On moments-based Heisenberg inequalities

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Abstract. In this paper we revisit the quantitative formulation of the Heisenberg uncertainty principle. The primary version of this principle establishes the impossibility of refined simultaneous measurement of position $\mathbf{x}$ and momentum $\mathbf{u}$ for a (1-dimensional) quantum particle in terms of variances: $\langle\|\mathbf{x}\|^2\rangle\langle\|\mathbf{u}\|^2\rangle \geq 1/4$. Since this inequality applies provided each variance exists, some authors proposed entropic versions of this principle as an alternative (employing Shannon's or Rényi's entropies). As another alternative, we consider moments-based formulations and show that inequalities involving moments of orders other than 2 can be found. Our procedure is based on the Rényi entropic versions of the Heisenberg relation together with the search for the maximal entropy under statistical moments' constraints ($\langle\|\mathbf{x}\|^a\rangle$ and $\langle\|\mathbf{u}\|^b\rangle$). Our result improves a relation proposed very recently by Dehesa *et al.* [1] where the same approach was used but starting with the Shannon version of the entropic uncertainty relation. Furthermore, we show that when $a = b$, the best bound we can find with our approach coincides with that of Ref. [1] and, in addition, for $a = b = 2$ the variance-based Heisenberg relation is recovered. Finally, we illustrate our results in the cases of d-dimensional hydrogenic systems.

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INTRODUCTION

The well-known Uncertainty Principle (UP) establishes the existence of an irreducible lower bound for the uncertainty in the result of a simultaneous measurement of non-commuting observables. In its initial formulation, the UP expresses in terms of the variances of the position $\mathbf{x}$ and the momentum $\mathbf{u}$ of a particle. However, such a formulation applies provided the variances exist, which is not always the case (see e.g. [2]). Recently, in order to be able to formulate the principle quantitatively in such cases, various information-theoretic quantities have been used as uncertainty measures. They describe the spread of the quantum-mechanical probability distribution more appropriately than the variance; in particular, they do not depend on any specific point of the probability domain. Thus, various alternative formulations of the UP have been proposed using the Shannon [3], Rényi [4, 5, 6] and Tsallis [7, 8] entropies as well as the entropic moments

[9] and the Fisher information [10, 11, 12], which have been employed in atomic and molecular physics for different purposes (see e.g. [13, 14, 15, 16]). These information-theoretic quantities are generally claimed to be not physical observables because they cannot be expressed as expectation values of any Hermitian operator of a quantum system[1]. Here we propose another formulation of UP which generalizes the variance-based one by use of the position and momentum *power moments* of arbitrary order (i.e., not necessarily equal to 2) as uncertainty measures; these measures often characterize some fundamental and/or experimentally accessible quantities of the system.

In parallel, physics still needs of statistical tools to describe complex systems such as atomic or molecular systems, chemical reactions, etc [18, 19, 20, 21, 22, 23, 1]. Some of the measures we employ here, work in both conjugated spaces (position/momentum). The motivation for using statistical moments is twofold: firstly they measure the spread of a distribution, and secondly they can be linked to physical quantities, e.g. atomic Thomas–Fermi or Dirac exchange [1]. Finally, in order to build a complexity measure that is invariant to a stretching factor applied to the distribution (and thus compressing in the conjugated domain), we will be interested in studying quantities of the form $\langle \|\mathbf{x}\|^a \rangle^{\frac{2}{a}} \langle \|\mathbf{u}\|^b \rangle^{\frac{2}{b}}$ with (a,b) not necessarily equal to $(2,2)$. In particular, in the present work we derive lower bounds for such kind of products corresponding to arbitrary powers.

The paper is organized as follows. First we briefly describe the entropic formulation of the uncertainty principle in terms of Rényi's entropies. Then, we propose an approach to reformulate the uncertainty principle using statistical moments of arbitrary orders. Our approach follows that used by both Bialynicki-Birula in [3] and Dehesa *et al.* in [1] to recover respectively the variance-based formulation and a moments-based formulation from the Shannon entropic-based expression. Later, we apply our results to d-dimensional hydrogenic systems. Finally, some conclusions and open problems are discussed.

