Fisher entropy and uncertaintylike relationships in many-body systems

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General model-independent relationships among radial expectation values of the one-particle densities in position and momentum spaces for any quantum-mechanical system are obtained. They are derived from the Stam uncertainty principle and the recently reported lower bounds to the Fisher information entropy of both densities. The results are usually expressed in terms of some uncertainty products of the system. The accuracy of the bounds is numerically analyzed for neutral atoms within a Hartree-Fock framework.
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I. INTRODUCTION

The study of the main physical properties of many-fermion systems involves, as basic variables, the one-particle densities in both position and momentum spaces $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$, respectively, as shown in the density-functional theory [1]. Throughout this work, the normalization

$$\int \rho(\mathbf{r})d\mathbf{r}=\int \gamma(\mathbf{p})d\mathbf{p}=N \tag{1}$$

will be considered for an N-particle system. For atoms, some of the radial expectation values of the aforementioned densities, namely,

$$\langle r^a\rangle \equiv \int r^a \rho(\mathbf{r})d\mathbf{r}, \quad \langle p^a\rangle \equiv \int p^a \gamma(\mathbf{p})d\mathbf{p}, \tag{2}$$

are experimentally accessible and/or physically meaningful. Let us remember here that (i) the Langevin-Pauli diamagnetic susceptiblity χ is proportional to the mean-square radius as $\chi=-\frac{1}{6}\alpha^2\langle r^2\rangle$, where α is the fine-structure constant [2]; (ii) the electron-nucleus attraction energy is given by $E_{eN}=-Z\langle r^{-1}\rangle$ (Z being the nuclear charge) [2], which is also related to the nuclear magnetic screening constant or diamagnetic screening factor [3]; (iii) the electron kinetic energy is half the mean-square momentum [2], i.e., $T=\langle p^2\rangle/2$; (iv) the Breit-Pauli relativistic correction T_{rel} to the kinetic energy T, due to the mass variation, is given at first order by [4] $T_{\mathrm{rel}}=-\alpha^2\langle p^4\rangle/8$; and (v) the height of the peak of the Compton profile $J(0)$, within the impulse approximation, is $\langle p^{-1}\rangle/2$ [2]. More recently, the so-called logarithmic expectation values $\langle r^a \ln r\rangle$ and $\langle p^a \ln p\rangle$ have been shown to be also relevant in the description of some features of this kind of system, not only in an information-theoretic framework [5] but also in the description of physical processes such as elastic electron scattering by nuclei [6], in which the quantity $\langle \ln r\rangle = 4\pi\int_0^\infty r^2 \ln r \rho(r)dr$ determines the behavior of the phase shifts at high energy and low angular momentum. Thus we see the interest of studying those quantities in order to better describe the corresponding one-particle densities $\rho(\mathbf{r})$ and $\gamma(\mathbf{p})$, as well as to rigorously correlate properties between conjugate spaces, with the aim of applying all the information coming from both spaces to the simultaneous study of both densities.

Not many relationships involving radial expectation values of conjugate spaces are found in the literature; see, e.g., Ref. [7] for a recent summary. Probably the most celebrated uncertainty expression is the one which correlates the mean-square values of radius and momentum, namely [7,8],

$$\langle r^2\rangle\langle p^2\rangle \geq \tfrac{9}{4}N^2, \tag{3}$$

which is essentially a three-dimensional generalization of the Heisenberg uncertainty principle; notice that equality is reached for the case of Gaussian wave functions.

More recently, a generalization of the above expression involving the uncertainty products defined by

$$\Delta(a,b)\equiv(\langle r^a\rangle/N)^{1/a}(\langle p^b\rangle/N)^{1/b}, \tag{4}$$

for $a,b\neq 0$, with the limiting cases

$$\Delta(a,0)\equiv(\langle r^a\rangle/N)^{1/a}\exp(\langle \ln p\rangle/N),$$
$$\Delta(0,b)\equiv \exp(\langle \ln r\rangle/N)(\langle p^b\rangle/N)^{1/b}, \tag{5}$$

$$\Delta(0,0)\equiv \exp[(\langle \ln r\rangle+\langle \ln p\rangle)/N], \tag{6}$$

has been obtained [9] by using information-theoretic methods related to the so-called Boltzmann-Shannon entropy [10], giving rise to the inequality

$$\Delta(a,b)\geq\left[\frac{\pi ab}{16\Gamma(3/a)\Gamma(3/b)}\right]^{1/2}\left(\frac{3}{a}\right)^{1/a}\left(\frac{3}{b}\right)^{1/b}e^{1-(1/a)-(1/b)}, \tag{7}$$

valid only for $a,b>0$.

