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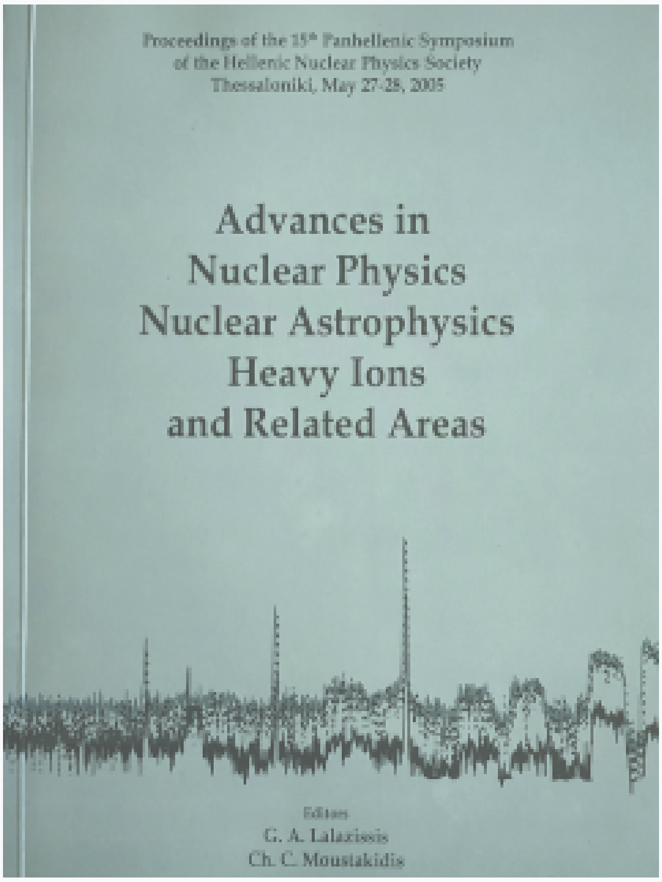

Information Entropy and Information Distances in Atoms, Nuclei and Bosonic Systems

K. Ch. Chatzisavvas, Ch. C. Moustakidis, C. P. Panos

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Information Entropy and Information Distances in Atoms, Nuclei and Bosonic Systems

K. Ch. Chatzisavvas, Ch. C. Moustakidis, C. P. Panos

Department of Theoretical Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece.

Abstract

The universal property for the information entropy $S = a + b \ln Z$ is verified for atoms using a systematic study with Roothaan-Hartree-Fock (RHF) wave functions with atomic number $Z = 2 - 54$. The above relation was proposed previously for atoms, nuclei, atomic clusters and correlated atoms in a trap. Kullback-Leibler relative entropy K and Jensen-Shannon divergence J are employed to compare RHF with Thomas-Fermi (TF) density of atoms as well as another phenomenological density obtained by Sagar et al. Two-body density distributions in position- and momentum-space are used to calculate and compare the corresponding information entropies for correlated and uncorrelated nuclei and bosonic systems (correlated atoms in a trap). It is seen that short-range correlations (SRC) increase the values of S. One-body information entropy entropy S_1 is compared with two-body information entropy and a conjecture is made for N-body information entropy S_N. The entropy K and the divergence J are also used to evaluate the information distance between correlated and uncorrelated densities both at the one- and the two-body levels for nuclei and trapped Bose gases.

1 Theoretical framework

The information entropy for a continuous probability distribution $p(x)$ in one dimension is defined by the expression

$$S = -\int p(x) \ln p(x)\, dx, \quad \text{where} \int p(x)\, dx = 1 \tag{1}$$

S is measured in bits if the base of the logarithm is 2 and nats (natural units of information) if the logarithm is natural. It represents the information content of a probability distribution as well as a measure of uncertainty of the corresponding state. It is noted that the information and the thermodynamic entropy are different concepts but can be connected employing some assumptions.

For a three-dimensional system the information entropy in position-space has the form

$$S_r = -\int \rho(\mathbf{r}) \ln \rho(\mathbf{r})\, d\mathbf{r} \tag{2}$$

and momentum-space is

$$S_k = -\int n(\mathbf{k}) \ln n(\mathbf{k})\, d\mathbf{k} \tag{3}$$

where $\rho(\mathbf{r})$, $n(\mathbf{k})$ are the density distributions in position- and momentum-space respectivelly, normalized to unity.

An important step was the discovery of an entropic uncertainty relation (EUR), which for a three-dimensional system is

$$S = S_r + S_k \geq 3\,(1 + \ln \pi) \simeq 6.434 \tag{4}$$

This inequality, for the information entropy sum in conjugate spaces, is a joint measure of uncertainty of a quantum mechanical distribution, since a highly localized $\rho(\mathbf{r})$ is associated with a diffuse $n(\mathbf{k})$, leading to low S_r and high S_k and vice versa.

The lower bound in (4) is attained for gaussian density distributions. Expression (4) is an information-theoretical uncertainty relation stronger than Heisenberg's, for two reasons: first EUR leads to Heisenberg's uncertainty relation but the inverse is not true. Second, the right-hand-side of EUR does not depend on the state of the system, while in Heisenberg's relation does depend. It is also noted that expression (4) does depend on the unit of length in measuring $\rho(\mathbf{r})$ and $n(\mathbf{k})$ i.e. the sum S_r+S_k is invariant to uniform scaling of coordinates.

