |\Psi(\vec{r}, \vec{r}_2, \ldots, \vec{r}_N)|^2 d\vec{r}_2 \ldots d\vec{r}_N, \tag{1}$$

with Ψ its spinless wave function. The one-particle density in momentum space is defined similarly,

$$\gamma(\vec{p}) = \int |\tilde{\Psi}(\vec{p}, \vec{p}_2, \ldots, \vec{p}_N)|^2 d\vec{p}_2 \ldots d\vec{p}_N, \tag{2}$$

now in terms of the DN-dimensional Fourier transform $\tilde{\Psi}$ of Ψ. In what follows, (i) normalization to unity will be considered, so that $\int \rho(\vec{r}) d\vec{r} = \int \gamma(\vec{p}) d\vec{p} = 1$, (ii) it is understood that all integrals are performed over the whole D-dimensional space $\mathbb{R}^D$, and (iii) atomic units (a.u.) will be used, so $\hbar = m = e = 1$.

These densities are interpreted, taking into account the aforementioned normalization, as probability distributions of finding a particle at a specific region within the respective domains of the densities (position or momentum).

Different expectation values and density functionals have been considered in order to quantify the extent to which a one-particle density is more or less localized/delocalized. The last concept is strongly related to that of 'uncertainty', in the Heisenberg sense, regarding the accuracy in the knowledge of the particle's position and momentum at a given time.

The well-known Heisenberg relation, given by [9–11]

$$\langle r^2 \rangle \langle p^2 \rangle \geq \frac{D^2}{4} \tag{3}$$

for arbitrary D-dimensional quantum systems, is expressed in terms of second order 'radial expectation values' of the one-particle densities, where

$$\langle r^a \rangle \equiv \int r^a \rho(\vec{r}) d\vec{r} \tag{4}$$

with $r \equiv |\vec{r}|$, and similarly for $\langle p^a \rangle$. The real exponent a will be referred as 'order' of the radial expectation value, whose range of allowed values will be imposed by the conditions of convergence of the involved integrals. For densities with finite value at the origin, the condition $a > -D$ has to be taken into account, according to the expression of the volume element $d\vec{r} = r^{D-1} dr \, d\Omega_D$, where $\Omega_D = 2\pi^{D/2}/\Gamma(D/2)$ is the D-dimensional solid angle.

The previous Heisenberg relation was later generalized to arbitrary uncertainty products $\langle r^a \rangle^{1/a} \langle p^b \rangle^{1/b}$ with positive orders a and b, firstly for three-dimensional systems [12] and later extended to arbitrary dimensionality D [15]. Thus, two different steps were considered, both them based on the concept of 'Shannon entropy', a density functional defined by [24]

$$S(\rho) \equiv -\int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r} \tag{5}$$

which is a measure of 'spreading/delocalization' of the probability distribution. As suggested by the notion of uncertainty previously discussed, the Shannon entropies in position and momentum spaces, namely $S(\rho)$ and $S(\gamma)$, fulfil the uncertainty relation given in Ref. [13]:

$$S(\rho) + S(\gamma) \geq D(1 + \ln \pi), \tag{6}$$

what means that it is not possible to deal, simultaneously, with arbitrary low values of both entropies or, in other words, with extremely accurate values of the position and momentum variables. The above inequality will be referred as BBM, because of its pioneering authors Bialynicki-Birula and Mycielski.

On the other hand, variational upper bounds to each one of the above entropies, in terms of one radial expectation value of positive order, were known [25] for three-dimensional distributions. Nevertheless, the variational procedure allows a straightforward extension to arbitrary dimensionality, giving rise to upper bounds $S_a^*(\rho)$ and $S_b^*(\gamma)$ in terms of $\langle r^a \rangle$ and $\langle p^b \rangle$ respectively. The use of these bounds together with the BBM one provide us with a set of lower bounds to uncertainty products [15]

$$\langle r^a \rangle^{1/a} \langle p^b \rangle^{1/b} \geq C(a, b, D), \quad a, b > 0 \tag{7}$$

with $C(a, b, D)$ an analytical expression provided in Ref. [15]. A very recent improvement to the above inequality has been achieved [22] by considering a Rényi-like inequality instead of the Shannon-like BBM one, giving rise to a lower bound $C(a, b, q, D)$ with a new parameter 'q', providing the original bound as $C(a, b, q = 1, D) = C(a, b, D)$. The optimization of this new bound with respect to the parameter q improves the results provided for the particular value $q = 1$.

