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Application of information theory in atoms, nuclei and atomic clusters

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Abstract

The position- and momentum-space information entropies of the electron distributions of atomic clusters are calculated using a Woods-Saxon single particle potential. The same entropies are also calculated for nuclear distributions according to the Skyrme parametrization of the nuclear mean field. It turns out that a similar functional form $S = a + b \ln N$ for the entropy as function of the number of particles N holds approximately for atoms, nuclei and atomic clusters. It is conjectured that this is a universal property of a many-fermion system in a mean field.

Information-theoretical methods have played in recent years an important role in the study of quantum mechanical systems [1-10] in two cases: first in the clarification of fundamental concepts of quantum mechanics and second in the synthesis of probability densities in position and momentum spaces. In the first case an important step was the discovery of an entropic uncertainty relation (EUR) by Bialynicki-Birula and Mycielski [1] which for a three-dimensional system has the form:

$$S_r + S_k \geq 3(1 + \ln \pi), \quad (\hbar = 1) \quad (1)$$

(see also ref. [11] for the one-dimensional case). In (1) S_r is the Shannon information entropy in position-space:

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

S_k is the corresponding entropy in momentum-space:

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

and $\rho(\mathbf{r})$, $n(\mathbf{k})$ are the position- and momentum-space density distributions respectively, which are normalized to one. However, for a normalization to the number of

particles N , the following EUR holds [4]:

$$S_r + S_k \geq 3N(1 + \ln \pi) - 2N \ln N = 6.434N - 2N \ln N \quad (4)$$

Inequality (1), 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. Expression (1) is an information-theoretical uncertainty relation stronger than Heisenberg's [1]. We also note that expression (1) does not 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, while the individual entropies S_k , S_r are not. The bound (4) is attained by Gaussian wavefunctions.

In [9] a different definition for the information entropy was employed. It is based on a phase-space distribution associated with the ground-state density of a many fermion system. Various phenomenological models for the density distribution were used for a number of nuclei. Nuclear densities calculated within various microscopic mean field approaches were also employed. It turned out that the entropy increases from crude phenomenological models of the nucleus to more sophisticated (microscopic) ones. It was concluded that the larger the information entropy, the better the quality of the nuclear density distribution. It seems that the concept of information entropy is useful for the study of quantum many body systems. In the present work we use an alternative definition i.e. relations (2) and (3).

This paper addresses the problem of what are the values of $S_r + S_k$ for different many fermion systems (atoms, nuclei, clusters). There is a growing belief in recent years that information-theoretic methods will play an increasing role in the future for the study of quantum mechanical systems. It is also interesting to find the extent of $\rho(\mathbf{r})$ and $n(\mathbf{k})$ for different fermionic systems.

Gadre [2] derived the following approximate expression for the information entropies of electron distributions in atoms:

$$S_r + S_k \simeq 6.65N - N \ln N \quad (5)$$

using Thomas-Fermi theory and Gadre et al [3] derived :

$$S_r + S_k \simeq 6.257N - 0.993N \ln N \quad (6)$$

with Hartree-Fock calculations. Here, N is the number of electrons.

Panos and Massen [8] found the following expression for nuclear distributions, employing the simple harmonic oscillator (HO) model of the nucleus:

$$S_r + S_k \simeq 5.287N - 1.13N \ln N \quad (7)$$

where N is the number of nucleons in nuclei. Relations of the same functional form hold for S_r and S_k separately but the important quantity is $S_r + S_k$.

There is a striking similarity of (5), (6) and (7) with the EUR (4), indicating that the functional form

$$S = aN + bN \ln N \quad (8)$$

is universal for a many-fermion system in a mean field.

However, the above relations were derived for a normalization of $\rho(\mathbf{r})$ and $n(\mathbf{k})$ to the number of particles N . In the following we find it more convenient to normalize to one. There is a simple relationship between the two cases and we can easily transform one case to the other according to the relations:

$$S_r[norm = 1] = \frac{S_r[norm = N]}{N} + \ln N$$

$$S_k[norm = 1] = \frac{S_k[norm = N]}{N} + \ln N$$

Hence, we have for normalization to one, the following expressions:

$$S_r + S_k \simeq 6.65 + \ln N \quad (atoms, Thomas - Fermi) \quad (9)$$

$$S_r + S_k \simeq 6.257 + 1.007 \ln N \quad (atoms, Hartree - Fock) \quad (10)$$

$$S_r + S_k \simeq 5.287 + 0.870 \ln N \quad (nuclei - H.O.) \quad (11)$$

In the present work we extend our calculations for two other cases: the distribution of the valence electrons in atomic clusters using a Woods-Saxon single particle potential and the nuclear distribution in nuclei employing the Skyrme parametrization of the nuclear mean field.

In atomic (metallic) clusters the effective radial electronic potential was derived by Ekardt [12] in his spherical-jellium-background-model study of the self-consistent charge density and the self-consistent effective one-particle potential, using the local density approximations. Ekardt's potentials for neutral sodium clusters were parametrized in ref. [13] by a Woods-Saxon potential of the form:

$$V_{WS}(r) = -\frac{V_0}{1 + \exp[\frac{r-R}{a}]} \quad (12)$$

with $V_0 = 6 \text{ eV}$, $R = r_0 N^{1/3}$, $r_0 = 2.25 \text{ \AA}$ and $a = 0.74 \text{ \AA}$. For a detailed study regarding the parametrization of Ekardt's potentials see ref. [14].

