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An Application of the Information Entropy to Nuclei

S. E. Massen

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

Abstract.

Shannon's information entropies in position- and momentum- space and their sum S are calculated for various s-p and s-d shell nuclei using a correlated one-body density matrix depending on the harmonic oscillator size b_0 and the short range correlation parameter y which originates from a Jastrow correlation function. It is found that the information entropy sum for a nucleus depends only on the correlation parameter y through the simple relation $S = s_{0A} + s_{1A} y^{-\lambda_{sA}}$, where s_{0A}, s_{1A} and λ_{sA} depend on the mass number A. Finally, we propose a method to determine the correlation parameter from the above property of S as well as the linear dependence of S on the logarithm of the number of nucleons.

1 Introduction

The uncertainty in position space (Δx) and in momentum space (Δp_x) are usually associated with the standard deviation of a set of measurement of the position and the momentum. That definition of the uncertainty is the most appropriate when the distribution is nearly a Gaussian. If the distribution deviates significantly from the Gaussian, i.e. having more than one peak, the standard deviation is not a good measure of the uncertainty [1]. As uncertainty is the missing information of a distribution it should not surprise us that Information Theory provides a way to measure uncertainty. A measure of the uncertainty is Shannon's information entropy (SIE). For a continues probability distribution $p(x)$ it is defined as

$$S = -\int p(x) \ln p(x) dx, \quad \int p(x) dx = 1$$

This quantity is useful for the study of quantum systems [2–17] and appears in various areas: information theory, ergodic theory and statistical mechanics. It is closely related to the entropy and disorder in thermodynamics. Shannon regarded that entropy attached to the system as the amount of information carried by the system. It has already been connected with experimental and/or fundamental quantities (e.g., the kinetic energy and magnetic susceptibility in atomic physics [4] and the kinetic energy and mean square radius in nuclear and cluster physics [14, 16].

An important step in the past was the discovery in Ref. [2] of an entropic uncertainty relation [2] which for a three-dimensional system has the form

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

where

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

and

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

are the Shannon's information entropies in position- and momentum-space and $\rho(\mathbf{r})$, $n(\mathbf{k})$ are the density distribution (DD) and momentum distribution (MD), respectively, normalized to unity.

Inequality (1) is an information-theoretical uncertainty relation stronger than Heisenberg's [2] and does not depend on the unit of length in measuring $\rho(\mathbf{r})$ and $n(\mathbf{k})$, i.e. the sum $S = S_r + S_k$ is invariant to uniform scaling of coordinates, while the individual entropies S_r and S_k are not. The physical meaning of S is that it is a measure of quantum-mechanical uncertainty and represents the information content of a probability distribution. Inequality (1) provides a lower bound for S which is attained for Gaussian wave functions.

Information entropies were employed in the past to study quantum-mechanical systems [2–10]. Recently [11, 13, 15] we studied the position- and momentum-space information entropies S_r and S_k, respectively, for the densities of various systems: the nucleon DD of nuclei, the valence electron DD of atomic clusters and the DD of trapped Bose alkali atoms. We found that the same functional form $S = a + b \ln N$ for the entropy sum as function of the number of particles N holds approximately for the above systems in agreement with Refs. [3, 4] for atomic systems. In Ref. [12] we used another definition of information entropy according to phase-space considerations [18] and we derived an information-theoretic criterion for the quality of a nuclear DD, i.e. the larger S the better the quality of nuclear model. In Ref. [19] the DD, the MD and the Shannon's information entropies have been calculated for nuclei using three different cluster expansions. The parameters of the various expressions have been determined by least-squares fit of the theoretical charge form factor

to the experimental one. It was found that the larger the entropy sum the smaller the value of χ^2, indicating that the maximal S is a criterion of the quality of a given nuclear model according to the maximum entropy principle. Only two exceptions to that rule were found out of many cases examined. Before proceeding, it is appropriate to mention that additional applications of entropy have attracted interest in recent years [7,8], but in a different spirit, in nuclear physics problems, such as in analysis of shell model eigenvectors. However, it is noted that in Ref. [8] the authors define a correlational entropy. This is a von Neumann entropy, which they apply in the framework of the nuclear shell model.