The Rényi entropy [23] constitutes a generalization of the Shannon one, and it is defined as follows:

$$R_q(\rho) \equiv \frac{1}{1-q} \ln \omega_q(\rho) \tag{8}$$

where the quantity

$$\omega_q(\rho) \equiv \int \rho^q(\vec{r}) d\vec{r} \tag{9}$$

is the 'frequency moment of order q' [26] of the distribution. The frequency moments play a central role in the description of many-fermion systems in terms of the one-particle density. In this sense, it is worthy to remark the relevance, within a Density Functional Theory (DFT) framework, of those with orders $q = 4/3$ and $5/3$. They correspond, essentially, to the exchange and kinetic energy terms of the energy functional [1]. The frequency moment of order 2, namely $\omega_2(\rho) = \int \rho^2(\vec{r})d\vec{r}$ is known as the 'disequilibrium' [27] of the probability distribution, which quantifies the departure from the equiprobability situation (equilibrium). In addition, the problem of fully characterize the distribution by frequency moments was also addressed by considering the so-called Hausdorff moment problem [28].

Concerning the Rényi entropies $R_q(\rho)$, two comments are in order: (i) the limiting case $q \to 1$ provides the Shannon entropy as $R_1(\rho) = S(\rho)$ [23], and (ii) similarly to the uncertainty inequality BBM, there exists a Rényi-like one given by [14]

$$R_q(\rho) + R_t(\gamma) \geq \ln\left[(2\pi)(2q)^{\frac{1}{2(q-1)}}(2t)^{\frac{1}{2(t-1)}}\right]^D \quad \text{as far as} \quad \frac{1}{q} + \frac{1}{t} = 2 \tag{10}$$

The BBM inequality is recovered for the particular case $q = t = 1$. Apart from the just mentioned case, it is clear that one of the orders must be above unity while the other is below one. In what follows, let us choose the parameters in such a way that $q \geq 1 \geq t$. The opposite order will be considered by exchanging the distributions ρ and γ.

III. LOWER BOUNDS TO UNCERTAINTY PRODUCTS

Let us notice that Eq. (10) can be expressed in terms of frequency moments as follows:

$$\frac{\omega_t^{\frac{1}{1-t}}(\gamma)}{\omega_q^{\frac{1}{q-1}}(\rho)} \geq \left[(2\pi)(2q)^{\frac{1}{2(q-1)}}(2t)^{\frac{1}{2(t-1)}}\right]^D \tag{11}$$

Due to the physical interest of the frequency moments, the variational procedure has been also employed in order to bound them in terms of physical observables. In Ref. [29], lower (upper) bounds on the D-dimensional frequency moments of order above (below) unity are given, in terms of two radial expectation values, not necessarily of positive order. These two bounds (ω_q^* and ω_t^*) translate into upper ones once writen in terms of Rényi entropies, because of the sign of the factors appearing before the logarithms. In this way we obtain

$$[\omega_t^*(\gamma)]^{2q-1}\omega_q^*(\rho) \geq \left[\left(\frac{\pi}{q}\right)^{q-1}(2q-1)^{q-\frac{1}{2}}\right]^D \equiv f(q,D) \tag{12}$$

where

$$\omega_q^*(\rho) = F(a,b,q,D)\left[\frac{\langle r^b\rangle^{q(a+D)-D}}{\langle r^a\rangle^{q(b+D)-D}}\right]^{1/(a-b)}, \;\; a>b>-D\frac{q-1}{q} \tag{13}$$

and

$$\omega_t^*(\gamma) = G(c,d,t,D)\left[\langle p^c\rangle^{-t(d+D)+D}\langle p^d\rangle^{t(c+D)-D}\right]^{1/(c-d)}, \;\; c>D\frac{1-t}{t}>d \tag{14}$$

for any $0<t\leq 1\leq q$ verifying $\dfrac{1}{q}+\dfrac{1}{t}=2$. The analytical expressions of both $F(a,b,q,D)$ and $G(c,d,t,D)$ can be found in Ref. [29].

We observe that Eq. (12) together with the expressions (13)-(14) provide a relationship including four radial expectation values, two in position space ($\langle r^a\rangle$ and $\langle r^b\rangle$) and the other two in momentum space ($\langle p^c\rangle$ and $\langle p^d\rangle$). Such a so general expression is given by

$$\frac{\langle r^a\rangle^{\epsilon_a}\langle p^c\rangle^{\epsilon_c}\langle p^d\rangle^{\epsilon_d}}{\langle r^b\rangle^{\epsilon_b}} \geq H(a,b,c,d,\lambda,D), \tag{15}$$

The notation employed and the constraints on the parameters are detaileded below.

