Improved lower bounds for uncertaintylike relationships in many-body systems

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We show that employing more stringent inequalities in the derivation of uncertaintylike relationships can improve their accuracy. In particular, Eq. (23) due to Romera *et al.* [Phys. Rev. A **59**, 4064 (1999)] can be further improved using the Faris inequalities rather than using the Hölder inequalities.
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In a recent paper [1], Romera *et al.* have considered the Fisher information entropy [2] and its application in the derivation of general uncertaintylike relationships in quantum mechanics [1,3,4]. Basically, these authors have discussed the following uncertainty products:

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

where radial expectation values are defined as

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

for the normalized one-particle densities in position space $\rho(\mathbf{r})$ and momentum space $\gamma(\mathbf{p})$,

$$\int \rho(\mathbf{r})d\mathbf{r} = \int \gamma(\mathbf{p})d\mathbf{p} = N. \tag{3}$$

In particular, these authors have discussed in depth the uncertaintylike relationships involving Δ_{-1}, Δ_{-2}, and Δ_2, where $\Delta_a \equiv \Delta(a,a)$. From the definition in Eq. (1), one can explicitly write

$$\Delta_{-1} \equiv \frac{N^2}{\langle r^{-1}\rangle\langle p^{-1}\rangle}, \tag{4}$$

$$\Delta_2 \equiv \frac{\sqrt{\langle r^2\rangle\langle p^2\rangle}}{N}, \tag{5}$$

$$\Delta_{-2} \equiv \frac{N}{\sqrt{\langle r^{-2}\rangle\langle p^{-2}\rangle}}. \tag{6}$$

After some manipulation, Romera *et al.* showed [1] that

$$\Delta_{-1} \geqslant \frac{4\Delta_{-2}\Delta_2}{\sqrt{(4\Delta_2)^2 + (\Delta_{-2})^{-2} - 4\dfrac{\langle r^2\rangle\langle r^{-2}\rangle + \langle p^2\rangle\langle p^{-2}\rangle}{N^2}}}. \tag{7}$$

Using the following two inequalities (due to the Hölder inequality [5]):

$$\frac{\langle r^2\rangle\langle r^{-2}\rangle}{N^2} \geqslant 1, \quad \frac{\langle p^2\rangle\langle p^{-2}\rangle}{N^2} \geqslant 1, \tag{8}$$

these authors could further show that [1]

$$\Delta_{-1} \geqslant \frac{4\Delta_{-2}\Delta_2}{\sqrt{(4\Delta_2)^2 + (\Delta_{-2})^{-2} - 8}}. \tag{9}$$

However, we contend that Eq. (7) can be further improved by simply using the Faris inequalities [6]

$$4\langle p^2\rangle \geqslant \langle r^{-2}\rangle, \quad 4\langle r^2\rangle \geqslant \langle p^{-2}\rangle. \tag{10}$$

From Eqs. (5), (6), and (10), one readily has

$$\frac{4\langle p^2\rangle\langle p^{-2}\rangle}{N^2} \geqslant \frac{\langle r^{-2}\rangle\langle p^{-2}\rangle}{N^2} \equiv (\Delta_{-2})^{-2}, \tag{11}$$

$$\frac{4\langle r^2\rangle\langle r^{-2}\rangle}{N^2} \geqslant \frac{\langle r^{-2}\rangle\langle p^{-2}\rangle}{N^2} \equiv (\Delta_{-2})^{-2}. \tag{12}$$

Equations (11) and (12) are more sensitive with respect to dynamical changes in densities than Eq. (8) because of the explicit dependence on Δ_{-2} instead of a constant. This conclusion is only valid if and only if [7]

$$\Delta_{-2} \leqslant \frac{1}{2}, \tag{13}$$

which is apparent upon examining Eqs. (8), (11), and (12). Equation (13) is empirically proven for all neutral atoms with nuclear charge $Z \leqslant 92$ (Table I).

If Eq. (13) *is* true in general, then Eq. (20) of Ref. [1],

$$\frac{2\Delta_2}{x+6+\sqrt{x(x+8)}} \leqslant \Delta_{-2} \leqslant \frac{2\Delta_2}{x+6-\sqrt{x(x+8)}}, \tag{14}$$

$$x \equiv 4(\Delta_2)^2 - 9, \tag{15}$$

can be further simplified as

$$\frac{2\Delta_2}{x+6+\sqrt{x(x+8)}} \leqslant \Delta_{-2} \leqslant \frac{1}{2}. \tag{16}$$

Due to the following celebrated inequality [1,4]:

TABLE I. Improved lower bounds to Δ_{-1} from Eq. (7) involving the uncertainty products Δ_2, Δ_{-2}, and Δ_{-1}. All numbers are in atomic units. The data for Δ_2, Δ_{-2}, and Δ_{-1} are from Ref. [1].

