Improved lower bounds for uncertainty-like relationships in many-body systems

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We show that employing more stringent inequalities in the derivation of uncertainty-like 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 uncertainty-like relationships in quantum mechanics [1,3,4]. Basically, these authors have discussed the following uncertainty products:

\[
\Delta(a,b) = \left( \frac{\langle r^a \rangle}{N} \right)^{1/a} \left( \frac{\langle p^b \rangle}{N} \right)^{1/b},
\]

(1)

where radial expectation values are defined as

\[
\langle r^a \rangle = \int r^a \rho(r)d\mathbf{r}, \quad \langle p^a \rangle = \int p^a \gamma(p)d\mathbf{p},
\]

(2)

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

\[
\int \rho(r)d\mathbf{r} = \int \gamma(p)d\mathbf{p} = N.
\]

(3)

In particular, these authors have discussed in depth the uncertainty-like relationships involving \( \Delta_{-1} \), \( \Delta_{-2} \), and \( \Delta_2 \), where \( \Delta_n = \Delta(a,a) \). From the definition in Eq. (1), one can explicitly write

\[
\Delta_{-1} = \frac{N^2}{\langle r^{-1} \rangle \langle p^{-1} \rangle},
\]

(4)

\[
\Delta_2 = \frac{\sqrt{\langle r^2 \rangle \langle p^2 \rangle}}{N},
\]

(5)

\[
\Delta_{-2} = \frac{N}{\sqrt{\langle r^{-2} \rangle \langle p^{-2} \rangle}}.
\]

(6)

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

\[
\Delta_{-1} \geq \frac{4\Delta_{-2}\Delta_2}{\sqrt{(4\Delta_2)^2 + (\Delta_{-2})^{-2} - 4\langle r^2 \rangle \langle p^2 \rangle \langle p^{-2} \rangle / N^2}}.
\]

(7)

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

\[
\frac{\langle r^2 \rangle \langle p^{-2} \rangle}{N^2} \geq 1, \quad \frac{\langle p^2 \rangle \langle p^{-2} \rangle}{N^2} \geq 1,
\]

(8)

these authors could further show that [1]

\[
\Delta_{-1} \geq \frac{4\Delta_{-2}\Delta_2}{\sqrt{(4\Delta_2)^2 + (\Delta_{-2})^{-2} - 4}}.
\]

(9)

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

\[
4\langle p^2 \rangle \geq \langle r^{-2} \rangle, \quad 4\langle r^2 \rangle \geq \langle p^{-2} \rangle.
\]

(10)

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

\[
\frac{4\langle p^2 \rangle \langle p^{-2} \rangle}{N^2} \geq \langle r^{-2} \rangle \langle p^{-2} \rangle = (\Delta_{-2})^{-2},
\]

(11)

\[
\frac{4\langle r^2 \rangle \langle p^{-2} \rangle}{N^2} \geq \langle r^{-2} \rangle \langle p^{-2} \rangle = (\Delta_{-2})^{-2}.
\]

(12)

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

\[
\Delta_{-2} \leq \frac{1}{2},
\]

(13)

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

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

\[
\frac{2\Delta_2}{x + 6 + \sqrt{x(x + 8)}} \leq \Delta_{-2} \leq \frac{2\Delta_2}{x + 6 - \sqrt{x(x + 8)}},
\]

(14)

\[
x = 4\Delta_2^2 - 9,
\]

(15)

can be further simplified as

\[
\frac{2\Delta_2}{x + 6 + \sqrt{x(x + 8)}} \leq \Delta_{-2} \leq \frac{1}{2}.
\]

(16)

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

\[
\frac{(A - B)(A + B)}{A^2 - B^2} \geq 1, \quad A \geq B > 0,
\]

(17)
TABLE I. Improved lower bounds to $\Delta_{-1}$ from Eq. (7) involving the uncertainty products $\Delta_{2}$, $\Delta_{-2}$, and $\Delta_{1}$. All numbers are in atomic units. The data for $\Delta_{2}$, $\Delta_{-2}$, and $\Delta_{-1}$ are from Ref. [1].

