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Abstract. Rigorous relationships among radial and logarithmic expectation values of an N-body system are obtained by means of information-theoretic methods. Especially interesting are the uncertainty expressions in terms of the product $\langle r^\alpha \rangle^{1/\alpha} \langle p^\beta \rangle^{1/\beta}$, which generalize the well known relation $\langle r^2 \rangle \langle p^2 \rangle \geqslant 9N^2/4$. Additionally, an inequality involving the uncertainty in the logarithmic radius and the logarithmic momentum is shown. For illustration, the accuracy of the inequalities found are numerically analysed in a Hartree–Fock framework for atomic systems. Finally, it is pointed out how these inequalities are improved in atoms by taking into account other physical quantities or by considering some semiempirical results on atomic information entropies.

The one-particle density $\rho(r)$ is a fundamental quantity in the study of the physical and chemical properties of many-fermion systems (Parr and Yang 1989). Since Hohenberg and Kohn (1964) formulated their theorem about the existence of a universal functional $E[\rho]$ for the energy of the many-fermion system, much effort has been paid in the study of the function $\rho(r)$.

The extension of this theory to the momentum space (Levy 1979, Henderson 1981, Pathak *et al* 1982, Das *et al* 1988), i.e. the description of physical quantities in terms of the momentum density $\gamma(p)$, greatly increased the interest in the study of the one-particle densities in both configuration and momentum spaces.

For atomic systems, it is known that some quantities related to the one-particle densities, like radial charge $\langle r^\alpha \rangle \equiv \int r^\alpha \rho(r) \, dr$ and momentum $\langle p^\alpha \rangle \equiv \int p^\alpha \gamma(p) \, dp$ expectation values, describe physically interesting and/or experimentally measurable quantities (Epstein 1973) such as, e.g. electron–nucleus attraction energy (essentially $\langle r^{-1} \rangle$), diamagnetic susceptibility (proportional to $\langle r^2 \rangle$), the height of the Compton profile peak in electron scattering (half of $\langle p^{-1} \rangle$) and kinetic energy and its relativistic correction due to the mass variation (essentially $\langle p^2 \rangle$ and $\langle p^4 \rangle$, respectively). Moreover, the mean logarithmic values $\langle \ln r \rangle$ and $\langle (\ln r)^2 \rangle$ as well as $\langle \ln p \rangle$ and $\langle (\ln p)^2 \rangle$ have been shown (Angulo and Dehesa 1992) to play a relevant role in the study of the atomic structure by using information-theoretic methods. Additionally, the quantity $\langle \ln r \rangle$ determines the high-energy behaviour of the phase shifts in electron scattering for low angular momentum (Lenz and Rosenfelder 1971, Friedrich and Lenz 1972).

Many relationships involving two or more radial expectation values are known (Gadre 1979, Gadre and Pathak 1981, Angulo and Dehesa 1991a,b, Angulo and Dehesa 1993). However, most of them relate values either in configuration or in momentum space. Among the inequalities which involve simultaneously both values $\langle r^\alpha \rangle$ and $\langle p^\alpha \rangle$, we should mention the well known uncertainty expression (Heisenberg 1927, Yue and Janmin 1984, Gadre and Chakravorty 1986)

$$\langle r^2 \rangle \langle p^2 \rangle \geqslant \tfrac{9}{4} N^2$$

(where the normalization is given by $\langle r^0 \rangle = \langle p^0 \rangle = N$, N being the number of particles of the system), as well as some other non-rigorous inequalities based on semiclassical results (Porras and Gálvez 1990). Atomic units ($\hbar = m = |e| = 1$, where $\hbar$ is Planck's constant and m and e are the mass and the charge of the electron, respectively) are used throughout this paper.

Here, we are going to obtain a family of more general uncertainty relationships among the quantities $\{\langle r^\alpha \rangle, \langle p^\alpha \rangle, \langle \ln r \rangle, \langle (\ln r)^2 \rangle, \langle \ln p \rangle, \langle (\ln p)^2 \rangle\}$. To do that, we use some information-theoretic methods (Shannon 1948a, b, Guiaşu 1977).