ENTROPIC UNCERTAINTY RELATIONS: A BRIEF REVIEW

To fix the notations, consider a d-dimensional state $\mathbf{x}$ of a continuous-state system, described by the wavefunction $\Psi(\mathbf{x})$, and its Fourier transform $\widehat{\Psi}(\mathbf{u}) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \Psi(\mathbf{x}) \exp(-\imath \mathbf{x}^t \mathbf{u})\, \mathrm{d}\mathbf{x}$ describing the distribution of the momentum $\mathbf{u}$ of the particle, assumed to be also continuous. Note that, by convention, we have adopted here $\hbar = 1$. Without loss of generality we will consider in the sequel of the paper that $\langle \mathbf{x} \rangle = \mathbf{0} = \langle \mathbf{u} \rangle$. Denoting by $r = \|\mathbf{x}\|$ and $p = \|\mathbf{u}\|$ the Euclidean norm of the d-dimensional position and the d-dimensional momentum, the well-known Heisenberg uncertainty principle writes

$$\langle r^2 \rangle \langle p^2 \rangle \geq \frac{d^2}{4}, \tag{1}$$

[1] See however [17] where Jizba claimed that Rényi's entropies are in fact observable, in terms of Lesche's condition.

where the expectation value of a general function $f(r)$ is defined as $\langle f(r)\rangle = \int_{\mathbb{R}^d} f(\|\mathbf{x}\|)\rho(\mathbf{x})\,\mathrm{d}\mathbf{x}$ with $\rho = |\Psi|^2$, and similarly for any function $g(p)$, with weight $\gamma = |\widehat{\Psi}|^2$.

The spread of the position distribution ρ (resp. momentum distribution γ) can be expressed very adequately via the Rényi's entropy of index $\lambda \geq 0$ [24, 25], or its corresponding entropy power, which are defined by

$$H_\lambda(\rho) = \frac{1}{1-\lambda}\log\int_{\mathbb{R}^d}[\rho(\mathbf{x})]^\lambda\,\mathrm{d}\mathbf{x} \tag{2}$$

and

$$N_\lambda(\rho) = \frac{1}{2\pi e}\exp\left(\frac{2}{d}H_\lambda(\rho)\right), \tag{3}$$

respectively. Note that $\lim_{\lambda\to 1} H_\lambda(\rho) = H(\rho) = -\int_{\mathbb{R}^d}\rho(\mathbf{x})\log\rho(\mathbf{x})\mathrm{d}\mathbf{x}$ is the Shannon's entropy, that can thus be viewed as a special case of Rényi's entropies.

A Rényi-entropy-based uncertainty relation has been recently shown [4, 5] to be valid, in the form

$$N_\alpha(\rho)N_{\alpha^*}(\gamma) \geq \mathscr{B}(\alpha) = \frac{\alpha^{\frac{1}{\alpha-1}}\alpha^{*\frac{1}{\alpha^*-1}}}{4e^2} \quad \text{with} \quad \mathscr{B}(1) = \frac{1}{4} \tag{4}$$

where

$$\alpha^* = \frac{\alpha}{2\alpha-1}, \tag{5}$$

with $\alpha \geq 1/2$. In the limit $\lambda \to 1$ and taking the logarithm of the above relation, the Shannon-entropy-based Bialynicki-Birula's version [3] is recovered. Moreover, as shown in [3], searching the maximum of the Shannon's entropy power $N(\rho) = N_1(\rho)$ subject to (s.t.) variance constraint $\langle r^2\rangle$ (that is known to be the entropy power of a Gaussian [25, 26]), and similarly for the momentum, one achieves

$$\langle r^2\rangle\langle p^2\rangle \geq d^2 N(\rho)N(\gamma) \geq \frac{d^2}{4} \tag{6}$$

and thus the Heisenberg relation is obtained from the entropic version. Heisenberg inequality is known to be sharp, and fortunately nothing is lost by this procedure. Indeed, equality between the entropy and its maximal value is reached if and only if ρ is Gaussian. Furthermore, if (and only if) ρ is Gaussian, γ is also Gaussian with the "appropriate" variance, and thus at the same time in the momentum space the maximum entropy is also achieved. Simultaneously, the Bialynicki-Birula inequality becomes an equality if and only if ρ is Gaussian, and thus the succession of inequalities are equalities.