Specially interesting is the case $a=b>0$, for which

$$\Delta_a\equiv\Delta(a,a)\geq[3\pi^{1/2}/4\Gamma(3/a)](3/ae)^{(2/a)-1} \tag{8}$$

for any $a>0$. Expression (3) appears as a particular case of Eq. (8) with the choice $a=2$, i.e., $\Delta_2\geq 3/2$.

In the same work [9], uncertaintylike relationships involving logarithmic expectation values and/or the logarithmic uncertainties

$$\Delta(\ln r) \equiv [N\langle(\ln r)^2\rangle - \langle \ln r\rangle^2]^{1/2},$$
$$\Delta(\ln p) \equiv [N\langle(\ln p)^2\rangle - \langle \ln p\rangle^2]^{1/2} \tag{9}$$

are also found and numerically analyzed. An extension of these results to systems of arbitrary dimensionality was given in Ref. [11].

In this work, a set of uncertaintylike expressions is obtained by means of another information-theoretic technique [12,13], based on the concept of Fisher information entropy (closely related to the Weizsäcker energy functional in the atomic case) as shown in Sec II. The main results concern (i) improved upper and lower bounds on radial expectation values using information of the complementary space (Sec. III), (ii) uncertainty products of nonpositive order (Sec. IV), and (iii) relationships involving two or more uncertainty products (also Sec. IV). For illustration, a brief numerical study of some of those model-independent relationships is carried out for atomic systems within a near-Hartree-Fock (NHF) framework. Finally, some concluding remarks are given.

II. BOUNDS ON THE FISHER INFORMATION ENTROPY

The so-called Fisher information entropy I_f of a three-dimensional density function $f(\mathbf{r}) = f(x,y,z)$ is defined as [14]

$$I_f \equiv \int [|\nabla f(\mathbf{r})|^2/f(\mathbf{r})]\, d\mathbf{r}, \tag{10}$$

and it measures the degree of spatial delocalization of such a distribution. The Stam uncertainty principle [15] establishes an upper bound to the entropy I_ρ of the one-particle density $\rho(\mathbf{r})$ in position space in terms of the mean-square momentum $\langle p^2\rangle$ (related to the kinetic energy of the system) in the form

$$I_\rho \leqslant 4\langle p^2\rangle, \tag{11}$$

and similarly for the entropy I_γ associated with the momentum space distribution $\gamma(\mathbf{p})$, now in terms of the mean-square value of the conjugate variable, i.e.,

$$I_\gamma \leqslant 4\langle r^2\rangle, \tag{12}$$

which is proportional to the diamagnetic susceptibility.

Recently, several lower bounds to the quantities I_ρ and I_γ have been derived by using different techniques [12,13]. Some of these bounds are expressed in terms of radial expectation values, while others additionally involve logarithmic expectation values. In this work, the combination of the above-mentioned upper and lower bounds on I_ρ and I_γ is carried out to provide rigorous relationships among expectation values on the conjugated spaces, i.e., between the $\mathbf{r}$ and $\mathbf{p}$ spaces.

Let us remark here that all the expressions shown in this work are also valid after the exchange of the conjugate variables $\mathbf{r}$ and $\mathbf{p}$. This fact will be taken into account in order to avoid the inclusion of many relationships which can be obtained by only performing such an exchange on the expressions written here.

III. RELATIONSHIPS AMONG RADIAL EXPECTATION VALUES

Two kinds of lower bounds to the functional I_ρ have been reported [12,13], the first one derived variationally [12] and the second one making use of different classical inequalities, such as Redheffer, Hölder, and Sobolev inequalities [13,16–18]. All them are expressed in terms of two or three radial expectation values $\langle r^a\rangle$. The main idea to carry out in this section is to combine the lower bounds to the Fisher information entropies with the upper bounds given by the Stam principle as shown by Eqs. (11) and (12). Then one obtains rigorous relationships among radial expectation values of both $\mathbf{r}$ and $\mathbf{p}$ spaces.