In the present work we focus on the entropy sum S of a nucleus using the analytical expressions of the DD and MD of Refs. [21–23]. The expressions of those distributions have been found for s-p and s-d shell nuclei using the factor cluster expansion of Clark and co-workers [24] and Jastrow correlation function which introduces short range correlations (SRC). Those expressions depend on the harmonic oscillator (HO) parameter and the correlation parameter. Finally, we propose a way to determine the correlation parameter of the model using the dependence of S on that parameter as well as the linear dependence on the logarithm of the number of nucleons. The HO parameter is determined equating the theoretical charge RMS radius of the nucleus with the experimental one.

The paper is organized as follows. In Section 2, the general definitions related to the correlated DD, MD as well as the dependence of the entropy sum on the correlation parameter are given. In Section 3, we present a method for the determination of the correlation parameter from the information entropy sum. Finally, in Section 4, the summary of the present work is given.

2 Correlated One-Body Density of s-p and s-d Shell Nuclei and Their Entropy

A general expression for the one-body density matrix of $N = Z$, s-p and s-d shell nuclei was derived in Refs. [22, 23] using the factor cluster expansion of Ristig, Ter Low and Clark [24]. That expression depends on the HO parameter b_0 ($b_0 = (\hbar/(m\omega))^{1/2}$), the occupation probabilities of the various states and the correlation parameter y that comes from the Jastrow type correlation function

$$f(r) = 1 - \exp[-y r_b^2], \quad r_b = r/b_0 \ , \tag{4}$$

which introduces short range correlations. The correlation function $f(r)$ for large values of r goes to 1 and goes to 0 for $r \to 0$. It is obvious that the effect of correlations introduced by the function $f(r)$ becomes large when the correlation parameter y becomes small and vice versa.

The diagonal part of the one-body density matrix is the DD $\rho(\mathbf{r})$. The Fourier transform of the DD is the form factor

$$F(q) = \int \exp[i\mathbf{q}\mathbf{r}]\rho(\mathbf{r})d\mathbf{r} \ , \tag{5}$$

while the MD $n(\mathbf{k})$ is given by the particular Fourier transform of the one-body density matrix

$$n(\mathbf{k}) = \frac{1}{(2\pi)^3} \int \exp[i\mathbf{k}(\mathbf{r}-\mathbf{r}')]\rho(\mathbf{r},\mathbf{r}')d\mathbf{r}d\mathbf{r}' \ . \tag{6}$$

The expressions of $\rho(\mathbf{r})$, $n(\mathbf{k})$ and $F(q)$ (in the two body approximation for the cluster expansion) have the forms

$$\rho(r) = \frac{N_0}{\pi^{3/2} b_0^3} \left[O_1(r_b) + O_2(r_b, y) \right] \ , \tag{7}$$

$$n(k) = \frac{N_0 b_0^3}{\pi^{3/2}} \left[\tilde{O}_1(k_b) + \tilde{O}_2(k_b, y) \right] \ , \tag{8}$$

and

$$F(q) = N_0 \left[\tilde{\tilde{O}}_1(q_b) + \tilde{\tilde{O}}_2(q_b, y) \right] \ , \tag{9}$$

where $k_b = k b_0$ and $q_b = q b_0$. The terms O_1, $\tilde{O}_1$ and $\tilde{\tilde{O}}_1$ come from the one-body term of the cluster expansion of the one-body density matrix and the terms O_2, $\tilde{O}_2$ and $\tilde{\tilde{O}}_2$ come from the two-body term. Their expressions as well as the expression of the normalization factor N_0 are given in Refs. [21–23].

From the expressions of $\rho(r)$ and $n(k)$ the Shannon's information entropies in position and momentum space and their sum $S = S_r + S_k$ can be calculated through Eqs. (2) and (3) for $\rho(r)$ and $n(k)$ normalized to 1.

For various values of the parameters b_0 and y and for the $N = Z$, s-p and s-d shell nuclei: ^{4}He, ^{12}C, ^{16}O, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar and ^{40}Ca we calculated S_r, S_k and $S \equiv S_A$, treating ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar as $1d$ shell nuclei. It is found that, for the above nuclei, S_r and S_k depend on both parameters, b_0 and y, while their sum S_A depends only on the correlation parameter y. The calculated values of S_A for the above mentioned nuclei versus $1/y$ are displayed by points in Figure 1.