- Defining $\lambda \equiv \dfrac{q-1}{q} = \dfrac{1-t}{t} \in (0,1)$, the orders of the expectation values are constrained as $a>b>-D\lambda$ and $c>D\lambda>d$. Because of the one-to-one correspondence between λ and each of the parameters q and t, we will replace both them by the new λ, whose non-negativity is worth noting. The limiting case $\lambda=0$ corresponds to the choice $q=t=1$, for which results derived from the BBM inequality are recovered.

- The lower bound $H(a,b,c,d,\lambda,D)$ is defined from those of the frequency moments (F and G) and that of the Rényi sum (f) as

$$H(a,b,c,d,\lambda,D) = \left[\frac{f\left(\frac{D}{D-\lambda},D\right)}{F\left(a,b,\frac{D}{D-\lambda},D\right)G^{\frac{D+\lambda}{D-\lambda}}\left(c,d,\frac{D}{D+\lambda},D\right)}\right]^{\frac{D-\lambda}{D}} \tag{16}$$

- Concerning the powers ϵ_i (all positive) to rising the radial expectation values, they are given by

$$\epsilon_a = \frac{D\lambda + b}{a - b},\ \ \epsilon_b = \frac{D\lambda + a}{a - b},\ \ \epsilon_c = \frac{D\lambda - d}{c - d},\ \ \epsilon_d = \frac{c - D\lambda}{c - d} \tag{17}$$

Especially remarkable are the equalities $\epsilon_b - \epsilon_a = \epsilon_c + \epsilon_d = 1$.

- The unique order with definite sign is $c > 0$ because of the constraint $c > D\lambda$. All others $\{a, b, d\}$ can be either positive or negative.

- For a given choice of orders $\{a, b, c, d\}$ fulfilling the appropriate constraints, it would be desirable to know the optimal allowed λ. We use the word 'optimal' in the sense of providing the highest bound allowed, attneding to the set of orders considered. Such an optimal value cannot be obtained analytically due to the functional dependence of the bound $H(\lambda)$, but it can be determined numerically instead.

- Nevertheless, any value $\lambda \in (0, 1)$ verifying $a > b > -D\lambda$ and $c > D\lambda > d$ is valid in order to get a lower bound for the four-moment uncertainty product. We will choose appropriate values, within those allowed, in order to get not very complicated expressions. The numerical optimization will be provided elsewhere.

The most general bound obtained by following the above procedure is

$$\begin{aligned} H(a,b,c,d,\lambda,D) = \ & \frac{(a-b)^{1+\lambda}}{(c-d)^{1-\lambda}} \left[\frac{\Gamma^2(D/2)}{4B\left(\frac{c-D\lambda}{\lambda(c-d)}, \frac{D\lambda-d}{\lambda(c-d)}\right) B\left(\frac{D\lambda+b}{\lambda(a-b)}, 1+\frac{1}{\lambda}\right)} \right]^{\lambda} \left[\frac{(1+\lambda)^{1+\lambda}}{(1-\lambda)^{1-\lambda}} \right]^{D/2} \times \\ & \times \left[\frac{(D\lambda+b)^{D\lambda+b}}{(D\lambda+a)^{D\lambda+a}} \right]^{\frac{1}{a-b}} \left[(D\lambda-d)^{D\lambda-d} (c-D\lambda)^{c-D\lambda} \right]^{\frac{1}{c-d}} \end{aligned} \tag{18}$$

where the symbol $B(x, y)$ denotes the beta function.

It is worthy to remark that the inequality obtained also holds after exchanging the position (r) and momentum (p) variables. This is equivalent to the choice of the parameters as $t > 1 > q$ in the initial stage, the uncertainty product having both r expectation values at the numerator as well as one of the p ones, with the other at the denominator.

IV. PARTICULAR CASES OF PHYSICAL INTEREST

The last inequality in the previous section provides us with a extremely wide set of lower bounds on uncertainty products. The general expression contains four radial expectation values, but particular cases with only three or two will be considered also. Emphasis will

be made on the products $\langle r^\alpha \rangle^{1/\alpha} \langle p^\beta \rangle^{1/\beta}$, having one of the orders negative, because the only known results in this sense, to our knowledge, correspond to products with both positive orders, as done e.g. in Refs. [15] and [22].