The well-known uncertainty expression given by Eq. (3) is obtained as a particular case by simultaneously using one of the variational bounds to I_ρ (or I_γ) and Eq. (11) [or Eq. (12)]. The consideration of other variational results provides different relationships among two or three radial expectation values of one space and one value of the conjugate space. Because (i) the variational bounds also appear as particular cases of the nonvariational ones, and (ii) those obtained from Redheffer's inequality (in terms of $\langle r^{-2}\rangle$ and/or $\langle r^{(b/2)-1}\rangle$ and $\langle r^b\rangle$) are much more accurate than those of Sobolev origin (in terms of N and/or two radial expectation values), we will center our attention on the expressions derived from the Redheffer type bounds to the Fisher information entropy. Using Eqs. (12) and (23) of Ref. [12], one obtains, respectively,

$$\langle p^2\rangle \geqslant [(b+4)^2/16]\,(\langle r^{(b/2)-1}\rangle^2/\langle r^b\rangle) \tag{13}$$

for any $b > -3$, and

$$\langle p^2\rangle \geqslant \frac{\langle r^{-2}\rangle}{16}\left[4 + \frac{[4+b(b+4)]\langle r^{(b/2)-1}\rangle^2}{\langle r^b\rangle\langle r^{-2}\rangle - \langle r^{(b/2)-1}\rangle^2}\right] \tag{14}$$

for any $b > -2$. Especially interesting are the particular cases corresponding to the choices $b = -2$, 0, and 2 in Eq. (13) and $b = 0$ in Eq. (14). Concerning Eq. (13), the uncertainty relationship given by Eq. (3) is obtained again for $b = 2$, while for the values $b = -2$ and 0 it provides, respectively, the following known expressions [19]:

$$\langle p^2\rangle \geqslant \langle r^{-2}\rangle/4\,, \tag{15}$$

$$N\langle p^2\rangle \geqslant \langle r^{-1}\rangle^2, \tag{16}$$

which can be rewritten in terms of uncertainty products as $\Delta(-2,2) \geqslant \frac{1}{2}$ and $\Delta(-1,2) \geqslant 1$, respectively. Taking $b = 0$ in Eq. (14), we find that

$$2\langle p^2\rangle\left[1 - \sqrt{1 - \frac{\langle r^{-1}\rangle^2}{N\langle p^2\rangle}}\right] \leqslant \langle r^{-2}\rangle \leqslant 2\langle p^2\rangle\left[1 + \sqrt{1 - \frac{\langle r^{-1}\rangle^2}{N\langle p^2\rangle}}\right]. \tag{17}$$

This expression improves the well-known bounds [19,17] $\langle r^{-1}\rangle^2/N \leqslant \langle r^{-2}\rangle \leqslant 4\langle p^2\rangle$, as can be easily shown. Indeed,

TABLE I. Comparison of the accuracies of the lower bounds to the uncertainty product Δ_2 given by Eqs. (3) and (21). Atomic units are used.

Z	Δ_2^2	Bound Eq. (21)	Accuracy (in %) Eq. (3)	Eq. (21)
1	3.000	2.500	75.00	83.33
2	3.390	2.634	66.37	77.71
6	28.88	4.736	7.79	16.40
20	191.5	19.41	1.18	10.14
30	138.2	11.41	1.63	8.25
48	257.7	14.34	0.87	5.56
65	483.0	26.64	0.47	5.52
92	750.9	33.18	0.30	4.42

TABLE II. Uncertainty products Δ_a $(a=-2,-1,2)$, and the accuracy of the lower and the upper bound to Δ_{-1} given by Eqs. (24) and (25), respectively. Atomic units are used.