It is seen that S_A is an increasing function both of $1/y$ and of the number of nucleons A of the nucleus, while S_A depends almost linearly on $1/y$. For that reason we fitted the numerical values of S_A with the form

$$S \equiv S_A(y) = s_{0A} + s_{1A}\ y^{-\lambda_{sA}} \ , \tag{10}$$

separately for each nucleus, that is the parameters s_{0A}, s_{1A} and λ_{sA} depend on the mass number A of the nucleus. The parameter s_{0A} is determined from the values of the information entropy sum in the HO case, i.e,

$$s_{0A} = S_A(\infty) \ ,$$

while the other two parameters are determined by least-squares fit of the values of S_A calculated from Eq. (10) to the corresponding ones calculated from

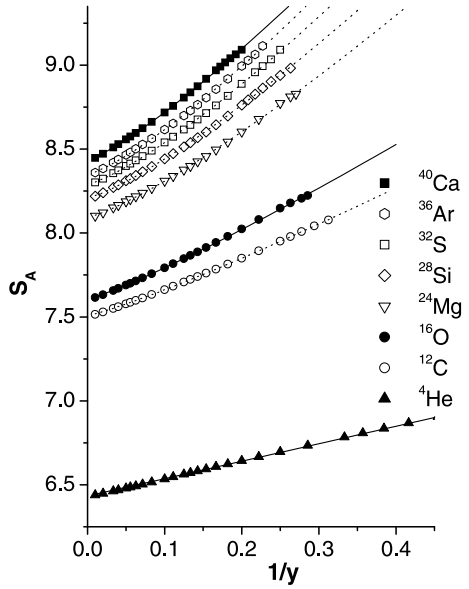

Figure 1. The information entropy sum S_A versus the correlation parameter $1/y$ for various s-p and s-d shell nuclei. The points correspond to the numerical values of $S_A(y)$ and the lines come from the fitting expression (10).

Eqs. (2) and (3). The values of the parameter s_{0A} and the best fit values of the parameters s_{1A} and λ_{sA} are displayed in Table 1, while the values of $S = S_A(y)$ found from Eq. (10) using the above values of the parameters are displayed by lines in Figure 1.

It is seen that the simple form of S_A, given by Eq. (10), reproduces very well the numerical values of S_A for all nuclei considered. Also, there is a systematic

Table 1. The values of the parameters s_{0A}, s_{1A} and λ_{sA} of the information entropy sum S_A of the relation (10) for various s-p and s-d shell nuclei.

Nucleus	s_{0A}	s_{1A}	λ_{sA}
^{4}He	6.4342	1.0410	1.0064
^{12}C	7.5086	2.1885	1.1548
^{16}O	7.6069	2.6464	1.1529
^{24}Mg	8.0933	3.7445	1.2390
^{28}Si	8.2096	4.1641	1.2548
^{32}S	8.2901	4.5837	1.2659
^{36}Ar	8.3490	4.9578	1.2681
^{40}Ca	8.4347	4.7275	1.2208

trend of the values of the parameters s_{0A}, s_{1A} and λ_{sA}. The parameter s_{0A} depends linearly on the logarithm of A. That is expected, as s_{0A} is equal to the information entropy sum in the HO case which depends linearly on the logarithm of the number of the nucleons [11]. The parameter λ_{sA} has smaller values in the closed shell nuclei ^{4}He, ^{16}O and ^{40}Ca than in the corresponding neighboring open shell ones. Finally, the parameter s_{1A} is almost a monotonic increasing function of A with an exception for the nucleus ^{40}Ca.

3 Determination of the Correlation Parameter from the Information Entropy

In recent works, it has been shown that the information entropy sum of a quantum system (electrons in atoms [3,4], nucleons in nuclei and valence electrons in atomic clusters [13] and correlated Bose atoms in a harmonic trap [15]) depends approximately linearly on the logarithm of the number of particles, given by the form

$$S = S(A) = a + b \ln A \,, \tag{11}$$

where a and b depend on the considered system.