Note now that the relation with Rényi's entropies given above concerns only indexes α and α^* so that 2α and $2\alpha^*$ are conjugated in the Hölder sense: $\frac{1}{2\alpha} + \frac{1}{2\alpha^*} = 1$. Zozor *et al.* then showed in [6] that the relation (4) extends for any couple (α,β) so that

$0 \leq \beta \leq \alpha^*$, with the bounds

$$N_\alpha(\rho)N_\beta(\gamma) \geq \mathscr{B}_{\mathrm{ZPV}}(\alpha,\beta) = \begin{cases} 1/e^2 & \text{for } (\alpha,\beta) \in [0;1/2]^2 \\ \mathscr{B}(\max(\alpha,\beta)) & \text{otherwise} \end{cases} \tag{7}$$

It is worth noting that on the "conjugated curve" $\beta = \alpha^* = \alpha/(2\alpha-1)$ in the (α,β) plane, the bound is sharp and attainable if (and only if) ρ is Gaussian [5, 6]. We also showed that for $\beta > \alpha^*$, no uncertainty principle exists [6], in the sense that it is possible to find states for which the positive product of Rényi's entropy powers can be made arbitrarily small. But below the conjugated curve we do not know yet neither the sharpest bound nor the states for which that bound is achieved.

Since this formulation suffers from the fact that the Rényi entropies are not physical observables, it is natural to search for another alternative based on uncertainty measures more directly connected to fundamental observables of the system such as e.g. the moments around the origin. This is done in the next section.

IMPROVED MOMENTS-BASED UNCERTAINTY RELATIONS

Following Angulo and Dehesa [27, 28] , as recently reviewed by Dehesa et al [1], it is known that

$$\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}} \geq \left(\frac{e\,d^{\frac{2}{a}}\,\Gamma^{\frac{2}{d}}\left(1+\frac{d}{2}\right)}{(ae)^{\frac{2}{a}}\,\Gamma^{\frac{2}{d}}\left(1+\frac{d}{a}\right)}\right)\left(\frac{e\,d^{\frac{2}{b}}\,\Gamma^{\frac{2}{d}}\left(1+\frac{d}{2}\right)}{(be)^{\frac{2}{b}}\,\Gamma^{\frac{2}{d}}\left(1+\frac{d}{b}\right)}\right) = \mathscr{D}(a,b) \tag{8}$$

for any $a,b \geq 0$. This immediately leads to the Heisenberg inequality when $a = b = 2$.

The basic idea to prove (8) is similar to that used to derive Heisenberg relation from the Bialynicki-Birula relation: search for the maximizer of the Shannon's entropy of ρ s.t. $\langle r^a\rangle$, and, separately, the maximizer of the entropy of γ s.t. $\langle p^b\rangle$. We will present the proof just below in a slightly more general context to achieve a (possibly) better bound. But previously, let us remark that such a bound cannot be sharp. If we denote $\Psi_{\max,a}$ the wave function that gives the maximizer of $N(\rho)$ s.t. $\langle r^a\rangle$ and $\widetilde{\Psi}_{\max,b}$ the one that maximizes $N(\gamma)$ s.t. $\langle p^b\rangle$, these two functions are not linked by a Fourier transform, namely $\widetilde{\Psi}_{\max,b} \neq \widehat{\Psi}_{\max,a}$, even if a and b are conjugated (except $a = b = 2$). Or, in other words, the sum of the maximal entropies is not here the maximum of the sum of entropies.