<table>
<thead>
<tr>
<th>$Z$</th>
<th>$\Delta_{-2}$</th>
<th>$\Delta_{1}$</th>
<th>$\Delta_{2}$</th>
<th>Accuracy $^a$ (in %)</th>
<th>Eq. (9) $^b$</th>
<th>Eq. (20)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.31623</td>
<td>0.58905</td>
<td>1.7321</td>
<td>52.6</td>
<td>60.3</td>
<td></td>
</tr>
<tr>
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<td>0.55372</td>
<td>1.8413</td>
<td>49.7</td>
<td>58.6</td>
<td></td>
</tr>
<tr>
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<td>36.7</td>
<td></td>
</tr>
<tr>
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<td>0.41000</td>
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<td>27.6</td>
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</tr>
<tr>
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<td>0.52219</td>
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</tr>
<tr>
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<td>0.48903</td>
<td>15.612</td>
<td>16.4</td>
<td>17.0</td>
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</tr>
<tr>
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<td>21.079</td>
<td>12.1</td>
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<tr>
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<td>0.044760</td>
<td>0.41726</td>
<td>27.402</td>
<td>10.5</td>
<td>11.0</td>
<td></td>
</tr>
</tbody>
</table>

$^a$Following Romera et al. [1], the accuracy of the expression $A \equiv B$ 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].

$$\Delta_{2} \geq \frac{3}{2}. \quad (17)$$

Then it also follows that

$$\frac{2\Delta_{2}}{x + 6 + \sqrt{x(x+8)}} \leq 1 \leq \frac{2\Delta_{2}}{x + 6 - \sqrt{x(x+8)}}, \quad (18)$$

which simply says that the upper bound of Eq. (14) is always less sensitive than $\frac{3}{2}$ if Eq. (13) is true in general. Equations (13) and (17) indicate a zero overlap between $\Delta_{-2}$ and $\Delta_{2}$. 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),

$$\Delta_{-2} \leq \frac{1}{2} \leq \min\{\Delta(-2,2), \Delta(2,-2)\}, \quad (19)$$

which suggests that $\Delta_{-2}$ 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

$$\Delta_{-1} \geq \frac{\Delta_{-2}\Delta_{2}}{\sqrt{(\Delta_{2})^2 - (4\Delta_{-2})^2}}, \quad (20)$$

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 $\Delta_{2}$ based on functions of $\Delta_{-2}$. All numbers are in atomic units. The data for $\Delta_{2}$ and $\Delta_{-2}$ are from Ref. [1].

<table>
<thead>
<tr>
<th>$Z$</th>
<th>$\Delta_{-2}$</th>
<th>$\Delta_{2}$</th>
<th>Accuracy $^a$ (in %)</th>
<th>Eq. (17) $^b$</th>
<th>Eq. (23) $^c$</th>
<th>Eq. (22)</th>
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<td>27.402</td>
<td>5.47</td>
<td>21.02</td>
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<td></td>
</tr>
</tbody>
</table>

$^a$Following Romera et al. [1], the accuracy of the expression $A \equiv B$ 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

$$(4\Delta_{-2}\Delta_{2})^2 \geq \frac{4\langle r^2 \rangle}{\langle r^2 - \frac{z}{2} \rangle} \left( \frac{4\langle r^2 \rangle}{\langle p^2 \rangle} \right) \geq 1, \quad (21)$$

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

$$\Delta_{2} \geq (4\Delta_{-2})^{-1}, \quad (22)$$

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

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

$$\Delta_{2} \geq \frac{z + \sqrt{z^2 + 12}}{4}, \quad (23)$$

$$z = 2\Delta_{-2} + (2\Delta_{-2})^{-1}, \quad (24)$$

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

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

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[7] We thank Dr. J. C. Angulo for this comment.