The question that arises is how that property can be used in practice. A possible way is to determine $S(A)$ for two nuclei (such that ^{4}He and ^{40}Ca) for which there are enough experimental data and then to find a and b of Eq. (11) from the relations

$$a = \frac{S(4)\ln 40 - S(40)\ln 4}{\ln 40 - \ln 4} \,, \tag{12}$$

$$b = \frac{S(40) - S(4)}{\ln 40 - \ln 4} \,. \tag{13}$$

$S(4)$ and $S(40)$ can be found calculating first the charge form factors of ^{4}He and ^{40}Ca from the relation

$$F_{ch}(q) = F(q) f_{cm}(q) f_p(q) f_{DF}(q) \,,$$

where $F(q)$ is the point form factor of the nucleus calculated from Eq. (5), $f_{cm}(q)$ is the Tassie-Barker [25] center-of-mass correction and $f_p(q)$ and $f_{DF}(q)$ are the correction for the finite proton size and the Darwin-Foldy relativistic correction, respectively [26].

The parameters b_0 and y for ^{4}He and ^{40}Ca are determined by least-squares fit of the theoretical $F_{ch}(q)$ to the experimental, with the constraint that the experimental charge RMS radius is to be reproduced. The values of the parameters b_0 and y as well as the values of χ^2 are displayed in Table 2. In the same table the values of b_0 and χ^2 in the HO case ($y = \infty$) are also shown. In that case b_0 is determined from the above mentioned constraint. The experimental and the theoretical $F_{ch}(q)$, calculated with and without SRC, for the two nuclei are shown in Figure 2.

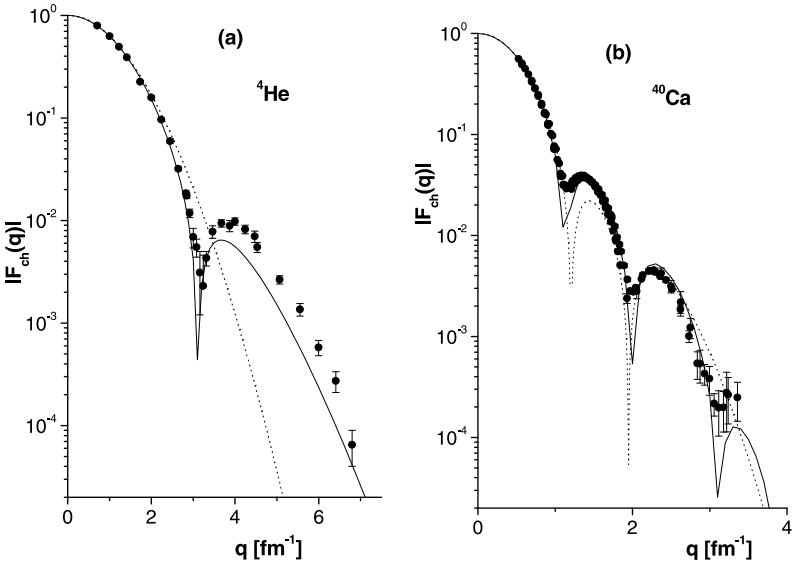

Figure 2. The charge form factors of nuclei ^{4}He (a) and ^{40}Ca (b). The solid lines correspond to the case when SRC are included and the parameters y and b_0 are determined by least squares fit of the theoretical charge form to the experimental with the constraint the calculated RMS charge radius is to be the experimental one. The dot lines correspond to the HO case when b_0 is determined from the experimental RMS charge radius. The experimental points for ^{4}He are from Ref. [28] and for ^{40}Ca from Ref. [29].

With the values of b_0 and y determined in the above described way, for the two nuclei ^{4}He and ^{40}Ca, we calculated the point $\rho(r)$ and $n(k)$ from Eqs. (7) and (8) and the Shannon's information entropies S_r and S_k from Eqs. (2) and (3) and their sum, $S(4)$ and $S(40)$. Substituting the values of $S(4)$ and $S(40)$ into Eqs. (13), the parameters a and b are determined. The calculated values

$$a = 5.4029 \quad \text{and} \quad b = 0.9360\ ,$$

are quite close to the values $a = 5.325$ and $b = 0.858$ which have been found in Ref. [21] with SkIII interaction.

