Information entropy and uncertainty in $D$-dimensional many-body systems

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Several entropic and uncertainty-like results for three-dimensional many-particle systems are extended to the case of arbitrary dimensionality $D$. This work deals with (i) upper bounds to information entropies and (ii) radial and logarithmic uncertainty-like relationships. The resulting expressions are given in an analytical compact form for any dimensionality. The first few low-dimensional cases ($D = 1, 2, 3, 4$) are emphasized.

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I. INTRODUCTION

The general density functional theory which begins with the Hohenberg-Kohn theorem [1] allows us to assume the existence of a universal functional $E[\rho]$ of the one-particle density $\rho(\mathbf{r})$ for the energy of many-fermion systems. This result has greatly emphasized the relevant role played by the quantity $\rho(\mathbf{r})$ in the study of the physical properties of such systems [2]. The extension of this theory to the momentum space [3] increases also the interest in a deeper knowledge of the one-particle momentum density $\gamma(\mathbf{p})$.

The further consideration of systems of dimensionality $D$, not necessarily equal to 3, is of fundamental importance, as it is observed in several fields of physics [4], such as condensed matter [5], magnetism [6], and atomic physics [7].

In this work, we will center our attention in the following density-dependent quantities of $D$-dimensional many-particle systems:

(i) radial expectation values, $\langle r^\alpha \rangle \equiv \int r^\alpha \rho(\mathbf{r})d^D r$;

(ii) mean logarithmic values, $\langle \ln r \rangle \equiv \int \ln r \rho(\mathbf{r})d^D r$ and $\langle (\ln r)^2 \rangle \equiv \int (\ln r)^2 \rho(\mathbf{r})d^D r$;

(iii) information entropy, $S_\rho \equiv -\int \rho(\mathbf{r}) \ln [\rho(\mathbf{r})]d^D r$;

and the corresponding momentum quantities $\langle p^\alpha \rangle$, $\langle (\ln p)^\alpha \rangle$, and $S_\gamma$ obtained from the momentum density $\gamma(\mathbf{p})$. Here, $\mathbf{r} = (x_1, x_2, \ldots, x_D)$, $\mathbf{r} = |\mathbf{r}|$, and $d^D r = dx_1 dx_2 \cdots dx_D$. The normalization is given by $\langle \sqrt{\mathbf{r}} \rangle = (\mathbf{p}^{\mathbf{r}}) = N$ ($N$ being the number of particles of the system).

The importance of the radial expectation values $\langle r^\alpha \rangle$ and $\langle p^\alpha \rangle$ in three-dimensional atomic systems is well known [8]. For instance, $\langle r^2 \rangle$ is related to the diamagnetic susceptibility, $\langle r^{-1} \rangle$ to the electron-nucleus attraction energy, $\langle r^{-2} \rangle$ to the height of the peak of the Compton profile, and $\langle p^2 \rangle$ and $\langle p^4 \rangle$ to the kinetic energy and its relativistic correction due to mass variation, respectively.

On the other hand, the mean logarithmic radius $\langle \ln r \rangle$ determines [9] the high-energy behavior of the phase shifts in electron scattering for low angular momentum, and together with other logarithmic expectation values and the information entropies $S_\rho$ and $S_\gamma$, it is important in the study of the structure and collisional phenomena [10,11] of atomic and molecular systems.

Recently [11,12] several relationships among the aforementioned quantities were obtained by means of information-theoretic methods. Among them, we should mention

(i) upper and lower bounds to the atomic information entropies $S_\rho$ and $S_\gamma$ in terms of radial and/or logarithmic expectation values [11],

(ii) uncertainty-like relationships among radial expectation values [12], and

(iii) uncertainty-like relationships among logarithmic expectation values [12].

The aim of this work is to extend these relationships to many-particle systems with arbitrary dimensionality. In Sec. II, the bounds to $S_\rho$ and $S_\gamma$ are extended. The same extension is carried out for radial and logarithmic uncertainty-like relationships in Secs. III and IV, respectively. Finally, some concluding remarks are given in Sec. V.

