Position-momentum uncertainty relations based on moments of arbitrary order

Steeve Zozor,[1,*] Mariela Portesi,[2,†] Pablo Sanchez-Moreno,[3,4,‡] and Jesus S. Dehesa[3,5,§]

[1] *Laboratoire Grenoblois d'Image, Parole, Signal et Automatique (GIPSA-Lab, CNRS), 961 rue de la Houille Blanche, F-38402 Saint Martin d'Hères, France*

[2] *Instituto de Física La Plata (CONICET), and Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, 1900 La Plata, Argentina*

[3] *Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, E-18071 Granada, Spain*

[4] *Departamento de Matemática Aplicada, Universidad de Granada, E-18071 Granada, Spain*

[5] *Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071 Granada, Spain*

(Received 7 December 2010; published 6 May 2011)

The position-momentum uncertainty-like inequality based on moments of arbitrary order for d-dimensional quantum systems, which is a generalization of the celebrated Heisenberg formulation of the uncertainty principle, is improved here by use of the Rényi-entropy-based uncertainty relation. The accuracy of the resulting lower bound is physico-computationally analyzed for the two main prototypes in d-dimensional physics: the hydrogenic and oscillator-like systems.

DOI: 10.1103/PhysRevA.83.052107 PACS number(s): 03.65.Ca, 02.50.−r, 05.90.+m, 03.65.Ta

I. INTRODUCTION

The uncertainty relations play a fundamental role not only in the foundations of quantum mechanics [1,2] but also for the quantum description of the internal structure of d-dimensional physical systems [1–5], as well as for the development of quantum information and computation [6,7]. The (position-momentum) uncertainty principle has attracted considerable attention since the early days of quantum mechanics [8,9] up to the present [1,2,10–12] because of its numerous scientific and technological implications. The first mathematical relation that expressed this principle in an exact and quantitative form is the celebrated Heisenberg relation [8,9], which uses the standard deviation or its square, the variance of position and momentum, as a measure of uncertainty; assuming $\langle \mathbf{x}\rangle = \langle \mathbf{p}\rangle = 0$ for notational simplicity, it reads

$$\langle r^2\rangle\langle p^2\rangle \geqslant \frac{d^2}{4} \qquad (1)$$

for d-dimensional quantum-mechanical states.

However, this relation is not only too weak but it is also often inadequate [12–16]. To overcome these problems, various alternative formulations of the uncertainty principle have been proposed by use of some information-theoretic uncertainty measures such as the Shannon entropy [17], Rényi entropies [18–20], Tsallis entropies [21,22], entropic momenta [23], and Fisher information [24–26], as recently surveyed [5,12,27].

Not so well known are the moment-based uncertainty relations developed by Angulo [28,29] in 1993, which can be recast [5] under the form

$$\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}} \geqslant \mathcal{D}(a,b) = \left(\frac{e\, d^{\frac{2}{a}}\, \Gamma^{\frac{2}{d}}\left(1+\frac{d}{2}\right)}{(ae)^{\frac{2}{a}}\, \Gamma^{\frac{2}{d}}\left(1+\frac{d}{a}\right)}\right) \times \left(\frac{e\, d^{\frac{2}{b}}\, \Gamma^{\frac{2}{d}}\left(1+\frac{d}{2}\right)}{(be)^{\frac{2}{b}}\, \Gamma^{\frac{2}{d}}\left(1+\frac{d}{b}\right)}\right) \qquad (2)$$

valid for all $(a,b) \in \mathbb{R}_+^2 = (0,+\infty)^2$. These relations, which offer a more general and versatile formulation of the uncertainty principle [note that it reduces to the Heisenberg inequality (1) in the particular case $a = b = 2$], has not received much attention despite the fact that the moments often completely characterize a probability density. Strictly speaking, in the d-dimensional case and when the characteristic function admits a Taylor expansion at any order, the assertion that the moments characterize a distribution is true concerning all the moments of the form $\int_{\mathbb{R}^d} \rho(\mathbf{x}) \prod_{i=1}^d [x_i^{k_i} dx_i]$ for all $k_i \in \mathbb{N}$. The assertion is no longer true when (some of) these moments do not exist and/or dealing only with fractional moments. For example, this appears for laws that are not exponentially decreasing (e.g., a power law such as Lévy noise). This is known as the Hamburger moment problem ([30], Chap. III, Sec. 8). Other similar relationships for particular values of the parameters have also been published [10,31,32]. Note also that quantities $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ are insensitive to a stretching factor in the position (or equivalently in the momentum). Moreover, for specific values of a and/or b, the moments are linked to physical quantities (e.g., atomic Thomas-Fermi or Dirac exchanges [5]). Thus, it may offer a useful tool to quantify complexity for atomic or chemical systems that can be complementary to those proposed, e.g., in [5,33–35].

In this work, we deal with relations (2) and improve them by use of a Rényi-entropy-based approach, in a way similar to the procedure followed by Bialynicki-Birula and Mycielski (BBM in short) [17] and Angulo [28,29] to obtain the relations (1) and (2), respectively, from the Shannon entropy. For this purpose, we first fix notations and briefly review the entropic

*steeve.zozor@gipsa-lab.grenoble-inp.fr
†portesi@fisica.unlp.edu.ar
‡pablos@ugr.es
§dehesa@ugr.es

uncertainty relations in Sec. II. Then, in Sec. III, we find moment-based formulations of the uncertainty principle that extend and generalize the relations (1) and (2). In Sec. IV, we carry out a computational analysis of our moment-based uncertainty relation for hydrogenic and oscillator-like systems, not only because they are the two main quantum prototypes in d-dimensional physics, but also because their position and momentum moments have known analytical expressions in terms of the hyperquantum numbers at all orders [36]. Finally, some conclusions are given in Sec. V. In the Appendixes, we provide help to clearly discuss the proof of the moment uncertainty relation described in Sec. III.

II. ENTROPIC UNCERTAINTY RELATIONS: A BRIEF REVIEW

Let us denote by $\Psi(\mathbf{x})$ and $\widehat{\Psi}(\mathbf{p})$ the wave functions of a d-dimensional quantum-mechanical system in the position and momentum spaces, respectively, so that

$$\widehat{\Psi}(\mathbf{p}) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \Psi(\mathbf{x}) \exp(-\imath \mathbf{x}^t \mathbf{p})\, d\mathbf{x},$$

where the units with $\hbar = 1$ are used. The corresponding position and momentum probability densities will be denoted as

$$\rho(\mathbf{x}) = |\Psi(\mathbf{x})|^2 \quad \text{and} \quad \gamma(\mathbf{p}) = |\widehat{\Psi}(\mathbf{p})|^2,$$

respectively. These two density functions are known to be completely characterized by the knowledge of the moments $\langle r^a \rangle$ and $\langle p^b \rangle$ of all orders, respectively, where $r = \|\mathbf{x}\|$ and $p = \|\mathbf{p}\|$ denote the Euclidean norms of the d-dimensional position and momentum single-particle operators, respectively. The position expectation value $\langle f(r) \rangle$ is defined as

$$\langle f(r) \rangle = \int_{\mathbb{R}^d} f(\|\mathbf{x}\|) \rho(\mathbf{x})\, d\mathbf{x},$$

and similarly for the expectation value $\langle f(p) \rangle$ with the momentum density $\gamma(\mathbf{p})$.

For notational simplicity, we assume that $\mathbf{x}$ and $\mathbf{p}$ have zero mean, so that the variance-based Heisenberg uncertainty relation takes the form (1). Nowadays it is well known that there exist other uncertainty relations that are much more stringent. They are based on information-theoretic quantities such as the Shannon and Rényi entropies and the Fisher information, which provide complementary measures of the position and momentum probability spreading. Let us recall here the definition of the Rényi entropy of (real) index $\lambda \geqslant 0$, $\lambda \neq 1$ [37,38],

$$H_\lambda(\rho) = \frac{1}{1-\lambda} \ln \int_{\mathbb{R}^d} [\rho(\mathbf{x})]^\lambda d\mathbf{x} = \frac{2\,\lambda}{1-\lambda} \ln \|\Psi\|_{2\lambda}, \qquad (3)$$

which represents an alternative generalized measure of uncertainty (lack of information) of a random variable with probability density $\rho = |\Psi|^2$. Here, $\|\cdot\|_s$ denotes the L^s norm for functions $\|\Psi\|_s = [\int_{\mathbb{R}^d} |\Psi(\mathbf{x})|^s d\mathbf{x}]^{1/s}$. Note that $\lim_{\lambda\to 1} H_\lambda(\rho) = H(\rho) = -\int_{\mathbb{R}^d} \rho(\mathbf{x}) \ln \rho(\mathbf{x}) d\mathbf{x}$ is the Shannon entropy, which can thus be viewed as a special case of the family of Rényi entropies (we will write $H = H_1$).

To derive an entropic formulation of the uncertainty relation, the point to start with is the Beckner relation that links the L^s norm of a (wave) function $\Psi(\mathbf{x})$ to the L^q norm of its Fourier transform $\widehat{\Psi}(\mathbf{p})$, where $\mathbf{x}$ and $\mathbf{p}$ are continuous in $\mathbb{R}^d$, d being the dimension, and s and q being conjugated numbers in the Hölder sense: $1/s + 1/q = 1$. This relation states that for any $s \in [1;2]$ and $q = s/(1-s)$,

$$\|\widehat{\Psi}\|_q \leqslant (C_{s,q})^d \|\Psi\|_s, \qquad (4)$$

where

$$C_{s,q} = \left(\frac{2\pi}{s}\right)^{-\frac{1}{2s}} \left(\frac{2\pi}{q}\right)^{\frac{1}{2q}} \qquad (5)$$

is the Babenko-Beckner constant. Thus, by taking the logarithm of the relation (4) with $s = 2\alpha$ and $q = 2\alpha^*$, one achieves the relation [18,19]

$$H_\alpha(\rho) + H_{\alpha^*}(\gamma) \geqslant d \left(\ln(2\pi) + \frac{\ln(2\alpha)}{2(\alpha-1)} + \frac{\ln(2\alpha^*)}{2(\alpha^*-1)} \right), \qquad (6)$$

where α and α^* are two real parameters related by $\frac{1}{\alpha} + \frac{1}{\alpha^*} = 2$, from which we define $\alpha^*(\alpha) = \alpha/(2\alpha - 1)$. In principle, $\alpha \in [\frac{1}{2}\,;\,1]$, but it can be seen that by symmetry (exchanging the roles of Ψ and $\widehat{\Psi}$), this relation holds for any $\alpha \geqslant 1/2$. When $\alpha \to 1$, then $\alpha^* \to 1$ and thus the BBM relation [17] dealing with Shannon entropies is recovered,

$$H(\rho) + H(\gamma) \geqslant d[1 + \ln(\pi)]. \qquad (7)$$

The entropic uncertainty relations given in (6) and (7) can be recast in the more convenient product form,

$$N_\alpha(\rho) N_{\alpha^*}(\gamma) \geqslant \mathcal{B}(\alpha), \qquad (8)$$

with

$$\mathcal{B}(\alpha) = \frac{\alpha^{\frac{1}{\alpha-1}} \alpha^{*\,\frac{1}{\alpha^*-1}}}{4e^2} \quad \text{for } \alpha \neq 1 \quad \text{and} \quad \mathcal{B}(1) = \tfrac{1}{4}, \qquad (9)$$

using the so-called Rényi λ-entropy power

$$N_\lambda = \frac{1}{2\pi e} \exp\left(\frac{2}{d} H_\lambda\right), \qquad (10)$$

where the limiting case $\lambda \to 1$ corresponds to the Shannon entropy power $N = N_1$. BBM showed also that his primary relation (7) using Shannon entropies *does imply* the Heisenberg relation (1). To show this, it suffices to search for the maximizer of $N(\rho)$ under variance constraint $\langle r^2 \rangle$ fixed, which is known to be a Gaussian of covariance matrix $\frac{\langle r^2 \rangle}{d} I$ for which the entropy power is $\frac{\langle r^2 \rangle}{d}$ [38,39]. The same work is then done (separately) for the momentum, i.e., for $N(\gamma)$ subject to $\langle p^2 \rangle$ fixed, to finally achieve

$$\langle r^2 \rangle \langle p^2 \rangle \geqslant d^2 N(\rho) N(\gamma) \geqslant \frac{d^2}{4} \qquad (11)$$

and thus the Heisenberg relation. The Heisenberg inequality is known to be sharp and, fortunately, nothing is lost in this process. 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 simultaneously in the momentum space the maximum entropy is achieved. In other words, the sum of the maximum entropies corresponds to the maximum of the sum here. Simultaneously, the BBM inequality becomes an equality if and only if ρ is Gaussian, and thus the succession of inequalities are equalities.