In addition, physically relevant products with three and four radial expectation values will be also analyzed. It is worth mentioning that some of these quantities are physically relevant and/or experimentally accesible in three-dimensional atomic systems. Some examples are [30]:

- The kinetic energy T, given by $T = \dfrac{\langle p^2 \rangle}{2}$, with its relativistic correction, proportional to $\langle p^4 \rangle$.

- The height of the peak of the Compton profile $J(q)$, experimentally accessible from electron scattering experiments, is $J(0) = \dfrac{\langle p^{-1} \rangle}{2}$.

- The diamagnetic susceptibility χ, proportional to $\langle r^2 \rangle$.

- The electron-nucleus attraction energy (absolute value) $E_{eN} = Z \langle r^{-1} \rangle$, with Z being the nuclear charge.

For illustration, the accuracy of the universal bounds to uncertainty products will be analyzed for ground-state neutral atoms throughout the whole Periodic Table (nuclear charge $Z = 1 - 103$). In doing so, accurate near-Hartree-Fock wavefunctions [31, 32] will be employed to compute the radial expectation values.

A. Two-moment products

Much attention has been paid to the products $\langle r^\alpha \rangle^{1/\alpha} \langle p^\beta \rangle^{1/\beta}$ with $\alpha, \beta > 0$. Let us notice that we can provide lower bounds on them by using Eq. (18), choosing appropriately two powers (orders) as zero, what simplifies the expression to a two-moment one because of the normalization to unity.

We distinguish the following three cases, according to the signs of α and β:

1. Both orders positive: the procedure here considered, based on the extremization of frequency moments with two constraints, would be equivalent to the extremization of the Rényi entropies with one-moment and normalization constraints. Such is the

technique employed in Ref. [22] and, consequently, the results in that case are here the same as in the aforementioned reference.

2. Both orders negative: such a choice is no longer possible, according to the constraints on the orders of the radial expectation values considered. Let us remind that necessarily $c > 0$, and consequently we cannot choose two negative orders and the other two equal to zero.

3. One positive and one negative: such a choice is allowed, providing results which constitute a novelty to our knowledge. Now we obtain lower bounds to the products considered in this section, with $\alpha > 0 > \beta$ or conversely.

If we choose $a = d = 0$ in Eq, (18), then

$$\langle r^b\rangle^{1/b}\langle p^c\rangle^{1/c} \geq \left[\frac{(-b)^{1+\lambda}}{c^{1-\lambda}}\right]^{\frac{1}{D\lambda}} \left[\frac{\Gamma^2(D/2)}{4B\left(\frac{c-D\lambda}{\lambda(c-d)},\frac{D\lambda-d}{\lambda(c-d)}\right)B\left(\frac{D\lambda+b}{\lambda(a-b)},1+\frac{1}{\lambda}\right)}\right]^{\frac{1}{D}} \left[\frac{(1+\lambda)^{1+\lambda}}{(1-\lambda)^{1-\lambda}}\right]^{\frac{1}{2\lambda}} \times \\ \times(D\lambda+b)^{-\frac{1}{b}-\frac{1}{D\lambda}}(D\lambda)^{\frac{1}{b}+\frac{1}{c}}(c-D\lambda)^{\frac{1}{D\lambda}-\frac{1}{c}} \tag{19}$$

for any $c > D\lambda > -b > 0$. The analogous relationship also holds after exchanging the variables r and p.

Attending to the above comments on the physical relevance of radial expectation values, especially interesting appears the three-dimensional ($D = 3$) bound

$$\frac{\langle p^2\rangle^{1/2}}{\langle r^{-1}\rangle} \geq \frac{7^{7/4}}{2^{2/3}3^{11/12}5^{4/3}} = 0.81080 \tag{20}$$

This equation involves the kinetic and the electron-nucleus attraction energy. Exactly the same bound is valid for the quotient $\langle r^2\rangle^{1/2}/\langle p^{-1}\rangle$, essentially between the diamagnetic susceptibility and the peak of the Compton profile.

According to the chosen orders, the parameter λ must belong to the interval $\left(\frac{1}{3},\frac{2}{3}\right)$. The bound just provided corresponds to the particular value $\lambda = 2/5$. An improvement on the accuracy of this bound can be achieved by optimizing the corresponding expression over the whole allowed interval.