In [1] we proposed a universal property for S for the density distributions of nucleons in nuclei, electrons in atoms and valence electrons in atomic clusters

$$S = a + b \ln N \tag{5}$$

where the parameters a, b depend on the system under consideration. The values of the parameters are the following

$$\begin{array}{lll} a=5.325 & b=0.858 & (nuclei) \\ a=5.891 & b=0.849 & (atomic\,clusters) \\ a=6.257 & b=1.007 & (atoms) \end{array} \tag{6}$$

In [2] relation (5) was found to hold for bosonic systems as well i.e. correlated atoms in a trap. The values of a, b are

$$\begin{array}{llll} a=6.029 & b=0.068 & 5\times 10^2 < N < 10^6 & (^{87}Rb) \\ a=5.961 & b=0.066 & 10^3 < N < 5\times 10^6 & (^{133}Cs) \end{array} \tag{7}$$

Another interesting result is the fact that the entropy of a N-photon state subjected to Gaussian noise increases linearly with the logarithm of N. It is remarkable that property (5) holds for systems of different sizes i.e. ranging from the order of fermis (10^{-13} cm) in nuclei to $10^4 \mathring{A}$ (10^{-4} cm) for bosonic systems, obeying different statistics and subject to various interactions.

Relation (5) was derived using one-body density distributions. In the present paper we introduce two-body density distributions $\rho(\mathbf{r}_1,\mathbf{r}_2)$ and the corresponding two-body momentum distributions $n(\mathbf{k}_1,\mathbf{k}_2)$. We intend to examine the properties of S at the two-body level for the correlated densities. The correlated nuclear systems or the trapped Bose gas are studied using the lowest order approximation [3,4]. Short-range correlations (SRC) are taken into account employing the Jastrow correlation function [5]. We are interested in investigating how S_2 is affected qualitatively and quantitatively by the same form of correlations in comparison with S_1, in view of the fact that the quantities $\rho(\mathbf{r}_1, \mathbf{r}_2)$ and $n(\mathbf{k}_1, \mathbf{k}_2)$ carry more direct information for correlations than the quantities $\rho(\mathbf{r})$ and $n(\mathbf{k})$, which are only indirectly affected by correlations.

A well known measure of distance of two continuous probability distributions $\rho^{(1)}(x)$, $\rho^{(2)}(x)$ is the Kullback-Leibler relative entropy [6]

$$K = \int \rho^{(1)}(x) \ln \frac{\rho^{(1)}(x)}{\rho^{(2)}(x)} dx \tag{8}$$

which can be easily extended for 3-dimensional systems. Our aim is to calculate K (distance) between $\rho^{(1)}(x)$ (correlated) and $\rho^{(2)}(x)$ (uncorrelated) densities both at the one- and the two-body levels in order to evaluate the effect of SRC (through the correlation parameter y) on the distance K. This is done for both systems under consideration: nuclei and correlated atoms in a trap. There is also an alternative definition of distance of two probability distributions introduced by Rao and Lin [7] i.e. a symmetrized version of K, the Jensen-Shannon divergence

$$J = H\left(\frac{\rho^{(1)}(x) + \rho^{(2)}(x)}{2}\right) - \frac{1}{2} H\left(\rho^{(1)}(x)\right) - \frac{1}{2} H\left(\rho^{(2)}(x)\right) \tag{9}$$

where $H(p) = -\sum_i \rho_i \ln \rho_i$ stands for Shannon's entropy. It is expected that for strong SRC the amount of distinguishability of the correlated from the uncorrelated distribution is larger than the corresponding one with small SRC. We may also see the effect of SRC on the number of trials L (coin tosses) needed to distinguish $\rho^{(1)}(x)$ and $\rho^{(2)}(x)$ (in sense described in [8]).

Shannon information entropy $S = S_r + S_k$ is calculated as function of the atomic number Z $(2 \leq Z \leq 54)$ in atoms. RHF electron wave functions [9] are used. The universal property $S = a + b \ln Z$ is verified. Thus we obtain a framework to be used as basis for further work on information-theoretic properties of atoms. We examine the problem of similarity index based on the concept of information distance K and J. The concept of similarity is an old one and related to the distinction between two or more objects. In this work we study K and J, which are connected with the concept of similarity or information distance. This enables us to compare various density distributions obtained using various models for atoms.

2 Results

2.1 Atoms

We use the RHF electron wave functions and obtain for the total information the relation

$$S = 6.257 + 1.069 \ln Z \tag{10}$$

Thus we verify a previous property obtained employing other wave functions and use this framework for new calculations. Next we calculate Kullback distance K between RHF density distributions and TF density of atoms, as well as another phenomenological density. It turns out that K is useful for the comparison of the above densities. Similar results are obtained for Jensen-Shannon divergence J.

2.2 Nuclei and trapped Bose gases

Our main conclusions are the following

(i) Increasing SRC the information entropy S and the information distances K and J increase.

(ii) There is a similar behavior of the entropies as functions of SRC for both systems (nuclei and trapped Bose gases) although they obey different statistics (fermions and bosons).

(iii) The relation $S_2 = 2S_1$ holds exactly for the uncorrelated densities in trapped Bose gase, while the above relations are almost exact for the uncorrelated densities and in the case of correlated densities both in nuclei and trapped Bose gas. For 3-body distributions $\rho(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ and $n(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ we extrapolate to $S_3 = 3(a + b \ln N)$ and generalizing for N-body distributions we have $S_N = N(a + b \ln N)$, conjectured for $N \geq 3$.

More details concerning the formalism, the results and more references of our work can be found in [10,11].

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