Z	Δ_{-2}	Δ_{-1}	Δ_2	Accuracy (in %) Eq. (24)	Eq. (25)
1	0.31623	0.58905	1.7321	52.6	87.9
2	0.28560	0.55372	1.8413	49.7	82.1
6	0.14854	0.42587	5.3738	33.5	29.3
15	0.11002	0.41000	9.5734	26.2	16.6
29	0.093713	0.52219	11.217	17.5	18.2
45	0.081761	0.48903	15.612	16.4	12.3
72	0.057027	0.46255	21.079	12.1	8.7
92	0.044760	0.41726	27.402	10.5	6.1

by taking into account the first terms of the Taylor expansion for the function $\sqrt{1-x}$ around $x=0$, we have

$$\frac{\langle r^{-1}\rangle^2}{N}\left[1+\frac{\langle r^{-1}\rangle^2}{2N\langle p^2\rangle}\right]\leqslant\langle r^{-2}\rangle\leqslant 4\langle p^2\rangle-\frac{\langle r^{-1}\rangle^2}{N}. \quad (18)$$

All the expressions shown in this section are also valid under the commutation of the conjugate spaces, i.e., replacing the variable **r** by **p**, and conversely. In this sense, the previous results involving $\langle r^{-2}\rangle$ transform into upper and lower bounds on the moment $\langle p^{-2}\rangle$.

Using the NHF atomic wave functions of Refs. [20,21], it is observed that, for atomic systems, the factor of improvement of the upper and lower bounds on $\langle r^{-2}\rangle$, as well as on $\langle p^{-2}\rangle$, is significantly higher than 1 only for light atoms. Nevertheless, it is worth realizing that the expressions found in this work also hold for any quantum-mechanical system, i.e., they may be applied to the study of molecules, nuclei, solids, etc.

IV. RELATIONSHIPS AMONG UNCERTAINTY PRODUCTS

The uncertainty products $\Delta(a,b)$ defined in Sec. I can also be analyzed, even for negative values of a and/or b, by making use of the aforementioned relationships. Two basic properties of the quantity $\Delta(a,b)$ are that it is an increasing and convex function of both a and b (as can be easily shown by using Hölder's inequality [17]) and, consequently, the product Δ_a is also an increasing and convex function of a.

In this sense, let us notice that $\Delta_{-1}\leqslant\Delta_2$. Now, taking into account that all the expressions in Sec. III are also valid under a commutation of the variables $\{\mathbf{r},\mathbf{p}\}$, let us multiply Eq. (16) by the same equation after the exchange $\mathbf{r}\leftrightarrow\mathbf{p}$, giving rise to the inequality

$$1/\Delta_2\leqslant\Delta_{-1}\leqslant\Delta_2, \quad (19)$$

which holds for any quantum system. To get an idea of the accuracy (we define the accuracy of the expression $A\leqslant B$ as the ratio A/B in percentage) of the above inequality, the atomic wave functions of Refs. [20,21] have been used to calculate the uncertainty products involved for all atoms with nuclear charge $Z=1$–92. We observe the poor quality of the upper bound (obtained from Hölder's inequality), its accuracy being only around 30% for hydrogen $(Z=1)$ and helium $(Z=2)$, and much lower (usually below 5%) for the rest of the atoms. However, the lower bound (obtained with the technique employed here) shows a better behavior. For $Z=1$–2, the accuracy is around 98%, and then slowly decreases from 60% $(Z=3)$ to 8% $(Z=92)$.

Working with Eq. (17) in a way similar to that with Eq. (16), the following upper and lower bounds to the uncertainty product Δ_{-2} in terms of Δ_2 are obtained:

$$\frac{2\Delta_2}{x+6+\sqrt{x(x+8)}}\leqslant\Delta_{-2}\leqslant\frac{2\Delta_2}{x+6-\sqrt{x(x+8)}} \quad (20)$$

where $x\equiv 4\Delta_2^2-9\geqslant 0$. The upper bound improves the Hölder bound: $\Delta_{-2}\leqslant\Delta_2$. A numerical study within the above-mentioned NHF framework for atomic systems reveals that such an improvement is still not enough to obtain accurate upper bounds. However, the accuracy of the new lower bound to Δ_{-2} in terms of Δ_2 is higher than 70% for hydrogen and helium, and oscillates between 20% and 45% for most of the remaining atoms of the periodic table.