Note now that the relation (8) with Rényi 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.* [20] then showed that the relation (8) extends for *any* pair (α,β) in $\mathbb{R}_+^2$ such that $\beta \leqslant \alpha^*(\alpha)$, simply noting that N_λ viewed as a function of λ is decreasing (and after decomposing the allowed domain for the parameters into three regions). This leads to

$$N_\alpha(\rho) N_\beta(\gamma) \geqslant \mathcal{Z}(\alpha,\beta), \tag{12}$$

where the bound is

$$\mathcal{Z}(\alpha,\beta) = \begin{cases} 1/e^2 & \text{for } (\alpha,\beta) \in [0;1/2]^2, \\ \mathcal{B}(\max(\alpha,\beta)) & \text{otherwise} \end{cases} \tag{13}$$

with $\mathcal{B}$ defined in Eq. (9).

Note that on the "conjugation curve" $\beta = \alpha^*(\alpha) = \alpha/(2\alpha - 1)$, the bound is sharp and attained if (and only if) ρ is Gaussian, since it is the (only) case of equality in the Babenko-Beckner relation (see Lieb's paper [40]). Finally, let us also mention that Zozor *et al.* [20] showed that for $\beta > \alpha^*$ no uncertainty principle exists, in the sense that the product of Rényi entropy powers is just trivially non-negative. But below the conjugation curve, i.e. for $\beta < \alpha^*$, neither the sharpest bound nor the states that saturate the uncertainty relation are known yet.

III. THE MOMENT-BASED UNCERTAINTY RELATIONS

The uncertainty relations (2) based on the moments $\langle r^a \rangle$ and $\langle p^b \rangle$ were obtained in [28,29,41] by use of two elements: the Shannon-entropy-based BBM relation (7) and the maximizer [41] of the Shannon entropy of the position (momentum) density subject to (s.t.) the constraint $\langle r^a \rangle$ ($\langle p^b \rangle$). Let us remark that such a bound cannot be sharp. If we denote by $\Psi_{\max,a}$ the wave function that gives the maximizer of $N(\rho)$ s.t. $\langle r^a \rangle$ and by $\widetilde{\Psi}_{\max,b}$ the wave function that maximizes $N(\gamma)$ s.t. $\langle p^b \rangle$, then these two functions are not linked by a Fourier transformation, namely $\widetilde{\Psi}_{\max,b} \neq \widehat{\Psi}_{\max,a}$, except for the particular case $a = b = 2$. Or, in other words, the sum of the maximal entropies here is not the maximum of the sum. When deriving the Heisenberg relation from the Bialynicki-Birula relation, although the maximization is made separately on each Shannon entropy, it appears that the square roots of the two maximizers are precisely linked by a Fourier transformation. Without going into detail here, let us consider the example of $\rho_{\max,a} = \arg\max H(\rho)$ s.t. $\langle r^a \rangle$, which is a generalized Gaussian of index a [42,43]. Its square root is thus a generalized Gaussian of index a and its Fourier transform is not a generalized Gaussian (i.e., its square is not the maximizer of the other Shannon entropy): it is linked to an α-stable law of stability index a [44].

In this section, we improve the relations (2) in a similar way but using the Rényi entropy (3), which includes the Shannon entropy as a particular case. Our procedure has the following steps:

(i) Start with the Rényi-entropy-based inequality (12), namely $N_\alpha(\rho) N_\beta(\gamma) \geqslant \mathcal{Z}(\alpha,\beta)$, with the bound $\mathcal{Z}$ defined in Eq. (13).

(ii) Search for the maximum Rényi entropy power $N_\alpha(\rho)$ s.t. $\langle r^a \rangle$. This will give rise to a relation of the form $\langle r^a \rangle^{2/a} \geqslant N_\alpha(\rho) \mathcal{M}(a,\alpha)$, where the bound $\mathcal{M}$ has to be obtained in terms of a and α (see Appendixes A and B).

(iii) Similarly (and separately) for the momentum, one will arrive at the relation $\langle p^b \rangle^{2/b} \geqslant N_\beta(\gamma) \mathcal{M}(b,\beta)$.

(iv) These will lead to $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geqslant N_\alpha(\rho) N_\beta(\gamma) \mathcal{M}(a,\alpha) \mathcal{M}(b,\beta) \geqslant \mathcal{M}(a,\alpha) \mathcal{M}(b,\beta) \mathcal{Z}(\alpha,\beta)$ for every pair $(a,b) \in \mathbb{R}_+^2$.

(v) Finally, the best bound we can find is $\mathcal{C}(a,b) = \max_{\alpha,\beta} \mathcal{M}(a,\alpha) \mathcal{M}(b,\beta) \mathcal{Z}(\alpha,\beta)$, where $\beta \leqslant \alpha^*(\alpha)$ [other restrictions come out that considerably reduce the (α,β) domain for searching the maximum; see Appendix C].

It can be shown (see Appendix C1) that the desired maximum is *on* the conjugation curve $\beta = \alpha^*(\alpha)$, and then $\mathcal{C}(a,b) = \max\limits_{\alpha} \mathcal{M}(a,\alpha) \mathcal{M}(b,\alpha^*) \mathcal{B}(\alpha)$.

As previously mentioned, the bound must be at least the same as the case of Dehesa *et al.* [5], since the latter corresponds to the particular situation $\alpha = \beta = 1$ in our computations.

The main result of the present effort is summarized here (and proved in the appendixes): For any $a \geqslant b > 0$, there exists an uncertainty principle that can be stated in the following way for arbitrary-order moments of the position and momentum observables in d-dimensional systems:

$$\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}} \geqslant \mathcal{C}(a,b) = \max_{\alpha \in D} \mathcal{B}(\alpha) \mathcal{M}(a,\alpha) \mathcal{M}(b,\alpha^*), \tag{14}$$

where $\mathcal{B}(\alpha)$ is defined in Eq. (9), $\alpha^* = \alpha/(2\alpha - 1)$,

$$D = \left(\max\left(\frac{1}{2}, \frac{d}{d+a} \right) ; 1 \right], \tag{15}$$

and the function $\mathcal{M}$ has the form

$$\mathcal{M}(l,\lambda) = \begin{cases} 2\pi e \left(\frac{l}{\Omega B\left(\frac{d}{l}, 1 - \frac{\lambda}{\lambda-1} - \frac{d}{l}\right)} \right)^{\frac{2}{d}} \left(\frac{-d\,(\lambda-1)}{d(\lambda-1)+l\lambda} \right)^{\frac{2}{l}} \left(\frac{l\lambda}{d(\lambda-1)+l\lambda} \right)^{\frac{2}{d(\lambda-1)}}, & 1 - \frac{l}{l+d} < \lambda < 1, \\ 2\pi e \left(\frac{l}{\Omega\, \Gamma\left(\frac{d}{l}\right)} \right)^{\frac{2}{d}} \left(\frac{d}{le} \right)^{\frac{2}{l}}, & \lambda = 1, \\ 2\pi e \left(\frac{l}{\Omega\, B\left(\frac{d}{l}, \frac{\lambda}{\lambda-1}\right)} \right)^{\frac{2}{d}} \left(\frac{d(\lambda-1)}{d(\lambda-1)+l\lambda} \right)^{\frac{2}{l}} \left(\frac{l\lambda}{d(\lambda-1)+l\lambda} \right)^{\frac{2}{d(\lambda-1)}}, & \lambda > 1, \end{cases} \tag{16}$$

with $\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ and $B(x,y)$ the beta function.

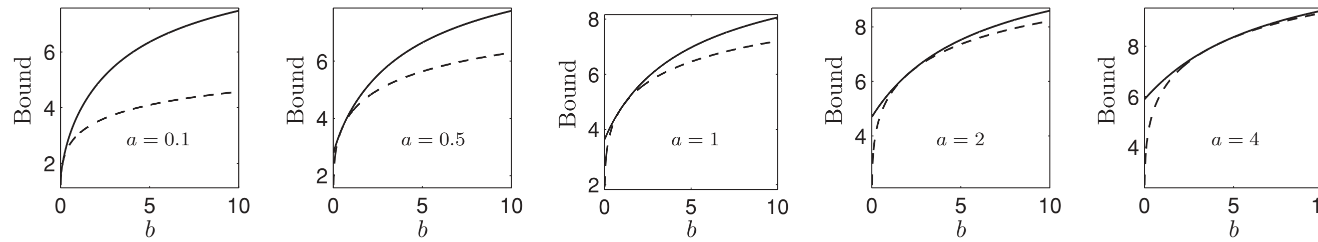

FIG. 1. Bound $\mathcal{C}(a,b)$ (solid line) given in (14) compared to $\mathcal{D}(a,b)$ in (2) (dashed line), vs b, for given $a = 0.1, 0.5, 1, 2,$ and 4, respectively, with $d = 5$. For each value of a, the new bound $\mathcal{C}$ is always above $\mathcal{D}$; both functions coincide when $b = a$.

Let us denote by $\alpha_{\rm opt}(a,b)$ the index that maximize $\mathcal{C}(a,b)$, i.e.

$$\alpha_{\rm opt}(a,b) = \arg\max_{\alpha\in D} \mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*). \tag{17}$$

The case $b \geqslant a > 0$ can be treated using the symmetry (proved in the Appendixes)

$$\alpha_{\rm opt}(b,a) = [\alpha_{\rm opt}(a,b)]^* \tag{18}$$

and then

$$\mathcal{C}(b,a) = \mathcal{C}(a,b). \tag{19}$$

The symmetry on $\alpha_{\rm opt}$ allows us also to conclude that $\alpha_{\rm opt}(a,a) = 1$ and thus the optimal bound from our approach coincides with that of Angulo, given in (2). Unfortunately, except for the case $a = b$, we have not been able yet to obtain an analytical expression for $\mathcal{C}(a,b)$.

Figure 1 depicts the bound $\mathcal{C}(a,b)$ for given values of a as a function of b compared to the bound $\mathcal{D}(a,b)$. From the figure, we see that the bound is substantially improved when $b \neq a$, especially as b departs considerably from a.