In Figure 1 the aforementioned quotients are displayed, as well as their lower bound in Eq. (20), for neutral atoms $Z = 1 - 103$. It is observed the similar path followed by both curves (computed from Eq. (20) and the corresponding one exchanging the conjugated variables), with a slightly higher structure observed in the curve defined in terms of $\langle r^2\rangle$ and

$\langle p^{-1}\rangle$ as compared to the conjugated one. The reason behind last comment is that these two expectation values enhance the contribution of the outermost (valence) region. This occurs because the factor r^2 enhances the contribution from electrons far from the nucleus, and the factor p^{-1} enhances that of low-speed electrons, that is those in the outermost region. An opposite effect occurs with operators r^{-1} and p^2, both them enhancing the surround of the nucleus (short distance and high speed).

The analysis of the presence of local extrema in these curves reveals (i) the systematic display of alkaline elements ($Z = 3, 11, 19, 37, 55, 87$) as local maxima, (ii) the same effect regarding most systems suffering from the so-called anomalous shell-filling ($Z = 24, 29, 42, 46, 78, 93, 97$), and (iii) all alkaline-earths ($Z = 4, 12, 20, 38, 56, 88$) correspond to local minima.

Additionally it is worthy to mention the behavior of the aforementioned products as (roughly) $Z^{0.27}$, induced numerically from Figure 1.

On the other hand, it is interesting to notice that the well-known lower bound $\langle r^2\rangle\langle p^2\rangle \geq 9/4$ can be improved by considering additional expectation values, from the use of Eq. (18) with an appropriate choice of the parameters. This will be discussed in Subsection IV.C.

B. Three-moment products

Relationships involving more than two radial expectation values have been obtained by means of different methods (Hölder's inequality [33], Stieltjes moment problem [26]). However, they are restricted to a given space (either position either momentum), but not combining simultaneously both conjugated spaces, as in the two-moment products of this work.

Restricting ourselves, for the sake of simplicity, to the four moments with orders -1 and 2 in both spaces, we have at our disposal four different three-moment combinations. Each one avoids the presence of one of these moments. We should keep in mind the validity of those bounds by exchanging the conjugated variables.

As in the two-moment case, there exists an allowed interval for the parameter λ according to the chosen orders. Nevertheless, we choose a particular value in each case, in order to get expressions as simple as possible. Some of those inequalities are given below:

$$\langle r^2\rangle^{3/2}\langle p^2\rangle^2\langle p^{-1}\rangle \geq \frac{4480}{3^{15/2}} = 1.18258, \quad \text{with } \frac{1}{3} = \lambda \in \left(0, \frac{2}{3}\right) \tag{21}$$

$$\frac{\langle p^2\rangle^{1/3}\langle r^2\rangle^{3/2}}{\langle p^{-1}\rangle^{7/3}} \geq \frac{(3/2)^6}{7^{4/3}} = 0.85065, \quad \text{with } \frac{1}{2} = \lambda \in \left(\frac{1}{3}, \frac{2}{3}\right) \tag{22}$$

$$\frac{\langle p^2\rangle^{5/3}\langle p^{-1}\rangle^{1/3}}{\langle r^{-1}\rangle^{3}} \geq \frac{27}{512}5^{5/3} = 0.77098, \quad \text{with } \frac{1}{2} = \lambda \in \left(\frac{1}{3}, \frac{2}{3}\right) \tag{23}$$

From Figure 2 the accuracy of the above bounds can be analyzed. Consider also the three inequalities exchanging the variables. Each of the above three inequalities and their conjugated counterparts are displayed, respectively, in Figures 2a, 2b and 2c.

It is observed that, as discussed for the two-moment products, the local extrema displayed in these figures follow the same trends according to the shell-filling pattern. Especially remarkable are the maxima associated to alkaline elements or some of those elements suffering an anomalous shell filling, while most minima correspond to alkaline-earths.

C. Four-moment products

There are two inequalities involving the four moments considered. Each inequality can be obtained from the other after exchanging the variables. We give here one of them:

$$\frac{\langle r^2\rangle^{1/3}\langle p^2\rangle^{5/3}\langle p^{-1}\rangle^{1/3}}{\langle r^{-1}\rangle^{7/3}} \geq \frac{243}{256}(5^5/7^4)^{1/3} = 1.03638, \quad \text{with } \frac{1}{2} = \lambda \in \left(\frac{1}{3}, \frac{2}{3}\right) \tag{24}$$

This product and its conjugated version are displayed in Figure 3. It is observed again the extreme similarity between the conjugated products, as well as their rough behavior as $Z^{5/4}$. The structure of the curves is justified with similar arguments to those previously done regarding other uncertainty products, according to the atomic shell-filling patterns.