Conversely, it is interesting to bound Δ_2 in terms of Δ_{-2}, as can be done by solving Eq. (20) in x, giving rise to

$$\Delta_2^2\geqslant\frac{y+10+\sqrt{(y+4)(y+16)}}{8}\geqslant\frac{9}{4}, \quad (21)$$

where $y\equiv[2\Delta_{-2}+(2\Delta_{-2})^{-1}]^2-4$, which again improves the basic relation $\Delta_2\geqslant\Delta_{-2}$ derived from the increasing behavior of the function Δ_a. The last inequality in Eq. (21) follows from the fact that $y\geqslant 0$, improving the lower bound given in Eq. (3). A comparative study of the accuracies of Eqs. (3) and (21) is given in Table I for some randomly chosen atoms. It is observed that, although the accuracy tends to decrease in both cases when increasing the nuclear charge, the new lower bound to Δ_2 given by Eq. (21) provides a much better bound than the well-known one given by Eq. (3), the improvement being especially important (at times a factor higher than 10) for heavy atoms. It is worthy to note here that the inequalities appearing in Eqs. (20) and (21) transform into equalities for $x=0$ and $y=0$, respectively, which occurs only for Gaussian wave functions, as pointed out in Sec. I, in which case $\Delta_{-2}=\frac{1}{2}$ and $\Delta_2=\frac{3}{2}$.

Finally, let us remark that it is possible to correlate more than two uncertainty products in a fashion similar to that described above. For illustration, consider Eq. (17) and separate the quantity $\langle r^{-1}\rangle$ as

$$\langle r^{-1}\rangle^2/N\langle p^2\rangle \leqslant 1-[\langle r^{-2}\rangle/2\langle p^2\rangle -1]^2. \tag{22}$$

Now, multiplying this expression by the same one after the commutation of conjugate variables, an inequality involving the uncertainty products Δ_{-2}, Δ_{-1}, and Δ_2 is obtained:

$$\Delta_{-1} \geqslant \frac{4\Delta_{-2}\Delta_2}{\left[(4\Delta_2)^2+\frac{1}{\Delta_{-2}^2}-\frac{4}{N^2}(\langle r^{-2}\rangle\langle r^2\rangle+\langle p^{-2}\rangle\langle p^2\rangle)\right]^{1/2}}, \tag{23}$$

which, taking into account that $\langle r^{-2}\rangle\langle r^2\rangle \geqslant N^2$ and $\langle p^{-2}\rangle\langle p^2\rangle \geqslant N^2$ (as can be easily obtained from Hölder's inequality [17]), gives rise to

$$\Delta_{-1} \geqslant \frac{4\Delta_{-2}\Delta_2}{\left[(4\Delta_2)^2+\frac{1}{\Delta_{-2}^2}-8\right]^{1/2}}. \tag{24}$$

Additionally, the property of convexity of the quantity Δ_a allows one to correlate the values involved in the previous equation easily, providing in this case an upper bound to Δ_{-1} in terms of Δ_{-2} and Δ_2, as

$$\Delta_{-1} \leqslant \tfrac{1}{4}[3\Delta_{-2}+\Delta_2]. \tag{25}$$

A numerical study of the above upper and lower bounds on Δ_{-1} within the NHF framework considered in this work for atomic systems shows that their accuracy tends to decrease when increasing the nuclear charge, especially when a new shell begins to be occupied. Concerning the lower bound, its accuracy is around 50% for hydrogen and helium, 20–35 % for $Z=3$–18, and 10–20 % for heavier atoms. On the other hand, the accuracy of the upper bound ranges from around 85% for $Z=1$–2, 15–40 % for $Z=3$–18, and 6–15% for $Z>18$ (with very few exceptions). The values for some specific atoms are given in Table II.

V. CONCLUSIONS

The combination of the Stam uncertainty principle, expressed in terms of Fisher information entropies, and the recently obtained lower bounds to such entropies in terms of radial expectation values, has provided a set of general uncertaintylike relationships, valid for any quantum-mechanical system. These results considerably extend previous ones of similar character in various senses: improving the accuracy in many cases (as has been theoretically proved), allowing one to involve radial expectation values of nonpositive order, giving not only lower but also upper bounds to uncertainty products and different radial expectation values, and involving not only one but two or even three uncertainty products.

The numerical analysis of the accuracy of these bounds reveals a large improvement, at times, of the expressions obtained with this technique with respect to the previously known ones. One notices, however, that still there is considerable room for improvement.

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