In the same spirit as [1], one can derive a bound for the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ from the more general uncertainty relation (7), instead of starting from the Shannon entropic version, and thus one can retain the better bound over the family. Such a bound must include that of Dehesa *et al.*, since the Bialynicki-Birula relation is included in (7). The program is then the following:

1. Start with (7), namely $N_\alpha(\rho)N_\beta(\gamma) \geq \mathscr{B}_{\mathrm{ZPV}}(\alpha,\beta)$.
2. Search for the maximum Rényi entropy power $N_\alpha(\rho)$ s.t. $\langle r^a\rangle$. The maximizers are stretched q-exponentials [29, 30] (see also [31] concerning the Shan-

non entropy), and the maximal entropy power gives an inequality of the form $\langle r^a\rangle^{2/a} \ge N_\alpha(\rho)\mathscr{M}(a,\alpha)$. The same work is done on $N_\beta(\gamma)$ s.t. $\langle p^b\rangle$, leading to $\langle p^b\rangle^{2/b} \ge N_\beta(\gamma)\mathscr{M}(b,\beta)$ (the expression for $\mathscr{M}$ is given below).

3. This leads to the family of inequalities $\langle r^a\rangle^{2/a}\langle p^b\rangle^{2/b} \ge N_\alpha(\rho)N_\beta(\gamma)\mathscr{M}(a,\alpha)\mathscr{M}(b,\beta) \ge \mathscr{M}(a,\alpha)\mathscr{M}(b,\beta)\mathscr{B}_{\mathrm{ZPV}}(\alpha,\beta)$, for any $\alpha > \frac{d}{d+a}$ and $\alpha^* \ge \beta > \frac{d}{d+b}$ (the restrictions are due to the validity domain of (7) and the existence of the entropy powers and moments [29]).
4. The best bound we can find is then $\mathscr{C}(a,b) = \max_{\alpha,\beta} \mathscr{M}(a,\alpha)\mathscr{M}(b,\beta)\mathscr{B}_{\mathrm{ZPV}}(\alpha,\beta)$.
5. Finally, studying the behavior of $\mathscr{M}(a,\alpha)$ that is increasing with α, and the behavior of $\mathscr{B}(\alpha)$, one can show that the maximum is achieved on the "conjugated" curve $\beta = \alpha^*$, and thus $\mathscr{C}(a,b) = \max_{\alpha} \mathscr{M}(a,\alpha)\mathscr{M}(b,\alpha^*)\mathscr{B}(\alpha)$. A rapid study of the behavior of $\mathscr{M}(a,\alpha)\mathscr{M}(b,\alpha^*)\mathscr{B}(\alpha)$ with α allows us to restrict the domain where the maximum is attained.

The final result can then be expressed as:

$$\langle r^a\rangle^{2/a}\langle p^b\rangle^{2/b} \ge \mathscr{C}(a,b) = \max_{\alpha\in D} \mathscr{B}(\alpha)\mathscr{M}(a,\alpha)\mathscr{M}(b,\alpha^*) \tag{9}$$

for any $a \ge b > 0$, where

$$D = \left(\max\left(\frac{1}{2}, \frac{d}{d+a}\right) ; 1\right], \tag{10}$$

the function $\mathscr{B}(\alpha)$ is given in (4), the parameter $\alpha^*(\alpha)$ is defined in Eq. (5), and

$$\mathscr{M}(l,\lambda) = \frac{2^{\frac{d-2}{d}}\, e\, l^{\frac{2\lambda}{d(\lambda-1)}}\, \lambda^{\frac{2}{d(\lambda-1)}}\, (d|\lambda-1|)^{\frac{2}{l}}}{[d(\lambda-1)+l\lambda]^{\frac{2}{l}+\frac{2}{d(\lambda-1)}} \left[B\left(\frac{d}{2}, \frac{\lambda}{|\lambda-1|} + \left(1-\frac{d}{l}\right)\mathbb{1}_{(1;+\infty)}\right)\right]^{\frac{2}{d}}} \tag{11}$$