Figure 2 depicts the optimal $\alpha = \alpha_{\rm opt}$ as a function of b in the same configurations as in Fig. 1. The curves illustrate that only for $a = b$ is the optimal bound obtained for $\alpha_{\rm opt} = 1$. For $a \neq b$, a finer study of $\mathcal{M}$ could allow us to even reduce the domain D where $\alpha_{\rm opt}$ lies.

IV. APPLICATION TO CENTRAL POTENTIAL PROBLEMS

Let us now apply and discuss the minimal uncertainty bound (14) for the two main prototypes of d-dimensional physics: hydrogenic and oscillator-like systems. But first, let us give a brief review on eigensolutions for quantum systems in central potentials.

A. Eigensolutions for central potentials: A brief review

In both hydrogenic and oscillator cases, the quantum systems are described by the physical solutions of the Schrödinger equation,

$$\left[-\tfrac{1}{2}\nabla^2 + V(r)\right]\Psi = E\,\Psi, \tag{20}$$

where $V(r)$ is a radial potential and where, without loss of generality, the mass is set to unity. It is well known [45] that the wave functions of a Hamiltonian with central potential can be separated out into a radial, $R_{E,l}(r)$, and an angular, $\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})$, part as

$$\Psi_{E,\{\mu\}}(\mathbf{x}) = R_{E,l}(r)\mathcal{Y}_{\{\mu\}}(\Omega_{d-1}). \tag{21}$$

The position $\mathbf{x} = (x_1,\ldots,x_d)$ is given in hyperspherical coordinates as $(r,\theta_1,\theta_2,\ldots,\theta_{d-1}) \equiv (r,\Omega_{d-1})$, where naturally $\|\mathbf{x}\| = r = \sqrt{\sum_{i=1}^d x_i^2} \in [0\,;+\infty)$ and $x_i = r(\prod_{k=1}^{i-1}\sin\theta_k)\cos\theta_i$ for $1 \leqslant i \leqslant d$ and with $\theta_i \in [0\,;\pi), i < d-1$, $\theta_{d-1} \in [0\,;2\pi)$. By convention, $\theta_d = 0$ and the empty product is the unity. The angular part, common to any central potential, is given by the hyperspherical harmonics [45,46] $\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})$, which are known to satisfy the eigenvalue equation

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

associated with the generalized angular momentum operator given by

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

The angular quantum numbers $\{\mu\} = \{\mu_1 \equiv l, \mu_2, \ldots, \mu_{d-1} \equiv m\}$ characterize the hyperspherical harmonics and satisfy the chain of inequalities $l \equiv \mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{d-2} \geqslant |\mu_{d-1}| \equiv |m|$.

The radial part $R_{E,l}(r)$ fulfills the second-order differential equation

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{d-1}{2r}\frac{\mathrm{d}}{\mathrm{d}r} + \frac{l(l+d-2)}{2r^2} + V(r)\right]R_{E,l}(r) = E\,R_{E,l}(r),$$

which only depends on the eigenenergy E, the dimensionality d, and the largest angular quantum number $l = \mu_1$.

Then, the quantum-mechanical position probability density for central systems is given by

$$\rho_{E,\{\mu\}}(\mathbf{x}) = |\Psi_{E,\{\mu\}}(\mathbf{x})|^2 = |R_{E,l}(r)|^2\,|\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})|^2. \tag{22}$$

It is worth remarking that this density function is normalized to unity. Let us note here that

$$\int_0^{+\infty} r^{d-1}|R_{E,l}(r)|^2\,dr = 1$$

and

$$\int_{[0;\pi)^{d-2}\times[0:2\pi)} |\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})|^2\,d\Omega_{d-1} = 1,$$

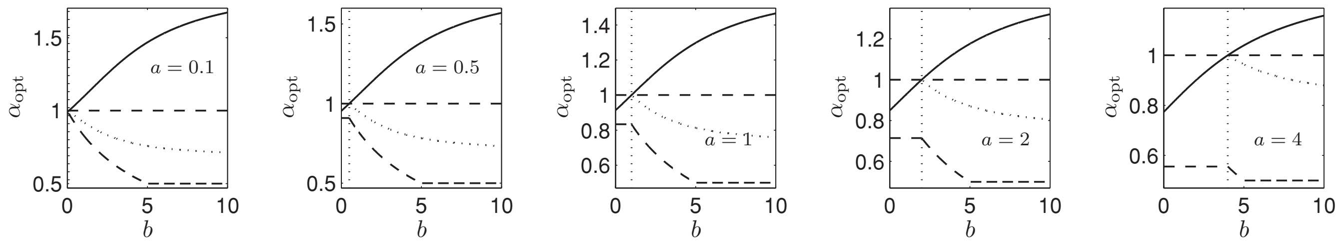

FIG. 2. $\alpha_{\rm opt}(a,b)$ (solid line) given in (17), vs b, for given $a = 0.1, 0.5, 1, 2$, and 4, respectively, with $d = 5$. The dotted vertical line indicates $b = a$. Thus, left to this line, $a \geqslant b > 0$ and $\alpha_{\rm opt}$ has to be searched in D, Eq. (15). This domain is indicated by the dashed lines. At the opposite, to the right of the vertical dotted line, $b > a$. Thus, symmetry Eq. (18) is used and $\alpha_{\rm opt}(b,a) = [\alpha_{\rm opt}(a,b)]^*$ is sought. Since $b > a > 0$, this parameter is also in domain D, Eq. (15) (where b replaces a); the dotted curve represents $\alpha_{\rm opt}(b,a)$ [the solid curve being $\alpha_{\rm opt}(a,b)$] and domain D is still represented by the dashed lines.

and that the volume element can be expressed in hyperspherical coordinates as

$$d\mathbf{x} = r^{d-1}\,dr\,d\Omega_{d-1} = r^{d-1}\,dr\left(\prod_{j=1}^{d-2}(\sin\theta_j)^{d-j-1}\,d\theta_j\right)d\theta_{d-1}.$$

Thus, the moment $\langle r^a\rangle$ for the d-dimensional density $\rho_{E,\{\mu\}}(\mathbf{x})$ has the expression

$$\langle r^a\rangle = \int_0^{+\infty} r^{d+a-1}|R_{E,l}(r)|^2\,dr, \tag{23}$$

which is only characterized by the position radial wave function $R_{E,l}(r)$ of the particle.

From the Fourier transform of $\Psi_{E,\{\mu\}}$, it is revealed that in the momentum domain the wave function $\widehat{\Psi}_{E,\{\mu\}}$ also separates under the form

$$\widehat{\Psi}_{E,\{\mu\}}(\mathbf{p}) = M_{E,l}(p)\,\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})$$

(see, e.g., [36,46,47]) with the same hyperspherical part, and the radial part is expressed from $R_{E,l}$ through the Hankel transform (e.g., [48,49]),

$$M_{E,l}(p) = p^{1-\frac{d}{2}}\int_0^{+\infty} r^{\frac{d}{2}}R_{E,l}(r)J_{l+\frac{d}{2}-1}(pr)\,dr \tag{24}$$

(J_ν is the Bessel function of the first kind and of order ν). Immediately, in the momentum space, the moment $\langle p^b\rangle$ has the expression

$$\langle p^b\rangle = \int_0^{+\infty} p^{d+b-1}|M_{E,l}(p)|^2\,dp, \tag{25}$$

which is only characterized by the momentum radial wave function $M_{E,l}(p)$ of the particle.

These expressions have allowed to find numerous information-theoretic properties [24,25,36,45,50,51] of general central potentials, particularly the Heisenberg [25] and Fisher-information [24,25] uncertainty relations, as recently reviewed [5].

B. Application to d-dimensional hydrogenic systems

Let us now examine the accuracy of the moments-based uncertainty relations (14) for the main prototype of d-dimensional systems, namely the hydrogenic atom. This system has been recently investigated in Ref. [36] in full detail from the information theory point of view. In this case, the potential has the form $V(r) = -\frac{1}{r}$ (without loss of generality, the atomic number is taken to be 1) and the energies are

$$E = -\frac{1}{2\eta^2}, \quad \eta = n + \frac{d-3}{2}, \quad n = 1,2,\ldots,$$

where η denotes the grand principal quantum number. The radial part of the eigenfunctions is completely calculable [36,50,51]. The radial wave function in position domain is expressed as

$$R_{E,l}(r) = \left(\frac{\eta}{2}\right)^{-\frac{d}{2}}\sqrt{\frac{\Gamma(\eta-L)}{2\eta\Gamma(\eta+L+1)}}\;\tilde{r}^{L-\frac{d-3}{2}} \times \exp\left(-\frac{\tilde{r}}{2}\right)\mathcal{L}_{\eta-L-1}^{2L+1}(\tilde{r}), \tag{26}$$

where $L = l + \frac{d-3}{2}$, $l = 0,\ldots,n-1$ is the grand orbital quantum number, $\tilde{r} = \frac{2r}{\eta}$ is a reduced (dimensionless) position, and $\mathcal{L}_p^q$ are the Laguerre polynomials. As is shown in Refs. [36,50,51], after the Hankel transform (24), the radial wave function in the momentum domain is expressed as

$$M_{E,l}(p) = 2^{2L+3}\sqrt{\frac{\Gamma(\eta-L)}{2\pi\Gamma(\eta+L+1)}}\,\Gamma(L+1)\,\eta^{\frac{d+1}{2}} \times \frac{\tilde{p}^l}{(1+\tilde{p}^2)^{L+2}}\;\mathcal{G}_{\eta-L-1}^{L+1}\left(\frac{1-\tilde{p}^2}{1+\tilde{p}^2}\right),$$

where $\tilde{p} = \eta p$ is the reduced (dimensionless) momentum and $\mathcal{G}_p^q$ are the Gegenbauer polynomials. From these expressions together with (23) and (25), it is shown [36] that the position and momentum moments of arbitrary orders, corresponding to a given eigenstate characterized by an energy E and an angular quantum number l (or equivalently by η and L), have the expressions

$$\langle r^a\rangle = \frac{\eta^{a-1}\Gamma(2L+a+3)}{2^{a+1}\Gamma(2L+2)} \times {}_3F_2(-\eta+L+1, -a-1, a+2\,;2L+2,\,1\,;1) \tag{27}$$

and

$$\langle p^b\rangle = \frac{4\,\Gamma(\eta+L+1)\,\Gamma\left(L+\frac{b+3}{2}\right)\,\Gamma\left(L+\frac{5-b}{2}\right)}{\eta^{b-1}\,\Gamma(\eta-L)\,\Gamma^2\left(L+\frac{3}{2}\right)\,\Gamma(2L+4)} \times {}_5F_4\left(L-\eta+1\,,\,L+\eta+1\,,\,L+1\,,\,L+\frac{b+3}{2}\,,\,L+\frac{5-b}{2}\,;\,2L+2\,,\,L+\frac{3}{2}\,,\,L+2\,,\,L+\frac{5}{2}\,;\,1\right) \tag{28}$$

for $b < 2L+5$, where ${}_pF_q$ are the generalized hypergeometric functions (see, e.g., [52], Sec. 2.19.14, Eq. (15) and reflective properties of hypergeometric functions). Note that the momentum wave function is not exponentially decreasing. The direct consequence is that not all moments exist in the momentum domain, which is reflected in the restriction for the values of b.

Thus, the uncertainty product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ can be computed and therefore studied analytically for hydrogenic systems in d dimensions. As an illustration, Fig. 3 depicts the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ computed from (27) and (28) for $(a,b)=(1,2)$ and Fig. 4 plots the case $(a,b)=(1,4)$ (both for $d=3$) when the system is in the state (E,l), together with the corresponding bound $\mathcal{C}(a,b)$ given in (14)–(16).