Rearranging Eq. (10) and replacing $S_A(y)$ by $S(A)$ from Eq. (11), we may write

$$y = \left(\frac{s_{1A}}{S(A) - s_{0A}}\right)^{1/\lambda_{sA}} . \tag{14}$$

Using the values of the parameters s_{0A}, s_{1A} and λ_{sA} given in Table 1 and the values of $S(A)$ calculated from Eq. (11), the correlation parameter y is determined for the other nuclei without any fit to experimental data. The HO pa-

rameter b_0, can be determined now for each nucleus from the relation

$$r_{exp}^2 = \langle r^2 \rangle - \frac{b_0^2}{A} + r_p^2 + \frac{\hbar^2}{2m^2c^2} \ , \tag{15}$$

where r_{exp}^2 is the experimental mean square charge radius of the nucleus and $\langle r^2 \rangle$ is the point mean square radius calculated from the correlated density distribution. The last three terms of Eq. (15) are the corrections due to the spurious center-of-mass motion, the finite proton size and the Darwin-Foldy relativistic correction, respectively.

The values of b_0 and y for the various s-p and s-d shell nuclei determined in the way above described, as well as the values of the least-squares errors, in the comparison of the theoretical $F_{ch}(q)$ to the experimental and the entropy sum S are displayed in Table 2. In the same table the values of b_0, χ^2 and S when SRC are not included (HO case) are also shown. From Table 2 we can see that there is a systematic behavior of the parameter y. The values of y are always smaller (that is large correlations) in the closed shell nuclei, ^{4}He, ^{16}O, ^{36}Ar and ^{40}Ca, than in the neighboring open shell ones. It is mentioned that ^{36}Ar is treated as 1d closed shell nucleus. The above behavior indicates that there should be a shell effect in the case of closed shell nuclei for the values of the correlation

Table 2. The values of the parameters b_0 (in fm) and y, the χ^2, the RMS charge radius $\langle r_{ch}^2 \rangle^{1/2}$ (in fm) and the information entropy sum S for various s-p and s-d shell nuclei. The theoretical RMS charge radii are equal to the experimental of Ref. [27].

Nucleus	Case	b_0	y	χ^2	$\langle r_{ch}^2 \rangle^{1/2}$	S
^{4}He	SRC	1.2497	3.7857	9.40	1.676	6.7068
	HO	1.3335	∞	53.46	1.676	6.4342
^{12}C	SRC	1.5617	7.1294	153.46	2.471	7.7351
	HO	1.6108	∞	181.31	2.471	7.5086
^{16}O	SRC	1.6451	5.1782	417.05	2.730	8.0044
	HO	1.7554	∞	202.09	2.730	7.6069
^{24}Mg	SRC	1.7609	7.8711	221.07	3.075	8.3839
	HO	1.8222	∞	226.41	3.075	8.0933
^{28}Si	SRC	1.7226	7.8711	322.63	3.086	8.5282
	HO	1.7860	∞	472.93	3.086	8.2096
^{32}S	SRC	1.7781	7.4140	669.72	3.248	8.6531
	HO	1.8559	∞	850.03	3.248	8.2901
^{36}Ar	SRC	1.7885	7.0790		3.327	8.7634
	HO	1.8801	∞		3.327	8.3490
^{40}Ca	SRC	1.8397	7.1632	168.44	3.479	8.8620
	HO	1.9526	∞	230.60	3.479	8.4347