II. BOUNDS TO INFORMATION ENTROPIES

Following the same technique as in Ref. [11], we obtain a family of upper bounds to $S_\rho$ and $S_\gamma$. The non-negativity of the relative entropy [13] $I(p, f)$ associated to two probability density functions $p(\mathbf{r})$ and $f(\mathbf{r})$, assuming that $\int p(\mathbf{r})d\mathbf{r} = \int f(\mathbf{r})d\mathbf{r} = N$, provides the above mentioned bounds. The relative entropy is defined as

$$I(p, f) \equiv \int p(\mathbf{r}) \ln \frac{p(\mathbf{r})}{f(\mathbf{r})}d\mathbf{r}. \quad (1)$$

Keeping in mind that $S_\rho = -\int p(\mathbf{r}) \ln [p(\mathbf{r})]d\mathbf{r}$ it is easy to show that

$$S_\rho \leq -\int p(\mathbf{r}) \ln [f(\mathbf{r})]d\mathbf{r} \equiv S_\rho^* \quad (2)$$
for any \( f(r) \) such that \( \int p(r)dr = \int f(r)dr = N \).

The consideration of spherically symmetric density functions \( f(r) \) allows us to replace the \( D \)-dimensional volume element \( dr \) by \( r^{D-3}\Omega_D dr \), where \( \Omega_D = 2\pi^{D/2}/\Gamma(D/2) \) is the \( D \)-dimensional solid angle, and where \( 0 \leq r < \infty \). Particularly interesting cases are \( \Omega_1 = 1 \), \( \Omega_2 = 2\pi \), and \( \Omega_3 = 4\pi \).

Here we will only extend Eqs. (15) and (36) of Ref. [11] to arbitrary dimensionality. The following expressions are obtained for a \( N \)-particle system:

\[
S_\rho \leq A_D(\alpha, z) + zN\ln(r^\alpha) + (D - \alpha z)(\ln r)
\]

(3a)

for all \( z > 0 \), \( \alpha > -D \), where

\[
A_D(\alpha, z) = N \left[ z + \ln \frac{\Omega_D \Gamma(z)}{\alpha z^{D-1}} \right]
\]

(3b)

and

\[
S_\rho \leq B_D + N\ln \Delta(\ln r) + D(\ln r),
\]

(4a)

where

\[
B_D = N \left[ \frac{1}{2} + \ln \left( \frac{\sqrt{2}\pi D}{N^2} \right) \right]
\]

(4b)

and

\[
\Delta(\ln r) = \sqrt{N((\ln r)^2) - (\ln r)^2}.
\]

(4c)

Similar expressions in terms of the corresponding momentum-space quantities are also valid.

For the first upper bound [Eqs. (3)], it is specially interesting the particular case \( z = D/\alpha \), because it provides an upper bound to \( S_\rho \) (or \( S_\gamma \)) in terms of only one radial expectation value \( \langle r^\alpha \rangle \) (or \( \langle p^\alpha \rangle \)) of positive order:

\[
S_\rho \leq A_D(\alpha, D/\alpha) + \frac{DN}{\alpha}(\ln r^\alpha)
\]

(5)

for \( \alpha > 0 \).

Some particular subcases of Eq. (5) are

\[
S_\rho \leq \begin{cases} 
N \left[ D + \ln \frac{\Omega_D(D-1)!}{\alpha^{D-1}} \right], & \alpha = 1 \\
\frac{DN}{2} \left[ 1 + \ln \frac{2\pi}{\alpha N^{1/4}} \right], & \alpha = 2 .
\end{cases}
\]

(6)

III. RADIAL UNCERTAINTYLIKE RELATIONSHIPS

A stronger version of Heisenberg’s uncertainty principle in terms of the information entropies \( S_\rho \) and \( S_\gamma \) of any quantum many-particle system is known [14], namely,

\[
S_\rho + S_\gamma \geq DN(1 + \ln \pi) - 2N\ln N,
\]

(7)

where \( D \) is the dimensionality of the system. This result, together with the above mentioned upper bounds [Eq. (5)] to \( S_\rho \) and \( S_\gamma \), in terms of one radial expectation value, allow us to obtain a set of radial uncertaintylike relationships [12], i.e., lower bounds to the product \( \langle r^\alpha \rangle^{1/\alpha} \langle p^\beta \rangle^{1/\beta} \) for any positive \( \alpha \) and \( \beta \) in the three-dimensional case.