We can see from both figures that, although not sharp, the bound $\mathcal{C}(a,b)$ 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 pairs (a,b) regardless of the dimensionality d. Since hydrogenic systems belong to the family of radial potential systems, this suggests that a 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 [24,25]. To give a further illustration, Fig. 5 depicts $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ as a function of b for fixed a, and for the ground state ($n=1$, $l=0$) in three dimensions. In all the cases shown, we observe the existence of a value of b that is "optimum" in the sense that the uncertainty product is close to the bound proposed here, corresponding to a situation of low generalized uncertainty. As b increases (up to $2L+5=5$ for the ground state in three dimensions), the uncertainty departs from our bound. Finally, one observes for the tested values of a that the lower bound has a concave behavior versus b, while the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ exhibits a convex behavior. This suggests the existence of an optimal value of b (function of a) in terms of low discrepancy from the bound.

C. Application to d-dimensional oscillator-like systems

Let us consider now a potential of the form $V(r)=\frac{1}{2}r^2$ (without loss of generality, the product mass squared pulsation is taken as unity). In this case, the energies are

$$E = 2n + l + \frac{d}{2}, \quad n = 0,1,\ldots \quad \text{and} \quad l = 0,1,\ldots$$

and the radial parts of the wave functions are again known [53]. They are expressed as

$$R_{E,l}(r) = \sqrt{\frac{2\Gamma(n+1)}{\Gamma(n+l+d/2)}}\; r^l\; \exp\left(-\frac{r^2}{2}\right)\, \mathcal{L}_n^{l+d/2-1}(r^2) \tag{29}$$

and $M_{E,l}(p) = R_{E,l}(p)$. Comparing (29) with (26), after a change of variables $\tilde r = r^2$, one can easily show from (27) that the statistical moments read

$$\langle r^a\rangle = \frac{\Gamma\left(l+\frac{d+a}{2}\right)}{\Gamma\left(l+\frac{d}{2}\right)}\,{}_3F_2\left(-n,-\frac{a}{2},\frac{a}{2}+1\,;\,L+\frac{d}{2},1\,;\,1\right)$$

and (30)

$$\langle p^b\rangle = \frac{\Gamma\left(l+\frac{d+b}{2}\right)}{\Gamma\left(l+\frac{d}{2}\right)}\,{}_3F_2\left(-n,-\frac{b}{2},\frac{b}{2}+1\,;\,L+\frac{d}{2},1\,;\,1\right)$$

(see also Ref. [54] for special cases).

Figure 6 describes the moments product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ using (30) for $(a,b)=(1,2)$, and Fig. 7 exhibits the case $(a,b)=(1,4)$ (both for $d=3$) together with the corresponding bound $\mathcal{C}(a,b)$ given in (14)–(16).

We can see from these figures also that even if not sharp, the bound $\mathcal{C}(a,b)$ is very close to the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ for the ground state ($n=0$ and $l=0$). The global behavior is similar to what happens for the hydrogenic systems: there is a discrepancy from the bound as n increases. But here,

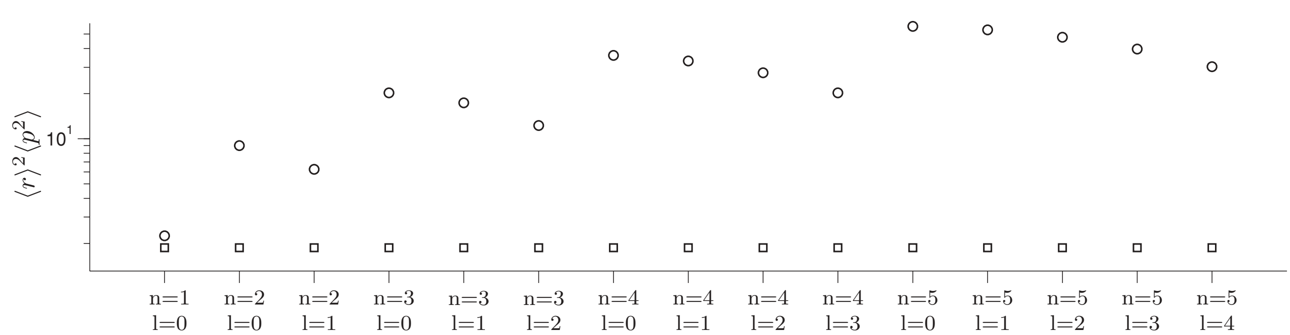

FIG. 3. Product $\langle r\rangle^2\langle p^2\rangle$, i.e., $(a,b)=(1,2)$ in Eqs. (27), (28) (circles) for the lowest-energy states and lower bound $\mathcal{C}(1,2)$, Eqs. (14)–(16), of this product (squares), for three-dimensional hydrogenic systems ($d=3$).

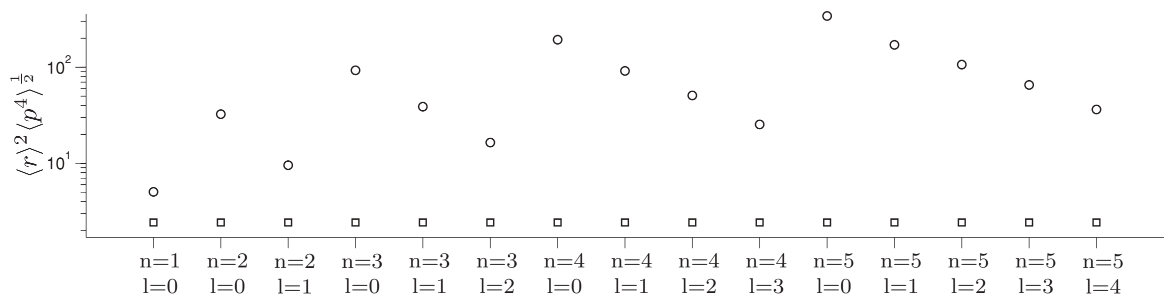

FIG. 4. Product $\langle r\rangle^2\langle p^4\rangle^{\frac{1}{2}}$, i.e., $(a,b) = (1,4)$ in Eqs. (27), (28) (circles) for the lowest-energy states and lower bound $\mathcal{C}(1,4)$, Eqs. (14)–(16), of this product (squares), for three-dimensional hydrogenic systems ($d = 3$).

the discrepancy increases also with l when n is fixed. The same behavior occurs for other pairs (a,b) and whatever the dimension d. In fact, when observing more finely $\langle r\rangle^2\langle p^2\rangle$ and $\langle r\rangle^2\langle p^4\rangle^{\frac{1}{2}}$, it appears that these products depend essentially on the energy level, i.e., the values of these products for a fixed value of $2n + l$ are very close (see, e.g., $n = 0, l = 2$ or $n = 1$, $l = 0$). This was true also for the hydrogenic systems, but it is more strongly pronounced for the harmonic oscillator. All these observations reinforce our "conjecture" that refinement can be found in the context of radial systems, for moments' orders other than $a = b = 2$, at least in terms of energy levels.

A further illustration is given by Fig. 8, where $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ versus b is depicted, for different fixed values of a in the case of the ground state ($n = 0$, $l = 0$).

Globally, the behavior of the moments' product compared to the bound observed here is similar to that of the hydrogenic systems. However, the discrepancy from the bound is less pronounced for the harmonic oscillator (in the ground state) than for the hydrogen systems. Note that the bound is achieved in the case in which $a = b = 2$. This case corresponds to the classical variance-based Heisenberg inequality. Moreover, the ground state of the oscillator leads to the Gaussian probability density function ρ (and γ): in this case, the variance-based Heisenberg inequality is saturated. One can again observe the convexity of the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ (in fact almost linear): together with the observed concavity of the lower bound, this reinforces our conjecture on the existence of an optimal value of $b(a)$ in terms of low discrepancy from the bound. This remains to be studied more systematically and more deeply.

V. DISCUSSION AND CONCLUSIONS

In this paper, we have proposed an improved version of the moment-based mathematical formulation of the position-momentum uncertainty principle for quantum systems that generalizes the seminal variance-based formulation of Heisenberg. The main result of this contribution is formalized in Eq. (14) together with Eqs. (9), (15), and (16): $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}} \geqslant \mathcal{C}(a,b)$. In contrast to the entropic uncertainty relations [like Eq. (12)], the present formulation is based on spreading measures that describe physical observables. The present approach suffers, however, from the fact that the lower bound $\mathcal{C}(a,b)$ found here for the product of the position and momentum moments for arbitrary a and b is not sharp. To tackle this issue, a variational approach may be envisaged, although it is a difficult task. Another alternative might be to employ appropriate Sobolev-like inequalities, as done for entropic formulations (see, e.g., Ref. [17–19,21]).

Our moment-based uncertainty relation is physico-computationally analyzed in some d-dimensional quantum systems. More specifically, the bound of the moment-based uncertainty relation is compared to the product of the moments for hydrogenic and oscillator-like systems. In both cases, analytic expressions of the moments exist in terms of hypergeometric functions [Eqs. (27), (28) and (30), respectively]. Our results suggest that the improvement of this relation for general central potentials seems possible regardless of the orders a and b of the moments, at least in terms of energy levels. Such an improvement exists in the variance-based context $a = b = 2$ [24,25], but for moments of arbitrary order this issue is a fully open problem that deserves to be variationally solved for both fundamental and applied reasons. This suggests

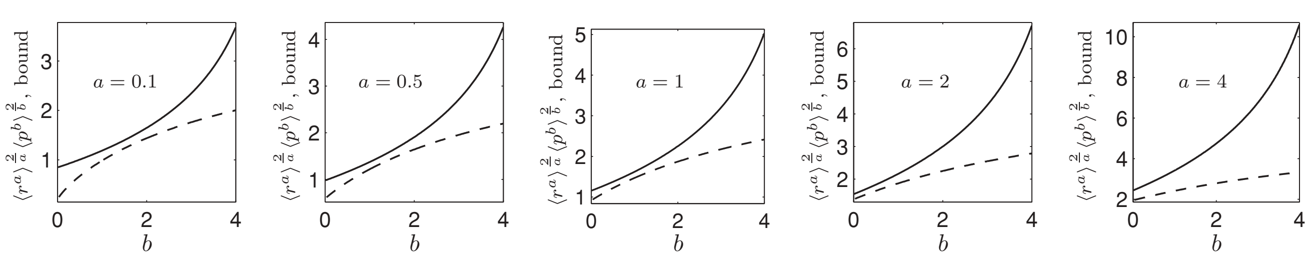

FIG. 5. Product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ (solid lines) in the ground state ($n = 1, l = 0$), for fixed $a = 0.1$, 0.5, 1, 2, and 4, respectively, and lower bound (dashed lines) for three-dimensional hydrogenic systems ($d = 3$).