				Accuracy [a] (in %)	
Z	Δ_{-2}	Δ_{-1}	Δ_2	Eq. (9) [b]	Eq. (20)
1	0.31623	0.58905	1.7321	52.6	60.3
2	0.28560	0.55372	1.8413	49.7	58.6
6	0.14854	0.42587	5.3738	33.5	36.7
15	0.11002	0.41000	9.5734	26.2	27.6
29	0.093713	0.52219	11.217	17.5	18.5
45	0.081761	0.48903	15.612	16.4	17.0
72	0.057027	0.46255	21.079	12.1	12.6
92	0.044760	0.41726	27.402	10.5	11.0

[a]Following Romera *et al.* [1], the accuracy of the expression $A \leqslant B$ as the ratio A/B (in percent).
[b]The data for this column are identical to that of Eq. (24) in Table II of Ref. [1].

$$\Delta_2 \geqslant \frac{3}{2}. \tag{17}$$

Then it also follows that

$$\frac{2\Delta_2}{x+6+\sqrt{x(x+8)}} \leqslant \frac{1}{2} \leqslant \frac{2\Delta_2}{x+6-\sqrt{x(x+8)}}, \tag{18}$$

which simply says that the upper bound of Eq. (14) is always less sensitive than $\frac{1}{2}$ if Eq. (13) *is* true in general. Equations (13) and (17) indicate a zero overlap between Δ_{-2} and Δ_2. In addition, if Eq. (13) *is* true in general, one then has a very interesting inequality based on the Faris inequalities [1,6], Eq. (10),

$$\Delta_{-2} \leqslant \frac{1}{2} \leqslant \min\{\Delta(-2,2),\Delta(2,-2)\}, \tag{19}$$

which suggests that Δ_{-2} only overlaps with $\Delta(-2,2)$ or $\Delta(2,-2)$ at the boundary value $\frac{1}{2}$. Given all these intriguing results, it is highly desirable to rigorously prove or disprove Eq. (13).

Substituting Eqs. (11) and (12) into Eq. (7), one immediately has

$$\Delta_{-1} \geqslant \frac{\Delta_{-2}\Delta_2}{\sqrt{(\Delta_2)^2-(4\Delta_{-2})^{-2}}}, \tag{20}$$

which is simpler than Eq. (9). Table I shows that Eq. (20) derived here is numerically more accurate than Eq. (9) derived by Romera *et al*. The numerical Hartree-Fock wave functions [8] were used to calculate the uncertainty products involved [1].

TABLE II. Comparison of the accuracies of the lower bounds to Δ_2 based on functions of Δ_{-2}. All numbers are in atomic units. The data for Δ_2 and Δ_{-2} are from Ref. [1].

			Accuracy [a] (in %)		
Z	Δ_{-2}	Δ_2	Eq. (17) [b]	Eq. (23) [c]	Eq. (22)
1	0.31623	1.7321	86.60	91.28	45.64
2	0.28560	1.8413	81.46	88.15	47.54
6	0.14854	5.3738	27.91	40.50	31.32
15	0.11002	9.5734	15.67	27.83	23.74
20	0.059872	13.838	10.84	31.84	30.17
29	0.093713	11.217	13.37	26.84	23.78
30	0.081313	11.756	12.76	28.73	26.15
45	0.081761	15.612	9.61	21.54	19.59
48	0.071069	16.053	9.34	23.59	21.91
65	0.050345	21.977	6.83	23.49	22.59
72	0.057027	21.079	7.12	21.84	20.80
92	0.044760	27.402	5.47	21.02	20.38

[a]Following Romera *et al.* [1], the accuracy of the expression $A \leqslant B$ as the ratio A/B (in percent).
[b]Equation (17) is equivalent to Eq. (3) of Ref. [1].
[c]Equation (23) is equivalent to Eq. (21) of Ref. [1].

Moreover, using the same Faris inequalities [6], Eq. (10), one can easily show that

$$(4\Delta_{-2}\Delta_2)^2 \equiv \left(\frac{4\langle p^2\rangle}{\langle r^{-2}\rangle}\right)\left(\frac{4\langle r^2\rangle}{\langle p^{-2}\rangle}\right) \geqslant 1, \tag{21}$$

which directly ensures the non-negativity of the argument of the square root in the denominator of Eq. (20)

$$\Delta_2 \geqslant (4\Delta_{-2})^{-1}. \tag{22}$$

Thus, Eq. (20) is always meaningful and real.

Interestingly, Eq. (22) is a new lower bound to Δ_2 in terms of Δ_{-2}. Table II shows that Eq. (22) is less sensitive than Eq. (21) of Ref. [1],

$$\Delta_2 \geqslant \frac{z+\sqrt{z^2+12}}{4}, \tag{23}$$

$$z \equiv 2\Delta_{-2}+(2\Delta_{-2})^{-1}, \tag{24}$$

but definitely much better than Eq. (17) for neutral atoms with nuclear charge $Z \geqslant 6$.

We have provided numerical evidence that demonstrates the benefit of a more sensitive choice of the inequalities in the derivation of the general uncertaintylike relationships in quantum mechanics. This should encourage more effort towards this direction in future research.

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