It should be noticed the possibility of obtaining a lower bound on the Heisenberg product $\langle r^2\rangle\langle p^2\rangle$ other than the constant one 9/4, but in terms of other two radial expectation values instead. In doing so, an appropriate choice of the orders and the (almost) free parameter in Eq. (18) may be done. In this sense, the aforementioned constant bound could be improved from the knowledge of the values of two radial expectation values other than those of order two.

V. CONCLUSIONS

The variational bounds on frequency moments in terms of radial expectation values, together with the Rényi uncertainty inequality, allow to obtain a great variety of lower bounds on uncertainty products defined in terms of radial expectation values. These bounds are of universal validity, and the main novelties are (i) the possibility of dealing with moments of negative order, and (ii) the collection of results for products of more than two expectation values. The analysis for ground state atomic systems reveals (i) the deep similarity between results obtained from a given inequality and its conjugated one, and (ii) the display of atomic shell-filling patterns according to the location of local extrema in the curves displayed. Some of the results here studied are based on a specific choice of the (almost) free Rényi parameter, but they can still be improved by carrying out a numerical optimization on such a parameter. This will be done elsewhere.

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Figure Captions

Figure 1 Two-moment uncertainty products, one with order -1 and the other with order 2, and fit in terms of the nuclear charge Z, for one-particle densities of neutral atoms with $Z = 1 - 103$. Atomic units are used.

Figure 2 Three-moment uncertainty products with orders -1 and 2 as given by (a) Eq. (21), (b) Eq. (22) and (c) Eq. (23), and fits in terms of the nuclear charge Z, for one-particle densities of neutral atoms with $Z = 1 - 103$. Atomic units are used.

Figure 3 Four-moment uncertainty products with orders -1 and 2 in both conjugated spaces, and fit in terms of the nuclear charge Z, for one-particle densities of neutral atoms with $Z = 1 - 103$. Atomic units are used.