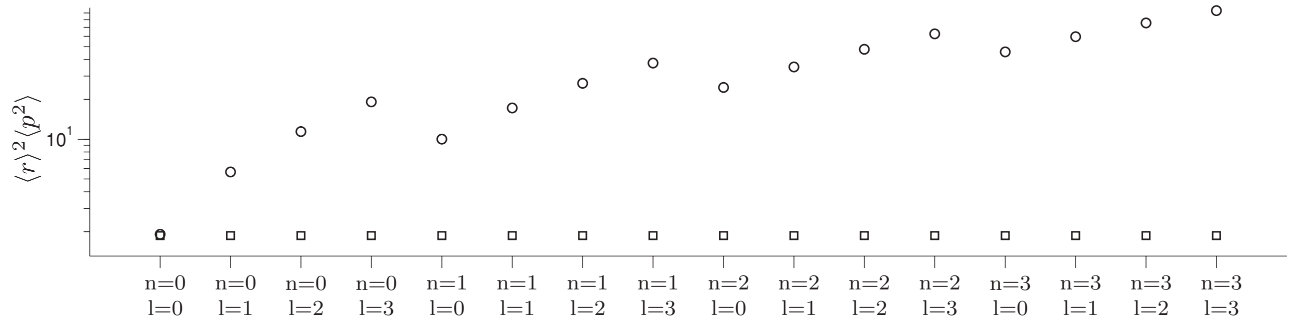

FIG. 6. Product $\langle r\rangle^2\langle p^2\rangle$, i.e., $(a,b) = (1,2)$ in Eqs. (30) (circles) for the lowest-energy states and lower bound $\mathcal{C}(1,2)$, Eqs. (14)–(16), of this product (squares) for three-dimensional harmonic oscillators ($d = 3$).

also that the product $\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}}$ can be envisaged as a useful tool to quantify the complexity and organization of various physical systems. However, the properties of such a complexity measure should be analyzed in more detail.

ACKNOWLEDGMENTS

S.Z. and M.P. are grateful to the CNRS (France) and CONICET (Argentina) for the cooperation grant that partially enabled this work. M.P. also acknowledges financial support by CONICET and ANPCyT. P.S.-M. and J.S.D. are very grateful to Junta de Andalucía (Spain) for the grants FQM-2445 and FQM-4643, and the Ministerio de Ciencia e Innovación (Spain) for the grant FIS2008-02380.

APPENDIX A: EVALUATION OF THE MAXIMIZERS OF THE RÉNYI ENTROPY POWER UNDER MOMENT CONSTRAINT

In Sec. III [steps (ii) and (iii)], we established the necessity of searching for the maximum of the Rényi entropy power $N_\alpha(\rho)$ subjected to given moment $\langle r^a\rangle$ and $N_\beta(\gamma)$ s.t. $\langle p^b\rangle$. This variational problem has been tackled and partially solved by Dehesa *et al.* [55]. Similar to what is done for variance constraint, the problem is to maximize the frequency entropic moment of order $\lambda > 0$, an increasing function of the entropy power, $\int_{\mathbb{R}^d} f(\mathbf{x})^\lambda d\mathbf{x}$ s.t. $\int_{\mathbb{R}^d} f(\mathbf{x})d\mathbf{x} = 1$ and $\int_{\mathbb{R}^d} \|\mathbf{x}\|^l f(\mathbf{x})d\mathbf{x} = \langle r^l\rangle$, with $l > 0$ and where $\|\mathbf{x}\| = r$ is the Euclidean norm of $\mathbf{x}$. Note that we work here with the variables $\mathbf{x}$ and r, but the results obtained will be valid in the momentum domain, changing $\mathbf{x}$ to $\mathbf{p}$ and r to p. Then, we have to maximize $\int_{\mathbb{R}^d}[f(\mathbf{x})^\lambda - \mu f(\mathbf{x}) - \nu\|\mathbf{x}\|^l f(\mathbf{x})]d\mathbf{x}$, where μ and ν are the Lagrange factors. From the corresponding Euler-Lagrange equation, one obtains that f must be of the form $f(\mathbf{x}) = (\frac{\mu+\nu\|\mathbf{x}\|^l}{\lambda})_+^{\frac{1}{\lambda-1}}$, where $(y)_+ = \max(y,0)$. With integrability arguments (f must be a probability density function (pdf) and thus positive and integrable), $\mu > 0$ and ν must have the sign of $1-\lambda$, and thus the pdf that maximizes the entropy power N_λ s.t. $\langle r^l\rangle$ can be recast under the form

$$f_{\lambda,l}(\mathbf{x}) = C[1-(\lambda-1)(\|\mathbf{x}\|/\delta)^l]_+^{\frac{1}{\lambda-1}}. \tag{A1}$$

This pdf is sometimes called a generalized Gaussian [56,57], but this terminology is not adequate. Indeed, when $\lambda \to 1$, this pdf tends to $f_{1,l}(\mathbf{x}) = C\exp(-\|\mathbf{x}/\delta\|^l)$, which is also sometimes called a generalized Gaussian (or also Kotz-type) [43,58,59] (and also sometimes a stretched exponential or a power exponential [59,60]). Furthermore, when $l = 2$, one can recognize in (A1) the well known q-Gaussian (also known as Student-t or Student-r depending on the sign of $1-\lambda$), where $q = 2-\lambda$ and thus the generalization (A1) is known under the terminology of *stretched q-exponential* [55,61] or even *generalized q-Gaussian of parameter* $q = 2-\lambda$ and (stretching) parameter l.

Constants C and δ are to be determined so that the constraints are satisfied. The normalization constraint reads

$$\begin{aligned} 1 &= C\int_{\mathbb{R}^d}\left[1-(\lambda-1)(\|\mathbf{x}\|/\delta)^l\right]_+^{\frac{1}{\lambda-1}}\,d\mathbf{x} \\ &= C\,\Omega\int_0^{+\infty} r^{d-1}\left[1-(\lambda-1)(r/\delta)^l\right]_+^{\frac{1}{\lambda-1}}\,dr \\ &= \frac{C\,\Omega\delta^d}{l|\lambda-1|^{d/l}}\int_0^{+\infty} t^{d/l-1}\left[1-\operatorname{sgn}(\lambda-1)\,t\right]_+^{\frac{1}{\lambda-1}}\,dt, \end{aligned}$$

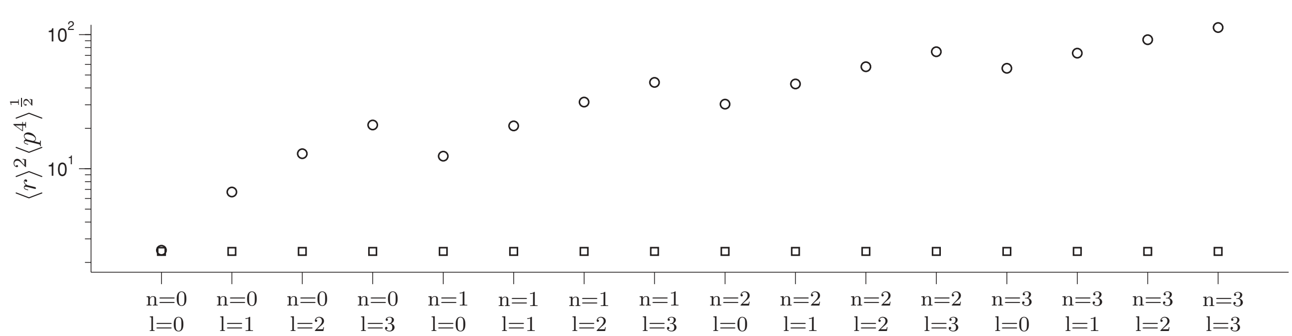

FIG. 7. Product $\langle r\rangle^2\langle p^4\rangle^{\frac{1}{2}}$, i.e., $(a,b) = (1,4)$ in Eqs. (30) (circles) for the lowest-energy states and lower bound $\mathcal{C}(1,4)$, Eqs. (14)–(16), of this product (squares) for three-dimensional harmonic oscillators ($d = 3$).

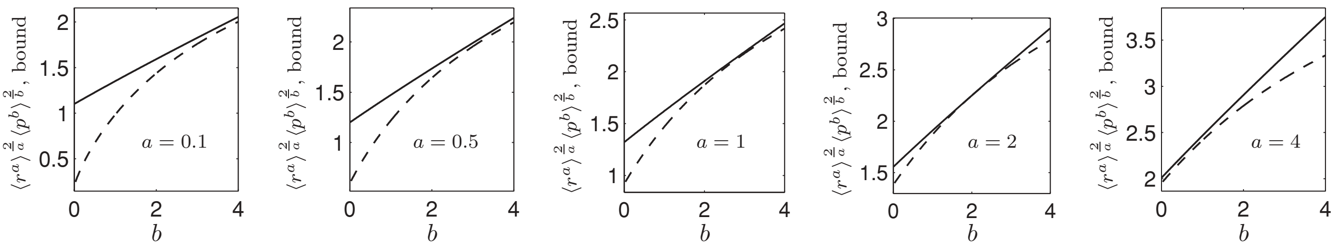

FIG. 8. Product $\langle r^a \rangle^{\frac{2}{a}} \langle p^b \rangle^{\frac{2}{b}}$ (solid lines) in the ground state ($n = 0, l = 0$), for fixed $a = 0.1, 0.5, 1, 2,$ and 4, respectively, and lower bound (dashed lines) for three-dimensional oscillators ($d = 3$).

where the second line comes from [62], Eq. 4.642, with $\Omega = \frac{2\pi^{d/2}}{\Gamma(d/2)}$, which is the surface of the d-dimensional unit sphere and where the third line comes from the change of variable $r = \delta(t/|1-\lambda|)^{1/l}$. The integral term, which we will denote $B_1(l,\lambda)$, is expressed via the beta function $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$, from [62], Eqs. 8.380-1 and 8.380-3, and one finally obtains

$$1 = \frac{C\,\Omega\delta^d}{l\,|\lambda-1|^{d/l}} B_1(l,\lambda), \tag{A2}$$

where

$$B_1(l,\lambda) = \begin{cases} B\left(\frac{d}{l}\,,\,\frac{\lambda}{\lambda-1}\right) & \text{if } \lambda > 1, \\ B\left(\frac{d}{l}\,,\,1+\frac{\lambda}{1-\lambda}-\frac{d}{l}\right) & \text{if } 1-\frac{l}{d} < \lambda < 1. \end{cases} \tag{A3}$$

Indeed, the integral converges provided that $\lambda > 1 - l/d$.

In the same vein, the power moment constraint reads

$$\begin{aligned} \langle r^l \rangle &= C \int_{\mathbb{R}^d} \|\mathbf{x}\|^l [1-(\lambda-1)(\|\mathbf{x}\|/\delta)^l]_+^{\frac{1}{\lambda-1}}\, d\mathbf{x} \\ &= C\,\Omega \int_0^{+\infty} r^{l+d-1}[1-(\lambda-1)(r/\delta)^l]_+^{\frac{1}{\lambda-1}}\, dr \\ &= \frac{C\,\Omega\delta^{l+d}}{l|\lambda-1|^{d/l+1}} \int_0^{+\infty} t^{d/l}[1-\operatorname{sgn}(\lambda-1)\,t]_+^{\frac{1}{\lambda-1}}\, dt, \end{aligned}$$

where the integral term, denoted $B_m(l,\lambda)$, is expressed via the beta function from [62], Eqs. 8.380-1 and 8.380-3, leading to

$$\langle r^l \rangle = \frac{C\,\Omega\delta^{l+d}}{l|\lambda-1|^{d/l+1}} B_m(l,\lambda), \tag{A4}$$

where

$$B_m(l,\lambda) = \begin{cases} B\left(\frac{d}{l}+1\,,\,\frac{\lambda}{\lambda-1}\right) & \text{if } \lambda > 1, \\ B\left(\frac{d}{l}+1\,,\,\frac{\lambda}{1-\lambda}-\frac{d}{l}\right) & \text{if } 1-\frac{l}{d+l} < \lambda < 1. \end{cases} \tag{A5}$$

Note that the existence of the latter integral implies a stronger restriction to λ than the one coming from the normalization. That is, we require now

$$\lambda > 1 - \frac{l}{d+l} = \frac{d}{d+l}. \tag{A6}$$

In both constraints, the case $\lambda = 1$ can be recovered by letting $\lambda \to 1^+$ or $\lambda \to 1^-$ from [63], Eq. 6.1.47 or [62], Eq. 8.328-1, $\lim_{y\to\infty} B(x,y)x^y = \Gamma(x)$]: it is not necessary to treat this case separately.