with $\mathbb{1}_A$ denoting the indicator function of set A. The case $b \ge a > 0$ can be treated using the symmetry

$$\arg\max_{\alpha} \mathscr{B}(\alpha)\mathscr{M}(a,\alpha)\mathscr{M}(b,\alpha^*) = \alpha_{\mathrm{opt}}(a,b) = (\alpha_{\mathrm{opt}}(b,a))^* \tag{12}$$

and

$$\mathscr{C}(b,a) = \mathscr{C}(a,b) \tag{13}$$

The symmetry on α_{opt} allows also to conclude that $\alpha_{\mathrm{opt}}(a,a) = 1$ and thus the optimal bound from our approach coincides with bound $\mathscr{D}(a,b)$ of Dehesa *et al.*, (8) in this case. Unfortunately, except for the case $a = b$, we were not able to give an analytical expression for $\mathscr{C}(a,b)$.

Figure 1 depicts the bounds $\mathscr{C}(a,b)$ for given a, as a function of b compared to $\mathscr{D}(a,b)$. This figure shows that the bound is substantially improved when $b \ne a$, especially when $b \to 0$ or $|a-b| \to \infty$.

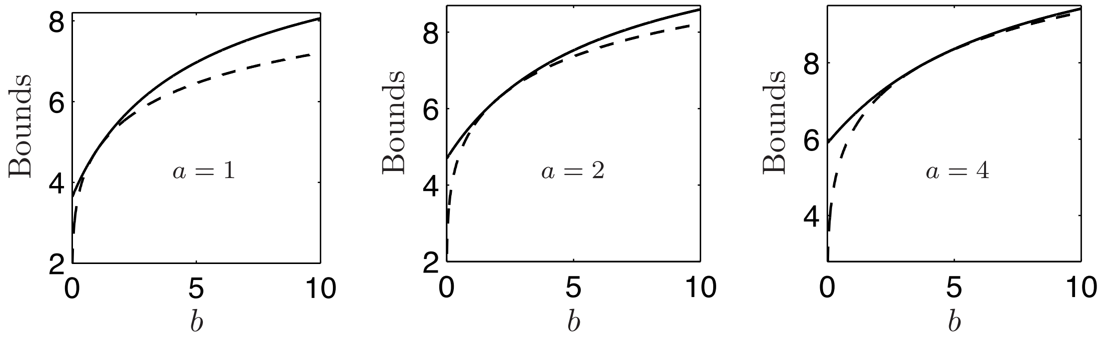

FIGURE 1. Bound $\mathscr{C}(a,b)$ (solid line) given in (9) compared to $\mathscr{D}(a,b)$ in (8) (dashed line), versus b, for given $a = 1$, $a = 2$ and $a = 4$ respectively.

APPLICATION TO HYDROGENIC SYSTEMS

Let us now examine the accuracy of the moments-based uncertainty relation (9) for the main prototype of d-dimensional systems, namely the hydrogenic atom. This system has been recently investigated in [20] in full detail. Therein one can find the explicit expressions not only for the quantum-mechanical wavefunctions of the ground and excited states of the system but also for the position and momentum power moments involved in relation (9) in terms of the dimensionality d and the hyperquantum numbers which completely characterize the states under study [20, 32, 33]. The resulting expressions permit to calculate the product $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$ in an explicit way. This product is depicted in Figure 2 for $(a,b) = (1,2)$ and Figure 3 for $(a,b) = (1,4)$, together with the corresponding bound $\mathscr{C}(a,b)$ given in (9)–(11).