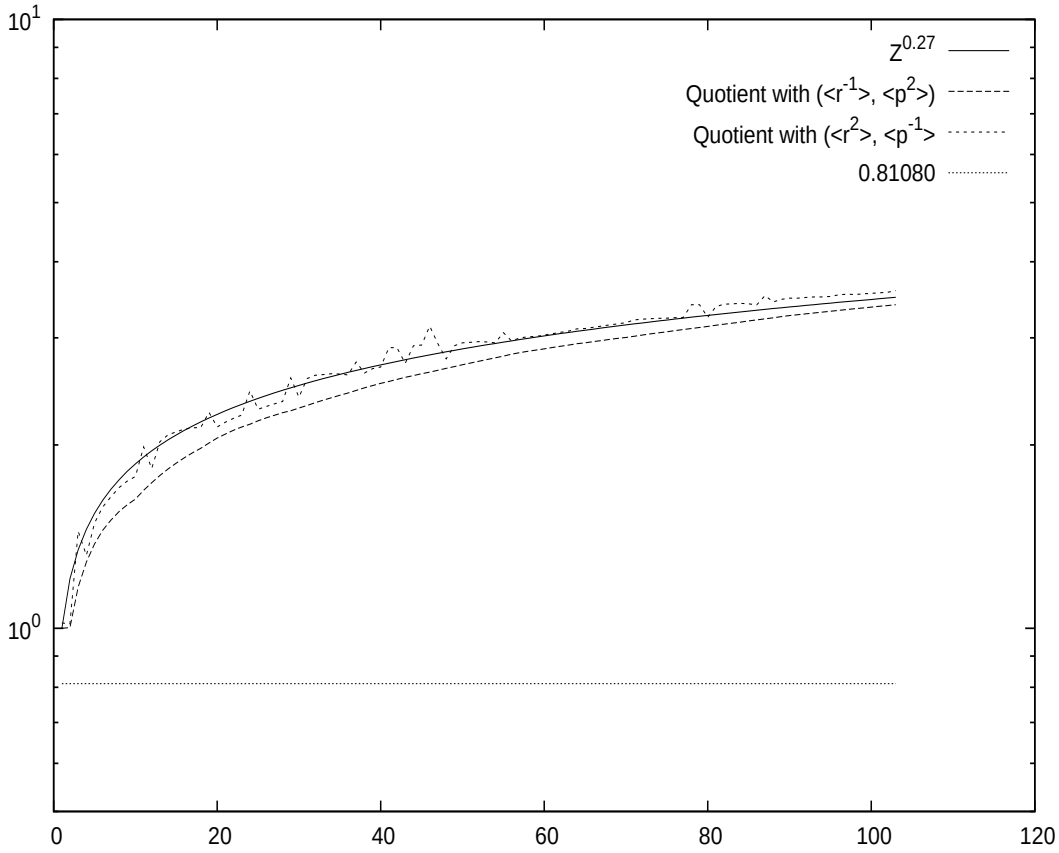
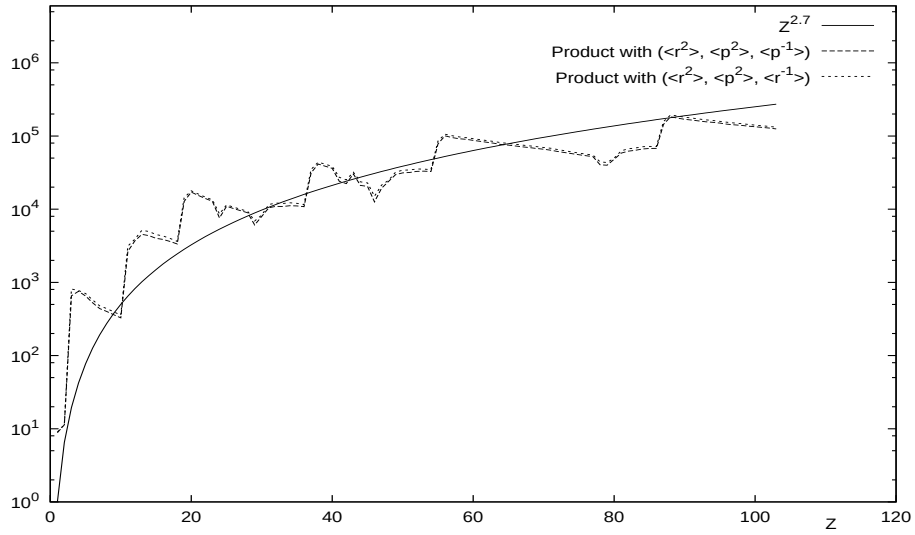


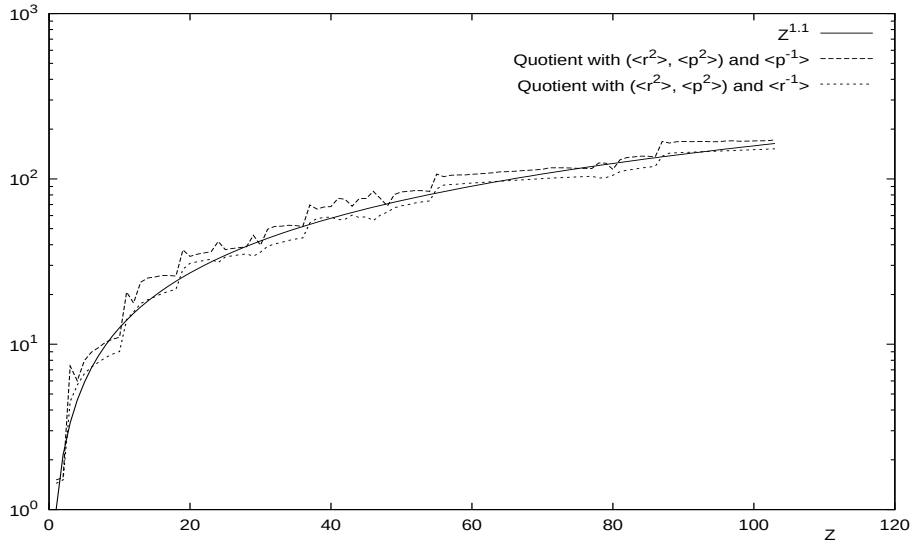
Figure 1 (J.C. Angulo)

Z

(a)



(b)



(c)