APPENDIX B: MAXIMAL ENTROPY POWER N_λ AND BOUND FOR THE MOMENT $\langle r^l \rangle$

Following the procedure proposed in Sec. III, we discuss here the bounds for the moments $\langle r^a \rangle$ and $\langle p^b \rangle$. From (A1), the maximal λ-norm of $f_{\lambda,l}(\mathbf{x})$ to the power λ takes the form

$$\begin{aligned} \|f_{\lambda,l}\|_\lambda^\lambda &= C^\lambda \int_{\mathbb{R}^d} [1-(\lambda-1)(\|\mathbf{x}\|/\delta)^l]_+^{\frac{\lambda}{\lambda-1}}\, d\mathbf{x} \\ &= C^\lambda\,\Omega \int_0^{+\infty} r^{d-1}[1-(\lambda-1)(r/\delta)^l]_+^{\frac{\lambda}{\lambda-1}}\, dr \\ &= \frac{C^\lambda\,\Omega\delta^d}{l|\lambda-1|^{d/l}} \int_0^{+\infty} t^{d/l-1}[1-\operatorname{sgn}(\lambda-1)\,t]_+^{\frac{\lambda}{\lambda-1}}\, dt. \end{aligned}$$

Then, from [62], Eqs. 8.380-1 and 8.380-3 we obtain

$$\|f_{\lambda,l}\|_\lambda^\lambda = \frac{C^\lambda\,\Omega\delta^d}{l|\lambda-1|^{d/l}} B_h(l,\lambda), \tag{B1}$$

where we have defined

$$B_h(l,\lambda) = \begin{cases} B\left(\frac{d}{l}\,,\,\frac{\lambda}{\lambda-1}+1\right) & \text{if } \lambda > 1, \\ B\left(\frac{d}{l}\,,\,\frac{\lambda}{1-\lambda}-\frac{d}{l}\right) & \text{if } 1-\frac{l}{d+l} < \lambda < 1, \end{cases} \tag{B2}$$

which adds no new restriction on λ. Thus, the maximal value of the Rényi entropy power is

$$\begin{aligned} N_\lambda(f_{\lambda,l}) &= \frac{1}{2\pi e}\left(\|f\|_\lambda^{\frac{\lambda}{1-\lambda}}\right)^{\frac{2}{d}} \\ &= \frac{1}{2\pi e}\left[C^{\frac{\lambda}{1-\lambda}}\left(\frac{\Omega\delta^d}{l|\lambda-1|^{d/l}}\right)^{\frac{1}{1-\lambda}} B_h^{\frac{1}{1-\lambda}}\right]^{\frac{2}{d}} \\ &= \frac{1}{2\pi e}\left[C^{-1}\left(\frac{C\Omega\delta^d}{l|\lambda-1|^{d/l}}B_1\right)^{\frac{1}{1-\lambda}}\left(\frac{B_h}{B_1}\right)^{\frac{1}{1-\lambda}}\right]^{\frac{2}{d}} \\ &= \frac{1}{2\pi e}\left[C^{-1}\left(\frac{B_h}{B_1}\right)^{\frac{1}{1-\lambda}}\right]^{\frac{2}{d}} \end{aligned}$$

from (A2) and where the arguments of B_1 and B_h are omitted for simplicity. Taking the ratio $\frac{\langle r^l \rangle^{d/l}}{1^{d/l+1}}$ from (A2) and (A4), one obtains

$$C^{-1} = \frac{\Omega}{l} B_1 \left(\frac{B_1}{B_m}\right)^{d/l} \langle r^l \rangle^{d/l},$$

which gives

$$N_\lambda(f_{\lambda,l}) = \frac{1}{2\pi e}\left[\frac{\Omega B_1}{l}\left(\frac{B_1}{B_m}\right)^{d/l}\left(\frac{B_h}{B_1}\right)^{\frac{1}{1-\lambda}}\langle r^l\rangle^{d/l}\right]^{\frac{2}{d}}.$$

One can simplify this expression a bit by considering the parameter

$$\mu = \mu(\lambda) = \frac{\lambda}{\lambda - 1} \tag{B3}$$

that governs the maximal entropy power, with $\mu > 1$ or $\mu < -d/l$. Noting that

$$\frac{B_1}{B_m} = \mathrm{sgn}(\mu)\frac{d + l\mu}{d} \quad \text{and} \quad \frac{B_h}{B_1} = \frac{l\mu}{d + l\mu} \tag{B4}$$

so that

$$N_\lambda(f_{\lambda,l}) = \frac{1}{2\pi e}\left[\frac{\Omega B_1(l,\lambda)}{l}\left(\frac{d + l\mu}{\mathrm{sgn}(\mu)\, d}\right)^{\frac{d}{l}} \times \left(\frac{d + l\mu}{l\mu}\right)^{\mu-1}\langle r^l\rangle^{d/l}\right]^{\frac{2}{d}}. \tag{B5}$$

We finally obtain that the Rényi entropy power of any pdf ρ, $N_\lambda(\rho) = \frac{1}{2\pi e}(\|\rho\|_\lambda^{\frac{\lambda}{1-\lambda}})^{\frac{2}{d}}$, s.t. fixed $\langle r^l\rangle$, is bounded from above by the maximum value $N_\lambda(f_{\lambda,l})$. Therefore, we can write

$$\langle r^l\rangle^{2/l} \geqslant N_\lambda(\rho)\mathcal{M}(l,\lambda), \tag{B6}$$

where the function $\mathcal{M}$ is expressed as

$$\mathcal{M}(l,\lambda) = \begin{cases} 2\pi e\left(\frac{l}{\Omega\, B(\frac{d}{l},\mu)}\right)^{\frac{2}{d}}\left(\frac{d}{d+l\mu}\right)^{\frac{2}{l}}\left(\frac{l\mu}{d+l\mu}\right)^{\frac{2(\mu-1)}{d}} & \text{if } \lambda > 1, \\ 2\pi e\left(\frac{l}{\Omega\,\Gamma(\frac{d}{l})}\right)^{\frac{2}{d}}\left(\frac{d}{le}\right)^{\frac{2}{l}} & \text{if } \lambda = 1, \\ 2\pi e\left(\frac{l}{\Omega\, B(\frac{d}{l},1-\mu-\frac{d}{l})}\right)^{\frac{2}{d}}\left(-\frac{d}{d+l\mu}\right)^{\frac{2}{l}}\left(\frac{l\mu}{d+l\mu}\right)^{\frac{2(\mu-1)}{d}} & \text{if } 1 - \frac{l}{l+d} < \lambda < 1, \end{cases} \tag{B7}$$

with

$$\mu = \frac{\lambda}{\lambda - 1} \tag{B8}$$

and where $\mathcal{M}(l,1) = \lim_{\lambda\to1}\mathcal{M}(l,\lambda)$ from the first and/or second expression of $\mathcal{M}$ and [63], Eq. 6.1.41.

APPENDIX C: GENERALIZED HEISENBERG-LIKE UNCERTAINTY RELATION

Using (B6) applied to r with $l = a$ and $\lambda = \alpha$ and applied to p with $l = b$ and $\lambda = \beta$, respectively, and using (12), we achieve the relation established in point (iv) of Sec. III,

$$\langle r^a\rangle^{\frac{2}{a}}\langle p^b\rangle^{\frac{2}{b}} \geqslant \mathcal{Z}(\alpha,\beta)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta) \tag{C1}$$

for all $a,b > 0$, $\alpha > \frac{d}{d+a}$, $\beta > \frac{d}{d+b}$, $\beta \leqslant \frac{\alpha}{2\alpha-1}$ and with the bounds $\mathcal{Z}$ and $\mathcal{B}$ given in Eqs. (13) and (B7).

A. The maximal bound is on the conjugation curve $\beta = \alpha^*$

We will now show that the pair (α,β) that maximizes $\mathcal{Z}(\alpha,\beta)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)$ is on the conjugation curve, namely for $\beta = \alpha^* = \alpha/(2\alpha - 1)$, for any values of a and b (under the existence condition for $\mathcal{M}$).

1. Function $\mathcal{M}(l,\lambda)$ is increasing with λ

Let us first consider the derivative of $\mathcal{M}(l,\lambda)$ versus λ.

For $\lambda > 1$, i.e., $\mu = \frac{\lambda}{\lambda-1} > 1$,

$$\begin{aligned}\frac{\partial}{\partial\mu}\ln\mathcal{M} &= \frac{\partial}{\partial\mu}\Bigg[-\frac{2}{d}\ln\Gamma(\mu) + \frac{2}{d}\ln\Gamma\left(\mu + \frac{d}{l}\right) - \frac{2}{l} \\ &\quad \times \ln(d + l\mu) + \frac{2(\mu-1)}{d}\ln\left(\frac{l\mu}{d + l\mu}\right)\Bigg] \\ &= \frac{2}{d}\Bigg[-\psi(\mu) + \psi\left(\mu + \frac{d}{l}\right) + \frac{l}{d + l\mu} - \frac{1}{\mu} \\ &\quad + \ln\left(\frac{l\mu}{d + l\mu}\right)\Bigg],\end{aligned}$$

where $\psi(x) = \frac{d}{dx}\ln\Gamma(x)$ is the digamma function.

Similarly, for $\lambda \in (1 - \frac{l}{l+d}; 1)$, i.e., $\mu < -d/l$,

$$\begin{aligned}\frac{\partial}{\partial\mu}\ln\mathcal{M} &= \frac{\partial}{\partial\mu}\Bigg[-\frac{2}{d}\ln\Gamma\left(1 - \mu - \frac{d}{l}\right) + \frac{2}{d}\ln\Gamma(1-\mu) \\ &\quad - \frac{2}{l}\ln(-d - l\mu) + \frac{2(\mu-1)}{d}\ln\left(\frac{l\mu}{d + l\mu}\right)\Bigg] \\ &= \frac{2}{d}\Bigg[-\psi(1-\mu) + \psi\left(1 - \mu - \frac{d}{l}\right) + \frac{l}{d + l\mu} \\ &\quad - \frac{1}{\mu} + \ln\left(\frac{l\mu}{d + l\mu}\right)\Bigg] \\ &= \frac{2}{d}\left[\psi\left(-\frac{d + l\mu}{l}\right) - \psi(-\mu) + \ln\left(\frac{l\mu}{d + l\mu}\right)\right],\end{aligned}$$

the last simplification coming from [62], Eq. 8.365-1.