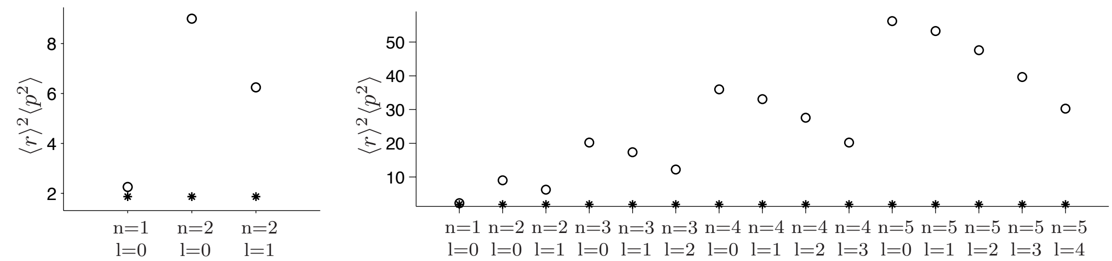

FIGURE 2. Product $\langle r\rangle^2\langle p^2\rangle$, i.e. for $(a,b) = (1,2)$ (circles), and lower bound $\mathscr{C}(a,b)$ of that product (stars), versus n and l for the 3-dimensional hydrogenic systems ($d = 3$). The plot on the left is a zoom of the one on the right.

We can see from this figure that although not sharp, the bound $\mathscr{C}(a,b)$ is close to the product $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$, for the ground state ($n = 1$ and $l = 0$). However, when n increases, the discrepancy from the bound increases (and decreases with l for fixed n). The same behavior occurs for other couples (a,b). Since hydrogenic systems of this kind belong to the family of radial potential systems, this suggests that refinement can be found in the context of radial systems as already done for the usual variance-based Heisenberg inequality, and for Fisher information-based versions [10, 11].

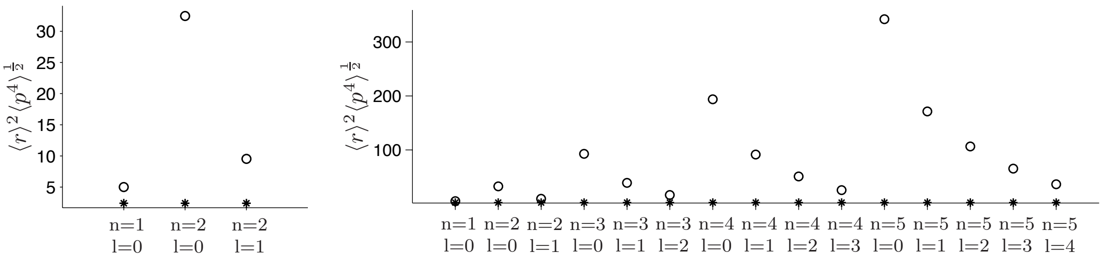

FIGURE 3. Product $\langle r\rangle^2\langle p^4\rangle^{\frac{1}{2}}$, i.e. for $(a,b) = (1,4)$ (circles), and lower bound $\mathscr{C}(a,b)$ of that product (stars), versus n and l for the 3-dimensional hydrogenic systems ($d = 3$). The plot on the left is a zoom of the one on the right.

CONCLUSIONS

In this paper we have proposed a moments-based mathematical realization of the position–momentum uncertainty principle that generalizes the variance-based Heisenberg uncertainty relation. In contrast to the entropic uncertainty relations, this novel formulation is based on uncertainty measures which describe physical observables. Our present approach suffers, however, from the fact that the lower bound for the product of position and momentum moments is probably not sharp, and that we have been unable (yet) to determine the minimizers. To solve this issue, a variational approach may be envisaged, although it seems a difficult task. Another alternative should be to employ appropriate Sobolev-like inequalities, as done for the entropic formulation (see e.g. [8]).

The moments-based uncertainty relation has been studied numerically for real hydrogenic systems. Although not presented here, we have also studied the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$. The results are similar, suggesting that such a product is a good candidate to assess the complexity of a system. To go further, the properties of such a complexity measure has to be analyzed in more detail.

Finally, let us point out that the improvement of the moments-based Heisenberg-like relations for the case of general central potentials is a fully open problem which deserves to be variationally solved for both fundamental and applied reasons.

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