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

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(Received 4 February 1994)

Several entropic and uncertaintylike 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 uncertaintylike 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.

PACS number(s): 31.15.+q, 02.50.Cw

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_γ obtained from the momentum density $\gamma(\mathbf{p})$. Here, $\mathbf{r} = (x_1, x_2, \ldots, x_D)$, $r = |\mathbf{r}|$, and $d^D r = dx_1 dx_2 \cdots dx_D$. The normalization is given by $\langle r^0\rangle = \langle p^0\rangle = N$ (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, $\langle p^{-1}\rangle$ 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_ρ and S_γ, 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_ρ and S_γ in terms of radial and/or logarithmic expectation values [11],

(ii) uncertaintylike relationships among radial expectation values [12], and

(iii) uncertaintylike 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_ρ and S_γ are extended. The same extension is carried out for radial and logarithmic uncertaintylike 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_ρ and S_γ. The nonnegativity 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

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

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

$$S_p \le -\int p(\mathbf{r}) \ln[f(\mathbf{r})] d\mathbf{r} \equiv S_p^* \qquad (2)$$

for any $f(\mathbf{r})$ such that $\int \rho(\mathbf{r})d\mathbf{r} = \int f(\mathbf{r})d\mathbf{r} = N$.

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

$$S_\rho \le A_D(\alpha, z) + zN\ln\langle r^\alpha\rangle + (D-\alpha z)\langle \ln r\rangle \quad (3a)$$

for all $z > 0$, $\alpha > -D$, where

$$A_D(\alpha, z) \equiv N\left[z + \ln\frac{\Omega_D\Gamma(z)}{|\alpha| z^z N^{z+1}}\right] \quad (3b)$$

and

$$S_\rho \le B_D + N\ln\Delta(\ln r) + D\langle\ln r\rangle, \quad (4a)$$

where

$$B_D \equiv N\left[\frac{1}{2} + \ln\left(\frac{\sqrt{2\pi}\Omega_D}{N^2}\right)\right] \quad (4b)$$

and

$$\Delta(\ln r) \equiv \sqrt{N\langle(\ln r)^2\rangle - \langle\ln r\rangle^2}\,. \quad (4c)$$

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_ρ (or S_γ) in terms of only one radial expectation value $\langle r^\alpha\rangle$ (or $\langle p^\alpha\rangle$) of positive order:

$$S_\rho \le A_D(\alpha, D/\alpha) + \frac{DN}{\alpha}\ln\langle r^\alpha\rangle \quad (5)$$

for $\alpha > 0$.

Some particular subcases of Eq. (5) are

$$S_\rho \le \begin{cases} N\left[D + \ln\frac{\Omega_D (D-1)!\langle r\rangle^D}{D^D N^{D+1}}\right], & \alpha = 1 \\ \frac{DN}{2}\left[1 + \ln\frac{2\pi\langle r^2\rangle}{N^{1+\frac{2}{D}}}\right], & \alpha = 2\,. \end{cases} \quad (6)$$

III. RADIAL UNCERTAINTYLIKE RELATIONSHIPS

A stronger version of Heisenberg's uncertainty principle in terms of the information entropies S_ρ and S_γ of any quantum many-particle system is known [14], namely,

$$S_\rho + S_\gamma \ge DN(1+\ln\pi) - 2N\ln N, \quad (7)$$

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

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

$$\langle r^{D/\alpha}\rangle^\alpha \langle p^{D/\beta}\rangle^\beta \ge \alpha^\alpha\beta^\beta \frac{\Gamma^2\left(1+\frac{D}{2}\right)}{\Gamma(1+\alpha)\Gamma(1+\beta)} e^{D-\alpha-\beta} N^{\alpha+\beta}. \quad (8)$$

Some particular cases of Eq. (8) are

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

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

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

$$\langle r^2\rangle\langle p^2\rangle \ge \frac{D^2}{4}N^2,$$

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

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

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

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

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

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_ρ and S_γ given by Eqs. (4) and the lower bound to $S_\rho + S_\gamma$ of Eq. (7), to get

$$\Delta(\ln r)\Delta(\ln p) \ge \frac{N^2\Gamma^2(D/2)}{8\pi}\exp\left\{D - 1 - D\frac{\langle\ln r\rangle + \langle\ln p\rangle}{N}\right\}.$$

The lowest dimensionality cases are

$$\Delta(\ln r)\Delta(\ln p) \geq \begin{cases} \frac{N^2}{8}\exp\left\{-\frac{\langle\ln r\rangle+\langle\ln p\rangle}{N}\right\}, & D=1 \\ \frac{N^2}{8\pi}\exp\left\{1-2\frac{\langle\ln r\rangle+\langle\ln p\rangle}{N}\right\}, & D=2 \\ \frac{N^2}{32}\exp\left\{2-3\frac{\langle\ln r\rangle+\langle\ln p\rangle}{N}\right\}, & D=3 \\ \frac{N^2}{8\pi}\exp\left\{3-4\frac{\langle\ln r\rangle+\langle\ln p\rangle}{N}\right\}, & D=4. \end{cases}$$

V. CONCLUDING REMARKS

The same mathematical technique which allowed us to obtain several bounds to information entropies and uncertaintylike 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 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.

ACKNOWLEDGMENTS

I am grateful to R. J. Yáñez and Professor J. S. Dehesa of the Departamento de Física Moderna of the Universidad de Granada for helpful comments and for their kind interest in this work. Also, I wish to acknowledge partial financial support from DGICYT under Project No. PB92-0927.

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