To summarize, noting that $\partial\mu/\partial\lambda = -1/(\lambda - 1)^2$,

$$\frac{\partial}{\partial\lambda}\ln\mathcal{M}(l,\lambda) = \frac{2}{d(\lambda-1)^2}\left[\psi(\mu) + \frac{1}{\mu} - \ln\mu - \psi\left(\mu + \frac{d}{l}\right) - \frac{1}{\mu + \frac{d}{l}} + \ln\left(\mu + \frac{d}{l}\right)\right] \quad \text{if } \lambda > 1, \tag{C2}$$

$$\frac{\partial}{\partial\lambda}\ln\mathcal{M}(l,\lambda) = \frac{2}{d(\lambda-1)^2}\left[\psi(-\mu) - \ln(-\mu) - \psi\left(-\mu - \frac{d}{l}\right) + \ln\left(-\mu - \frac{d}{l}\right)\right] \quad \text{if } 1 - \frac{l}{l+d} < \lambda < 1. \tag{C3}$$

Taking the limit $\lambda \to 1^+$ in Eq. (C2), or $\lambda \to 1^-$ in Eq. (C3), and $\mathcal{M}$ being continuous in $\lambda = 1$, we achieve $\frac{\partial}{\partial\lambda} \ln \mathcal{M}(l,\lambda)\big|_{\lambda=1} = \frac{1}{l}$.

Let us consider now the terms in the parentheses on the right-hand side Eq. (C2). They can be written as $g(\mu) - g(\mu + d/l)$, with

$$g(\mu) = \psi(\mu) + \frac{1}{\mu} - \ln \mu. \tag{C4}$$

Then, from [63], Eq. 6.4.1,

$$\begin{aligned} g'(\mu) &= \psi'(\mu) - \frac{1}{\mu} - \frac{1}{\mu^2} \\ &= \int_0^{+\infty} \frac{t}{1-e^{-t}} e^{-\mu t} dt - \int_0^{+\infty} e^{-\mu t} dt - \int_0^{+\infty} t\, e^{-\mu t} dt \\ &= \int_0^{+\infty} \frac{-1 + e^{-t} + te^{-t}}{1-e^{-t}} e^{-\mu t} dt. \end{aligned}$$

Now, it is easy to show that $-1 + e^{-t} + te^{-t} \leqslant 0$ for $t \geqslant 0$, which permits us to conclude that $g' \leqslant 0$ and thus that g is decreasing. As a conclusion, $g(\mu) - g(\mu + d/l) \geqslant 0$ and thus $\frac{\partial}{\partial\lambda} \ln \mathcal{M} \geqslant 0$: $\mathcal{M}$ is increasing in $(1\,;\, +\infty)$.

Similarly, the terms in parentheses on the right-hand side of Eq. (C3) ($\mu < -d/l < 0$ here) read $h(\mu) - h(\mu + d/l)$, with

$$h(\mu) = \psi(-\mu) - \ln(-\mu),$$

and they give from [63], Eq. 6.4.1

$$\begin{aligned} h'(\mu) &= -\psi'(-\mu) - \frac{1}{\mu} \\ &= \int_0^{+\infty} \frac{-t}{1-e^{-t}} e^{\mu t} dt + \int_0^{+\infty} e^{\mu t} dt \\ &= \int_0^{+\infty} \frac{1 - t - e^{-t}}{1-e^{-t}} e^{\mu t} dt. \end{aligned}$$

Then, it is easy to show that $1 - t - e^{-t} \leqslant 0$ for $t \geqslant 0$, which permits us to conclude that $h' \leqslant 0$ and thus that h is decreasing. As a conclusion, $h(\mu) - h(\mu + d/l) \geqslant 0$ and thus also for $\lambda \in (1 - \frac{l}{l+d}\,;\, 1)$ we have $\frac{\partial}{\partial\lambda} \ln \mathcal{M} \geqslant 0$: $\mathcal{M}$ is increasing.

2. $\mathcal{B}(\lambda)$ *increases with* $\lambda \in [1/2\,;1]$ *and decreases with* $\lambda > 1$

From (9) and $\lambda^* = \lambda/(2\lambda - 1)$, the derivative of $\mathcal{B}(\lambda)$ reads

$$\begin{aligned} \frac{\partial}{\partial\lambda} \ln \mathcal{B}(\lambda) &= \frac{\partial}{\partial\lambda}\left(\frac{\ln\lambda}{\lambda - 1} + \frac{\ln\lambda^*}{\lambda^* - 1}\right) \\ &= \frac{\partial}{\partial\lambda}\left(\frac{\ln\lambda}{\lambda - 1}\right) + \frac{\partial}{\partial\lambda^*}\left(\frac{\ln\lambda^*}{\lambda^* - 1}\right)\frac{\partial\lambda^*}{\partial\lambda} \\ &= \left(\frac{1}{\lambda(\lambda-1)} - \frac{\ln\lambda}{(\lambda-1)^2}\right) \\ &\quad - \left(\frac{1}{\lambda^*(\lambda^*-1)} - \frac{\ln\lambda^*}{(\lambda^*-1)^2}\right)\frac{1}{(2\lambda-1)^2}, \end{aligned}$$

that is,

$$\frac{\partial}{\partial\lambda} \ln \mathcal{B}(\lambda) = \frac{1}{(\lambda-1)^2}\left(2 - \frac{2}{\lambda} - \ln(2\lambda - 1)\right). \tag{C5}$$

A short study of the right-hand side shows that this quantity is positive if $\lambda \in [1/2\,;1]$ and negative if $\lambda \geqslant 1$: $\mathcal{B}$ increases with λ in $[1/2\,;1]$ and then decreases for larger values of λ.

3. *Domain where the maximal bound has to be searched*

Recall that starting from (C1), namely $\langle r^a\rangle^{\frac{2}{a}} \langle p^b\rangle^{\frac{2}{b}} \geqslant \mathcal{Z}(\alpha,\beta)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)$, the best bound is then so that $\mathcal{Z}(\alpha,\beta)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)$ is maximized as a function of α and β. Let us now consider the following sets in the (α,β) plane:

$$\begin{aligned} D_\alpha &= \{(\alpha,\beta) \in \mathbb{R}_+^2 | \alpha \geqslant 1, \beta \leqslant \alpha^*\}, \\ D_\beta &= \{(\alpha,\beta) \in \mathbb{R}_+^2 | \beta \geqslant 1, \alpha \leqslant \beta^*\}, \\ S_\alpha &= \{(\alpha,\beta) \in [0\,;\,1]^2 | \beta \leqslant \alpha\}, \\ S_\beta &= \{(\alpha,\beta) \in [0\,;\,1]^2 | \alpha \leqslant \beta\}, \\ S_1 &= S_\alpha \cup S_\beta, \end{aligned}$$

where $\alpha^* = \frac{\alpha}{2\alpha-1}$ and $\beta^* = \frac{\beta}{2\beta-1}$. These sets are represented in Fig. 9.

To study the best bound, we consider each subset:

(i) We first consider domain D_α and fix α. From Eq. (13), the bound is then $\mathcal{Z}(\alpha,\beta)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta) = \mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)$ and from the previous study of $\mathcal{M}$ we can know that it increases with β. Thus, the bound is maximum precisely *on* the conjugation curve $\beta = \alpha^*$.

(ii) By symmetry, in domain D_β and fixing β, one shows again that the bound is maximal on the conjugation curve $\alpha = \beta^*$.

(iii) In the domain S_1 we discuss the following cases:

(a) The maximum bound must be achieved on the line segment $\alpha = \beta$. Indeed, in S_α, the bound is given by $\mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)$ if $\alpha \geqslant 1/2$ and $\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)/e^2$ otherwise. Again, fixing α, the bound is increasing with β and thus is maximum for $\beta = \alpha$. This remains valid, by symmetry, in S_β, and thus in all S_1.

(b) For $\alpha \leqslant 1/2$, on the line segment $\alpha = \beta$ the bound is $\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha)/e^2$ and thus increases with α: it is maximum for $\alpha = 1/2$.

(c) For $\alpha \in (1/2\,;\,1]$, the bound is expressed as $\mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha)$ and tends to $\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha)/e^2$ for $\alpha \to 1/2$, $\mathcal{B}$ being an increasing function in $[1/2\,;1]$, and since $\mathcal{M}$ is increasing, the bound is then maximum for $\alpha = 1$.

In conclusion, on S_1 the maximum bound is achieved when $\alpha = \beta = 1$, which is again *on* the conjugation curve.

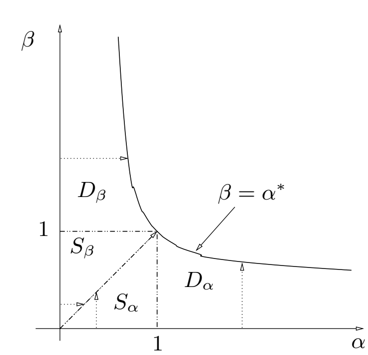

FIG. 9. Sets D_α, D_β, S_α, and S_β in the plane (α,β). The solid curve represents the pairs of conjugated parameters, i.e., $\beta = \alpha^*$. The dotted arrows indicate that $\mathcal{Z}(\alpha,\beta)\mathcal{M}(a,\alpha)\mathcal{M}(b,\beta)$ increases when the pair (α,β) moves along their directions in the sets where they are plotted.

B. Maximal bound and properties

The best bound of the generalized Heisenberg relation one can achieve by our approach is then

$$\mathcal{C}(a,b) = \max_{\alpha \in D(a,b)} \mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*), \tag{C6}$$

where the domain of search D is ruled by the restriction on the domain of existence of $\mathcal{M}$. We will come back to this domain later.

1. Symmetries

Let us denote by $\alpha_{\text{opt}}(a,b)$ the index that leads to $\mathcal{C}(a,b)$, i.e.,

$$\alpha_{\text{opt}}(a,b) = \arg\max_{\alpha} \mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*). \tag{C7}$$

Noticing that $\mathcal{B}(\alpha) = \mathcal{B}(\alpha^*)$, one immediately observes from (C7) that

$$\mathcal{C}(b,a) = \mathcal{C}(a,b), \tag{C8}$$

$$\alpha_{\text{opt}}(b,a) = [\alpha_{\text{opt}}(a,b)]^*. \tag{C9}$$

Thus, without loss of generality, one can restrict the study to the case with $a \geqslant b$.

2. Reduced domain of search

Consider the situation in which $a \geqslant b$.

If $\alpha > 1$, then $\alpha^* < 1$. We will show that the bound $\mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*)$ decreases with α, thus the maximum must satisfy $\alpha \leqslant 1$.