Here we extend this result from \( D = 3 \) to any \( D \). Now, Eq. (6) of Ref. [12] reads as

\[
\langle r^D/\alpha \rangle^{\alpha} \langle p^D/\beta \rangle^{\beta} \geq \frac{\Gamma^2(1 + D/2)}{(1 + \alpha)(1 + \beta)} e^{D - \alpha - \beta} N^{\alpha + \beta}.
\]

(8)

Some particular cases of Eq. (8) are

\[
\langle r \rangle \langle p \rangle \geq \frac{D_2}{e} \left( \frac{\Gamma(1 + D/2)}{\Gamma(1 + D)} \right)^{2/D} N^2,
\]

\[
\langle r^2 \rangle \langle p^2 \rangle \geq \frac{D_3}{2e} \left( \frac{\Gamma(1 + D/2)}{\Gamma(1 + D)} \right)^{2/D} N^3,
\]

\[
\langle r^2 \rangle \langle p \rangle^2 \geq \frac{D_3}{2e} \left( \frac{\Gamma(1 + D/2)}{\Gamma(1 + D)} \right)^{2/D} N^3,
\]

\[
\langle r^2 \rangle \langle p^2 \rangle \geq \frac{D_2}{4} N^2,
\]

and for different dimensionalties, Eq. (8) reads as

\[
\langle r^{1/\alpha} \rangle^{\alpha} \langle p^{1/\beta} \rangle^{\beta} \geq \frac{\pi^{\alpha+\beta} e^{1-\alpha-\beta}}{4}\frac{\alpha^\beta}{\Gamma(1 + \alpha)\Gamma(1 + \beta)} N^{\alpha + \beta} \quad (D = 1),
\]

\[
\langle r^{2/\alpha} \rangle^{\alpha} \langle p^{2/\beta} \rangle^{\beta} \geq \frac{e^{2-\alpha-\beta}}{\Gamma(1 + \alpha)\Gamma(1 + \beta)} N^{\alpha + \beta} \quad (D = 2),
\]

\[
\langle r^{3/\alpha} \rangle^{\alpha} \langle p^{3/\beta} \rangle^{\beta} \geq \frac{9\pi^{\alpha+\beta} e^{3-\alpha-\beta}}{16}\frac{\alpha^\beta}{\Gamma(1 + \alpha)\Gamma(1 + \beta)} N^{\alpha + \beta} \quad (D = 3),
\]

\[
\langle r^{4/\alpha} \rangle^{\alpha} \langle p^{4/\beta} \rangle^{\beta} \geq \frac{4\pi^{\alpha+\beta} e^{4-\alpha-\beta}}{\Gamma(1 + \alpha)\Gamma(1 + \beta)} N^{\alpha + \beta} \quad (D = 4).
\]

IV. LOGARITHMIC UNCERTAINTYLIKE RELATIONSHIPS

Following the same procedure described in the previous section, one can obtain a relationship involving only logarithmic expectation values. In doing so, we join the upper bounds to \( S_\rho \) and \( S_\gamma \) given by Eqs. (4) and the lower bound to \( S_\rho + S_\gamma \) of Eq. (7), to get

\[
\Delta(\ln r) \Delta(\ln p) \geq \frac{N^2\Gamma^2(D/2)}{8\pi} \exp \left\{ D - 1 - D \frac{(\ln r) + (\ln p)}{N} \right\}.
\]

The lowest dimensionality cases are
\[ \Delta (\ln r) \Delta (\ln p) \geq \begin{cases} 
\frac{N^2}{8} \exp \left\{ \frac{-(\ln r)^2 + (\ln p)^2}{N} \right\}, & D = 1 \\
\frac{N^2}{8 \pi} \exp \left\{ 1 - 2 \frac{\ln r + \ln p}{N} \right\}, & D = 2 \\
\frac{N^2}{32} \exp \left\{ 2 - 3 \frac{\ln r + \ln p}{N} \right\}, & D = 3 \\
\frac{N^2}{8 \pi} \exp \left\{ 3 - 4 \frac{\ln r + \ln p}{N} \right\}, & D = 4. 
\end{cases} \]

are given in a compact analytical form, independently of the number of dimensions involved, and are expressed in terms of physically meaningful and/or relevant density-dependent quantities. Finally, let us remark the usefulness of this kind of result in fields like statistical and quantum mechanics, in which sometimes it is necessary to deal with a large number of dimensions.

V. CONCLUDING REMARKS

The same mathematical technique which allowed us to obtain several bounds to information entropies and uncertainty-like relationships for three-dimensional many-particle systems can be applied to the study of quantum-mechanical problems involving an arbitrary dimensionality. The results, valid for any many-particle system, are given a compact analytical form, independently of the number of dimensions involved, and are expressed in terms of physically meaningful and/or relevant density-dependent quantities. Finally, let us remark the usefulness of this kind of result in fields like statistical and quantum mechanics, in which sometimes it is necessary to deal with a large number of dimensions.

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