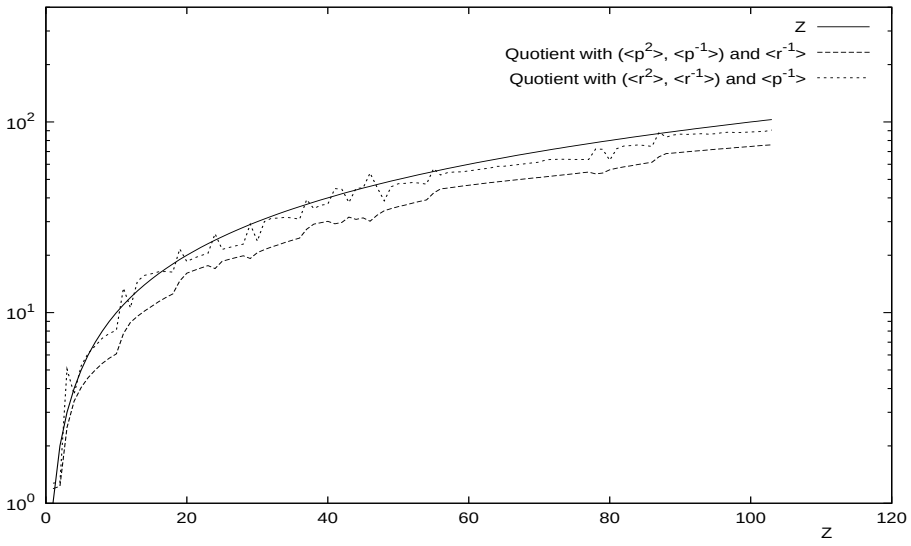


Figure 2 (J.C. Angulo)

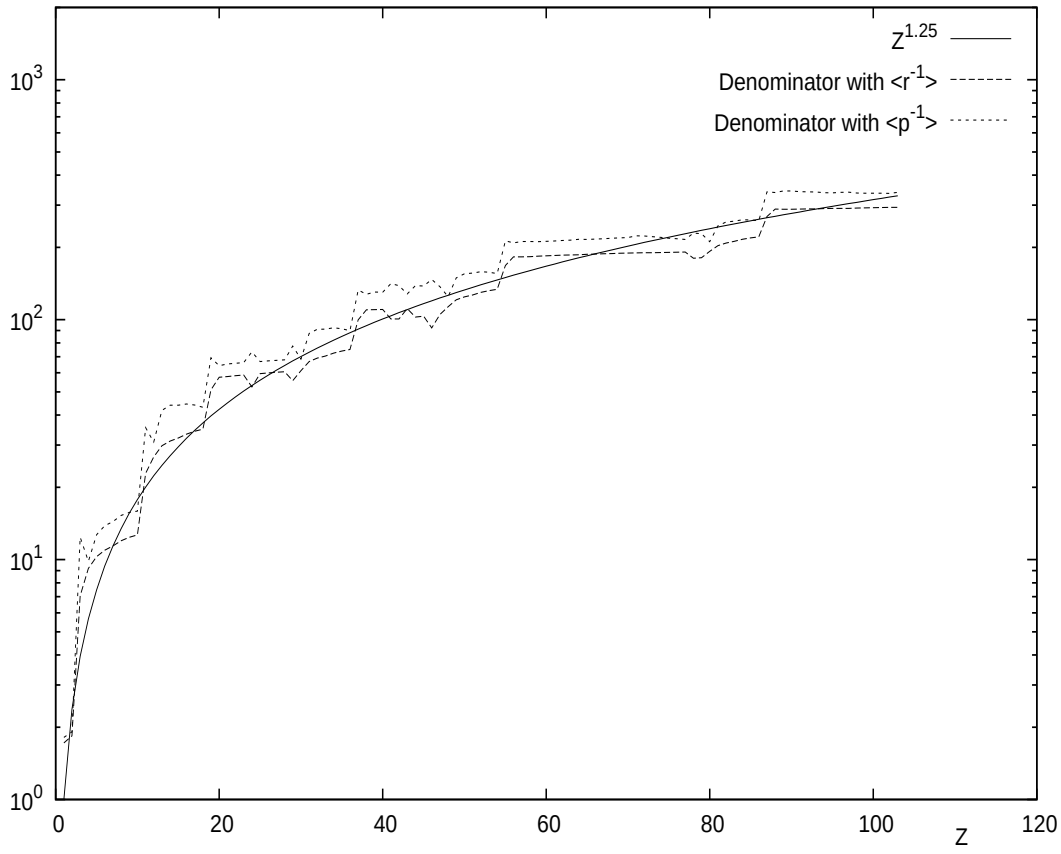


Figure 3 (J.C. Angulo)