We have already seen that $\mathcal{B}(\alpha)$ decreases when $\alpha > 1$. Consider then the part $\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*)$. Remembering that $\alpha^* = \frac{\alpha}{2\alpha-1}$, one has $\frac{\partial\alpha^*}{\partial\alpha} = -\frac{1}{(2\alpha-1)^2}$. Moreover, one has $\frac{1}{(\alpha^*-1)^2} = \frac{(2\alpha-1)^2}{(\alpha-1)^2}$ and $\mu(\alpha^*) = \frac{\alpha^*}{\alpha^*-1} = -\frac{\alpha}{\alpha-1} = -\mu(\alpha)$ from Eq. (B3). Then, from (C2)–(C3),

$$\begin{aligned}
&\frac{\partial}{\partial\alpha}\ln[\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*)]\\
&\quad= \frac{\partial}{\partial\alpha}\ln\mathcal{M}(a,\alpha) + \frac{\partial\alpha^*}{\partial\alpha}\frac{\partial}{\partial\alpha^*}\ln\mathcal{M}(b,\alpha^*)\\
&\quad= \frac{2}{d(\alpha-1)^2}\bigg(\frac{1}{\mu} - \frac{1}{\mu+d_a} - \psi(\mu+d_a)\\
&\qquad + \psi(\mu-d_b) + \ln(\mu+d_a) - \ln(\mu-d_b)\bigg),
\end{aligned}$$

where μ stands for $\mu(\alpha)$, $d_a = d/a$, and $d_b = d/b$. The goal is then to show the negativity of

$$\begin{aligned}
k(\mu,d_a,d_b) = {}&\frac{1}{\mu} - \frac{1}{\mu+d_a} - \psi(\mu+d_a) + \ln(\mu+d_a)\\
&+ \psi(\mu-d_b) - \ln(\mu-d_b),
\end{aligned} \tag{C10}$$

keeping in mind that $d_a \leqslant d_b$. To this end, we can view this function in terms of d_a for instance, and thus the sense of variation of $k(\mu,d_a,d_b) = -g(\mu+d_a) + g(\mu-d_b) + 1/\mu - 1/(\mu-d_b)$ is the same as the sense of variation of $-g(\mu+d_a) = -\psi(\mu+d_a) - \frac{1}{\mu+d_a} + \ln(\mu+d_a)$, introduced in Eq. (C4), versus d_a. We have shown that function g is decreasing and thus k is increasing with d_a. Since $d_a \leqslant d_b$, to show that k is negative, it is then sufficient to show that $k(\mu,d_b,d_b)$ is negative. From [62], Eq. 6.4.1,

$$\begin{aligned}
\frac{\partial k(\mu,d_b,d_b)}{\partial d_b} &= \frac{1}{\mu+d_b} + \frac{1}{(\mu+d_b)^2} - \psi'(\mu+g_g) + \frac{1}{\mu-d_b} - \psi'(\mu-d_b)\\
&= \int_0^{+\infty}\left[\left(1+t-\frac{t}{1-e^{-t}}\right)e^{-d_b t} + \left(1-\frac{t}{1-e^{-t}}\right)e^{+d_b t}\right]e^{-\mu t}dt\\
&= \int_0^{+\infty}[(1-e^{-t}-te^{-t})e^{-d_b t} + (1-t-e^{-t})e^{+d_b t}]\frac{e^{-\mu t}}{1-e^{-t}}dt.
\end{aligned}$$

Now, it is quite easy to show that the term in square brackets is decreasing with d_b since the derivative in d_b is negative (the factors of $e^{\pm d_b t}$ are negative). For $d_b = 0$, it is not difficult to show that the square bracket is negative, which permits us to conclude that for any d_b, the square bracket term is negative: $k(\mu,d_b,d_b)$ decreases with d_b.

Finally, $k(\mu,0,0) = 0$ and thus $k(\mu,d_b,d_b) \leqslant 0$, implying that for any $d_a \leqslant d_b$ one has $k(\mu,d_a,d_b) \leqslant 0$.

As claimed, $\frac{\partial}{\partial\alpha}\ln[\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*)] \leqslant 0$ for $\alpha > 1$. Together with the decrease of $\mathcal{B}$ when $\alpha > 1$, we conclude that the maximum of $\mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*)$ is attained for $\alpha < 1$.

As a conclusion, when $a \geqslant b$, the maximum is attained for $\alpha < 1$. Since we are on the conjugated curve, one also have $\alpha > 1/2$. Finally, from (C2) we must have $\alpha > \frac{d}{d+a}$.

In summary, for $a \geqslant b$,

$$\mathcal{C}(a,b) = \max_{\alpha \in \left(\max\left(\frac{1}{2},\frac{d}{d+a}\right);1\right]} \mathcal{B}(\alpha)\mathcal{M}(a,\alpha)\mathcal{M}(b,\alpha^*), \tag{C11}$$

where $\mathcal{B}$ and $\mathcal{M}$ are given by (9) and (B7), respectively.

[1] W. C. Price, *The Uncertainty Principle and Foundations of Quantum Mechanics*, edited by W. C. Price and S. S. Chissick (Wiley, New York, 1977).

[2] *Sixty-Two Years of Uncertainty: Historical, Philosophical, and Physical Inquiries into the Foundations of Quantum Mechanics*, edited by A. I. Miller (Plenum, New York, 1990).

[3] *Dimensional Scaling in Chemical Physics*, edited by D. R. Herschbach, J. Avery, and O. Goscinski (Springer-Verlag, New York, 2001).
[4] E. H. Lieb, *The Stability of Matter: From Atoms to Stars, Selecta of E. H. Lieb*, edited by W. Thirring (Springer-Verlag, Berlin, 2005).
[5] J. S. Dehesa, S. López-Rosa, and D. Manzano, in *Statistical Complexities: Application to Electronic Structure*, edited by K. D. Sen (Springer, Berlin, 2010).
[6] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
[7] V. Vedral, *Introduction to Quantum Information Science* (Oxford University Press, Oxford, 2006).
[8] W. Heisenberg, Z. Phys. A **43**, 172 (1927).
[9] E. H. Kennard, Z. Phys. **44**, 326 (1927).
[10] G. B. Folland and A. Sitaram, J. Fourier Anal. Appl. **3**, 207 (1997).
[11] P. Busch, T. Heinonen, and P. Lahti, Phys. Rep. **452**, 155 (2007).
[12] I. Bialynicki-Birula and L. Rudnicki, e-print arXiv:1001.4668.
[13] D. Deutsch, Phys. Rev. Lett. **50**, 631 (1983).
[14] J. B. M. Uffink and J. Hilgevoord, Found. Phys. **15**, 925 (1985).
[15] J. B. M. Uffink, Ph.D. thesis, University of Utrecht, Utrecht, The Netherlands (1990), see also references therein.
[16] J. Hilgevoord and J. B. M. Uffink, in *Proceedings of the International Conference on Microphysical Reality and Quantum Description*, edited by F. Selleri, A. van der Merwe, and G. Tarozzi (Reidel, Dordrecht, 1988), Vol. 1, pp. 91–114.
[17] I. Bialynicki-Birula and J. Mycielski, Commun. Math. Phys. **44**, 129 (1975).
[18] I. Bialynicki-Birula, Phys. Rev. A **74**, 052101 (2006).
[19] S. Zozor and C. Vignat, Physica A **375**, 499 (2007).
[20] S. Zozor, M. Portesi, and C. Vignat, Physica A **387**, 4800 (2008).
[21] A. K. Rajagopal, Phys. Lett. A **205**, 32 (1995).
[22] M. Portesi and A. Plastino, Physica A **225**, 412 (1996).
[23] H. Maassen and J. B. M. Uffink, Phys. Rev. Lett. **60**, 1103 (1988).
[24] E. Romera, P. Sánchez-Moreno, and J. S. Dehesa, J. Math. Phys. **47**, 103504 (2006).
[25] P. Sánchez-Moreno, R. González-Férez, and J. S. Dehesa, New J. Phys. **8**, 330 (2006).
[26] P. Sánchez-Moreno, A. R. Plastino, and J. S. Dehesa, J. Phys. A: Math. Theor. **44**, 065301 (2011).
[27] S. Wehner and A. Winter, New J. Phys. **12**, 025009 (2010).
[28] J. C. Angulo, J. Phys. A **26**, 6493 (1993).
[29] J. C. Angulo, Phys. Rev. A **50**, 311 (1994).
[30] D. V. Widder, *The Laplace Transform*, Princeton Mathematical Series (Princeton University Press, Princeton, NJ, 1946).
[31] E. Romera, J. C. Angulo, and J. S. Dehesa, Phys. Rev. A **59**, 4064 (1999).
[32] Y. A. Wang and E. A. Carter, Phys. Rev. A **60**, 4153 (1999).
[33] R. López-Ruiz, H. L. Mancini, and X. Calbet, Phys. Lett. A **209**, 321 (1995).
[34] S. López-Rosa, J. C. Angulo, and J. Antolín, Physica A **388**, 2081 (2009).
[35] S. López-Rosa, R. O. Esquievel, J. C. Angulo, J. Antolín, J. S. Dehesa, and N. Flores-Gallegos, J. Chem. Theor. Comput. **6**, 145 (2010).
[36] J. S. Dehesa, S. López-Rosa, A. Martínez-Finkelshtein, and R. J. Yáñez, Int. J. Quantum Chem. **110**, 1529 (2010).
[37] A. Rényi, in *Proceedings of the 4th Berkeley Symposium on Mathematical Statistics and Probability*, edited by J. Neyman, Vol. 1 (University of California Press, Berkeley, 1961), pp. 547-561.
[38] T. M. Cover and J. A. Thomas, *Elements of Information Theory* (Wiley, New York, 1991).
[39] J. A. Costa, A. O. Hero III, and C. Vignat, in *4th International Workshop on Energy Minimization Methods in Computer Vision and Pattern Recognition (EMMCVPR)*, Lecture Notes in Computer Sciences, edited by A. Rangarajan, M. A. T. Figueiredo, and J. Zerubia (Springer-Verlag, Lisbon, 2003), Vol. 2683, pp. 211–226.
[40] E. H. Lieb, Inventiones Mathematicae **102**, 179 (1990).
[41] J. C. Angulo and J. S. Dehesa, J. Chem. Phys. **97**, 6485 (1992).
[42] S. Nadarajah, J. Appl. Stat. **32**, 685 (2005).
[43] M. K. Varanasi and B. Aazhang, J. Acoust. Soc. Am. **86**, 1404 (1989).
[44] S. Zozor and C. Vignat, IEEE Trans. Signal Proc. **58**, 134 (2010).
[45] R. J. Yáñez, W. Van Assche, R. González-Férez, and J. Sánchez-Dehesa, J. Math. Phys. **40**, 5675 (1999).
[46] J. S. Avery, *Hyperspherical Harmonics and Generalized Sturmians* (Kluwer Academic, Dordrecht, 2002).
[47] R. J. Yáñez, W. Van Assche, and J. S. Dehesa, Phys. Rev. A **50**, 3065 (1994).
[48] R. Lord, Biometrika **41**, 44 (1954).
[49] J. S. Avery, J. Comput. Appl. Math. **233**, 1366 (2010).
[50] W. Van Assche, R. J. Yáñez, R. González-Férez, and J. S. Dehesa, J. Math. Phys. **41**, 6600 (2000).
[51] V. F. Tarasov, Int. J. Mod. Phys. B **18**, 3177 (2004).
[52] A. P. Prudnikov, Y. A. Brychkov, and O. I. Marichev, *Integrals and Series*, Vol. 2: Special Functions (Gordon and Breach Science Publishers, New York, 1986).
[53] J. D. Louck and W. H. Shaffer, J. Mol. Spectrosc. **4**, 298 (1960).
[54] J. D. Louck and W. H. Shaffer, J. Mol. Spectrosc. **4**, 334 (1960).
[55] J. S. Dehesa, F. J. Galvez, and I. Porras, Phys. Rev. A **40**, 35 (1989).
[56] C. Tsallis, R. M. Mendes, and A. R. Plastino, Physica A **261**, 534 (1998).
[57] A. Andai, J. Multivariate Anal. **100**, 777 (2009).
[58] S. Kotz and S. Nadarajah, Stat. Prob. Lett. **54**, 171 (2001).
[59] Y. Kano, J. Multivariate Anal. **51**, 139 (1994).
[60] T. J. Kozubowski, Statistics **36**, 219 (2002).
[61] C. Tsallis and E. K. Lenzi, Chem. Phys. **284**, 341 (2002).
[62] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, 7th ed. (Academic, San Diego, 2007).
[63] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1970).