A very important result concerning information entropies in quantum mechanics was shown in (Bialynicki-Birula and Mycielski 1975), where a lower bound to the sum $S_\rho + S_\gamma$ of the information entropies associated with the one-particle densities of a N-body system in position and momentum spaces is given in the form

$$S_\rho + S_\gamma \geqslant 3N(1 + \ln \pi) - 2N \ln N \equiv S_{\text{sum}} \tag{1}$$

where S_ρ and S_γ are defined by

$$S_\rho \equiv - \int \rho(r) \ln \rho(r) \, dr \qquad S_\gamma \equiv - \int \gamma(p) \ln \gamma(p) \, dp.$$

The same authors (Bialynicki-Birula and Mycielski 1975) pointed out that this inequality saturates only in the case of Gaussian wavefunctions.

Recently, rigorous upper bounds to the information entropy

$$S_f \equiv - \int f(x) \ln f(x) \, dx$$

of any density function $f(x)$ defined over $\mathbb{R}^3$ and normalized to N have been derived in terms of radial $\langle x^\alpha \rangle \equiv \int x^\alpha f(x) \, dx$ and logarithmic $\langle \ln x \rangle \equiv \int \ln x f(x) \, dx$ expectation values, where $x \equiv |x|$. These bounds are expressed in a quite simple form (Angulo and Dehesa 1992)

$$S_f \leqslant A_\alpha(z) + Nz \ln \langle x^\alpha \rangle + (3 - z\alpha) \langle \ln x \rangle \tag{2}$$

for any $z > 0$, $\alpha \neq 0$, and where

$$A_\alpha(z) \equiv N \ln \frac{4\pi \Gamma(z) e^z}{|\alpha| z^z N^{z+1}}.$$

An interesting case corresponds to $z = 3/\alpha$, for which the inequality does not contain the logarithmic expectation value

$$S_f \leqslant A_\alpha + 3N \ln \langle x^\alpha \rangle^{1/\alpha} \equiv S_f(1) \tag{3}$$

for $\alpha > 0$, and where $A_\alpha \equiv A_\alpha(3/\alpha)$.

Furthermore, another upper bound, which involves only logarithmic values, has been found (Angulo and Dehesa 1992)

$$S_f \leqslant B + N \ln \Delta \langle \ln x \rangle + 3 \langle \ln x \rangle \equiv S_f(2) \tag{4}$$

where

$$B \equiv \frac{N}{2}\left(1 + \ln\frac{32\pi^3}{N^4}\right)$$

and $\Delta(\ln x) \equiv \sqrt{N\langle(\ln x)^2\rangle - \langle\ln x\rangle^2}$ is the uncertainty in the logarithm of x.

Let us now consider the application of the rigorous inequalities (3) and (4) to the case of the atomic charge and momentum densities, $\rho(r)$ and $\gamma(p)$ respectively. In doing so, we should keep in mind that the normalization constraints $\int \rho(r)\,dr = \int \gamma(p)\,dp = N$ imply that the dimensions of $\rho(r)$ have to be the same as r^{-3}, and similarly for $\gamma(p)$ with respect to p^{-3}. The combination of the aforementioned inequalities together with (1) gives rise to the following general inequalities valid for any N-particle system

$$S_{\text{sum}} \leqslant S_\rho + S_\gamma \leqslant S_\rho(t) + S_\gamma(t) \tag{5}$$

with $t = 1, 2$, respectively. In the case $t = 1$, after a simple change of variable, one has

$$\langle r^{3/\alpha}\rangle^\alpha \langle p^{3/\beta}\rangle^\beta \geqslant \frac{9\pi}{16} \frac{\alpha^\alpha \beta^\beta e^{3-\alpha-\beta}}{\Gamma(\alpha+1)\Gamma(\beta+1)} N^{\alpha+\beta} \equiv C_{\alpha\beta} \tag{6}$$

for any $\alpha, \beta > 0$. Notice that the left-hand side of the above expression has dimensions of $\hbar^3$. The same occurs in the right-hand side if we remember that $\hbar = 1$ in the system of atomic units. The interesting expression $\langle r^2\rangle\langle p^2\rangle \geqslant 9N^2/4 = C_{22}$, reported by several authors (Heisenberg 1927, Yue and Janmin 1984, Gadre and Chakravorty 1986), is obtained as a particular case of the more general equation (6). Other particular cases are

$$\langle r\rangle\langle p\rangle \geqslant \frac{9\pi^{1/3}}{4e}N^2 = C_{11}$$

$$\langle r\rangle^2\langle p^2\rangle \geqslant \frac{27\pi^{1/3}}{8e}N^3 = C_{12}$$

$$\langle r^2\rangle\langle p\rangle^2 \geqslant \frac{27\pi^{1/3}}{8e}N^3 = C_{21}.$$