We solved numerically the Schrödinger equation for atomic clusters with $Z = 8, 18, 20, 34, 40, 58, 68, 70, 82, 92, 126$ and 168 valence electrons in the potential (12) and

found the wave functions of the single-particle states in configuration space and by Fourier transform the corresponding ones in momentum space. Using the above wave functions, we calculated the electron density $\rho(\mathbf{r})$ in position space and $n(\mathbf{k})$ in momentum space, which were inserted into equations (2), (3) and gave us the values of the information entropies S_r and S_k . Then we fitted the form $S = a + b \ln N$ to these values and obtained the expressions:

$$S_r \simeq 4.185 + 0.924 \ln N \quad (13)$$

$$S_k \simeq 1.706 - 0.075 \ln N \quad (14)$$

$$S_r + S_k \simeq 5.891 + 0.849 \ln N \quad (15)$$

The above relations hold for $8 \leq N \leq 168$.

Next the nuclear densities $\rho(\mathbf{r})$ and $n(\mathbf{k})$ for several nuclei (in the region $4 \leq N \leq 208$, where N is the number of nucleons) were obtained with Hartree-Fock calculations using the Skyrme parametrization of the nuclear mean field. There are various parametrizations of the Skyrme interaction, but they affect slightly the information entropies [9]. Thus we used the SKIII interaction [15]. Finally, we fitted the form $S = a + b \ln N$ to the values obtained with SKIII interaction and we found the expressions:

$$S_r \simeq 3.865 + 0.659 \ln N \quad (16)$$

$$S_k \simeq 1.460 + 0.199 \ln N \quad (17)$$

$$S_r + S_k \simeq 5.325 + 0.858 \ln N \quad (18)$$

The fit is in reasonably good agreement with its H.O. counterpart (comparison of relation (18) to (11)), though the individual entropies S_r and S_k do not match with the respective HO ones [8] that well. It seems that there is a delicate balance between the coordinate and momentum spaces, so that the interesting quantity is the sum $S = S_r + S_k$ (the net information content of the system) and not the individual entropies S_r and S_k .

In figure 1 we plot our fitted form $S = S_r + S_k = a + b \ln N$ for atoms (with Hartree-Fock, relation (10), upper curve), atomic neutral Na clusters (relation (15), middle curve) and nuclei (with Skyrme, relation (18), lower curve). These lines correspond to our fitted expressions, while the corresponding values of our numerical calculations are denoted by solid circles (clusters) and open circles (nuclei with SKIII interaction). The region of values of N is wider for nuclei, because in nuclei there are two kinds of particles (neutrons and protons), which fill separate potential wells, while in clusters there is only one kind of particles (electrons). Thus in clusters we go up to higher states than in nuclei.

A few comments seem appropriate: it is seen that formulas (7) and (18) violate the lower limit set in EUR (4) for the limit $N \rightarrow 1$. In fact relations (7) and (18) hold

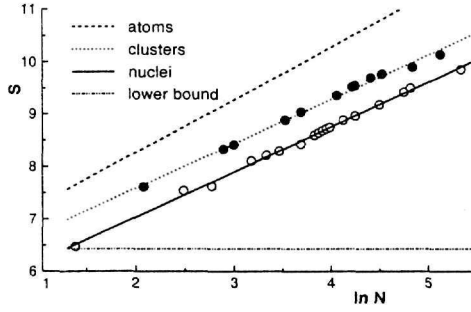


Fig. 1. Information entropy S as function of the number of particles N according to our fitted expression $S = a + b \ln N$ for atoms, clusters and nuclei. The corresponding values of our numerical calculations are denoted by solid circles (clusters) and open circles (nuclei). The limiting line corresponding to the lower bound, $S_r + S_k = 6.434$, is also shown.

only for the region $N \geq 4$, where the fitting has been performed. The case $N = 1$ has no meaning for nuclei. The same holds in the case of clusters, where relation (15) has been derived for the region $N \geq 8$. It is also noted that the right-hand-side of relation (4) gives a lower bound for $S_r + S_k$. The values of this sum calculated from relations (6), (7), which were derived from a specific model of the atom or nucleus, are greater than this lower bound as expected. It is also seen that in all examples the slope with $\ln N$ is substantially larger than the limiting slope of the EUR (4). This comes from the fact that this uncertainty relation underestimates the values of S for large systems i.e. formula (4) is not asymptotically correct [2].

Concluding, in the present paper we derive an interesting characteristic of information entropies S_r and S_k for various systems i.e. atoms (Thomas–Fermi theory, Hartree–Fock), nuclei (Harmonic Oscillator model, Skyrme force) and atomic clusters (Woods–Saxon potential). For all of these systems the entropies can be represented well by a function, which incorporates $\ln N$ linearly i.e. $S = a + b \ln N$ where N is the number of electrons in atoms or nucleons in nuclei or electrons in atomic clusters. We may conjecture that this is a universal property of a many-fermion system in a mean field. As stated in ref. [3], the information entropies seem to be a hidden treasure, as yet remains mostly unexplored.

Although it is not quite clear why S depends linearly on $\ln N$ and how to relate S with experimental properties of the different fermionic systems, we hope that the present work will stimulate further research on this matter. In atomic systems a connection with experiment has already been established. In this case S_r and S_k show a close relationship with fundamental and/or experimentally measurable quantities such as e.g. the kinetic energy and the magnetic susceptibility [16]. Both characteristics have been used in the study of the dynamics of atomic and molecular systems [17].

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