Now, let us consider the relationships in terms of the logarithmic uncertainties $\Delta(\ln r)$ and $\Delta(\ln p)$. They are obtained by taking into account the value $t = 2$ in (5). Then, one obtains that

$$\Delta(\ln r)\Delta(\ln p) \geqslant \frac{N^2}{32}\exp\left\{2 - 3\frac{\langle\ln r\rangle + \langle\ln p\rangle}{N}\right\} \equiv C_\Delta. \tag{7}$$

It is worthwhile pointing out that all these expressions are valid for any N-particle system (e.g. atoms, molecules, nuclei, clusters).

For completeness, let us analyse numerically the accuracy of the main inequalities (6) and (7) in the case of ground-state atomic systems. In doing so, we have used the atomic near-Hartree–Fock wavefunctions of (Clementi and Roetti 1974), which are a linear combination of Slater-type orbitals in position space. In table 1, the accuracy of the lower bounds $C_{11}, C_{12}, C_{21}, C_{22}, C_\Delta$ is shown. It is observed that the quality of the bounds rapidly decreases when the atomic number increases. At this moment, it is worth pointing out that

Table 1. Accuracy (in percent) of the lower bounds C_{11}, C_{12}, C_{21}, C_{22}, C_Δ (see text for details) for some neutral atoms of the periodic table. The atomic wavefunctions of (Clementi and Roetti 1974) have been used.

N	C_{11}	C_{12}	C_{21}	C_{22}	C_Δ
1	95.2	80.8	84.1	75.0	84.0
2	93.4	73.9	78.4	66.4	81.0
3	44.3	13.1	11.0	7.3	22.6
6	42.2	10.2	13.6	7.8	13.3
10	43.6	11.4	15.7	9.3	11.0
15	27.5	4.0	4.6	2.5	5.5
21	22.1	2.4	2.5	1.2	3.9
33	21.8	2.4	2.7	1.3	2.7

the atomic wavefunctions are not Gaussian, so the inequality (1) can never be saturated. Consequently, the inequalities (6) and (7) cannot be saturated in atoms.

Non-rigorously, one could improve these results by taking into account the numerical observation that $S_\rho + S_\gamma \geqslant N(5.91 - \ln N)$ for all neutral atoms from hydrogen through xenon, a much better lower bound for the sum of entropies $S_\rho + S_\gamma$ than that of (1). But this new inequality has not been rigorously proved. The corresponding expressions in this case are

$$\langle r^{3/\alpha}\rangle^\alpha \langle p^{3/\beta}\rangle^\beta \geqslant \frac{9}{16\pi^2} \frac{\alpha^\alpha \beta^\beta e^{5.91-\alpha-\beta}}{\Gamma(\alpha+1)\Gamma(\beta+1)} N^{\alpha+\beta+1} \equiv C'_{\alpha\beta}$$

$$\Delta(\ln r)\Delta(\ln p) \geqslant \frac{N^3}{32\pi^3} \exp\left\{4.91 - 3\frac{\langle \ln r\rangle + \langle \ln p\rangle}{N}\right\} \equiv C'_\Delta.$$

Then, the accuracy of the bounds C'_{11}, C'_{12}, C'_{21}, C'_{22}, C'_Δ oscillates between 50–99%, 12–83%, 11–88%, 5–74% and 40–96%, respectively, for all ground-state atoms from hydrogen through xenon. Finally, we should mention that it is also possible to correlate the quantities $\langle r^\alpha\rangle$, $\langle p^\beta\rangle$, $\langle \ln r\rangle$ and $\langle \ln p\rangle$ in forms other than those given by (6) and (7) by using inequalities (1) and (2).

In summary, several uncertainty relationships among different quantities of finite many-body systems have been obtained by means of information-theoretic methods. The new relationships substantially generalize the celebrated lower bound $\langle r^2\rangle\langle p^2\rangle \geqslant 9N^2/4$. The numerical study of these relationships in a Hartree–Fock framework reveals that, in neutral atoms, their accuracy rapidly decreases when increasing the atomic number. Finally, it is pointed out that it is possible to obtain non-rigorous but more accurate relationships in the atomic case by taking into account numerical estimates on atomic information entropies.

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