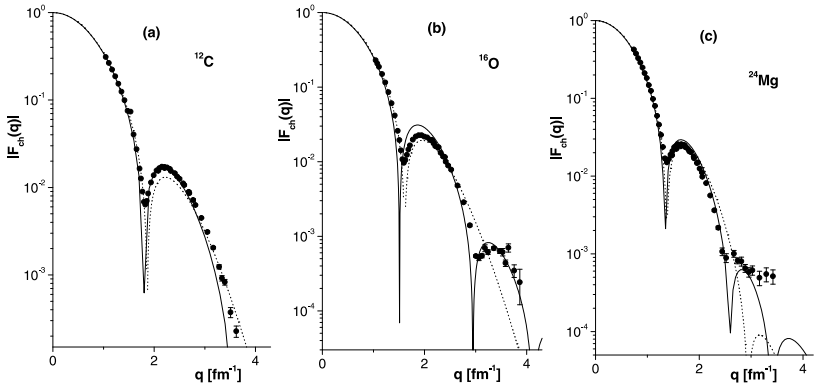

Figure 3. The charge form factors of nuclei ^{12}C (a), ^{16}O (b) and ^{24}Mg (c). The solid lines correspond to the case when SRC are included and the parameters y and b_0 are determined from Eq. (18) and the experimental RMS charge radius, respectively. The dot lines correspond to the HO case when the parameter b_0 is determined from the experimental RMS charge radius. The experimental points for ^{12}C and ^{16}O are from Ref. [30] and for ^{24}Mg from Ref. [31].

parameter y. Similar behavior was found in Ref. [22] where the determination of the parameters b_0 and y were made by individual fit of the theoretical $F_{ch}(q)$ to the experimental one. From the same table we can see that y is a monotonically increasing function of the number of nucleons of the closed shell nuclei.

The theoretical $F_{ch}(q)$ with and without SRC, as well as the experimental ones for various nuclei have been plotted versus the momentum transfer q in Figures 3 and 4. It is remarkable that without fit to the experimental charge form factors, the present method gives good form factors, reproducing the diffraction minima and maxima in the correct place. In nearly all cases, the χ^2 values found with SRC are better than the corresponding values in the HO case. However, the assessment of the quality of the calculated form factors should not be based solely on the values of the least-squares errors but also on the fulfillment of the requirement that all the diffraction minima are reproduced in the correct place. Thus, comparing the quality of the form factors calculated in the present method with the ones calculated with the harmonic oscillator model, we can say that the quality of the form factors are considerably better in the former case. All the diffraction minima (even the third one which seems to exist in the experimental data of ^{24}Mg, ^{28}Si and ^{32}S) are reproduced in the present method while in the harmonic oscillator model they are not. We note also that, in the case of the nucleus ^{36}Ar there are not experimental data for the form factor. The exception which appears in ^{16}O, where the value of χ^2 with SRC is worse compared with the value of χ^2 without SRC, should not be taken as a drawback of the present method. The reason is that there exist many experimental points at

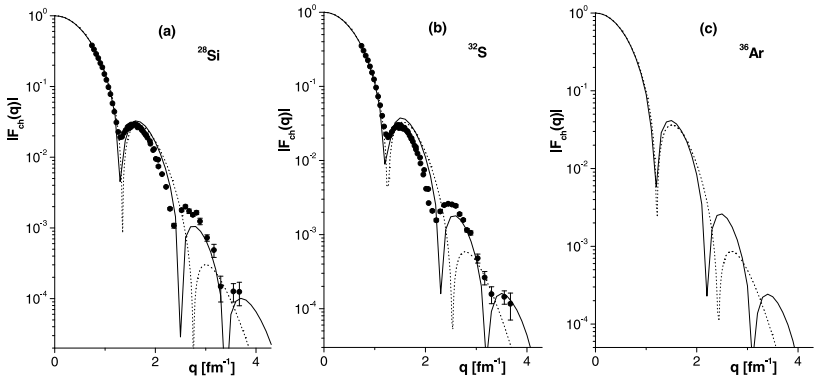

Figure 4. The charge form factors of nuclei ^{28}Si (a), ^{32}S (b) and ^{36}Ar (c). The various cases are as in Figure 4. The experimental points for ^{28}Si and ^{32}S are from Ref. [31].

low momentum transfer where the HO model gives good form factor, while there are a few experimental points at high momentum transfers where the present method reproduces these points very well, as well as all the diffraction minima and maxima. That can be seen in Figure 3b. If the experimental points were distributed uniformly, then the values of χ^2 calculated within the present method would be smaller than the ones calculated within the HO model. Thus, we should conclude that even in ^{16}O the theoretical $F_{ch}(q)$ calculated within the present method is better than that calculated within the HO model.

It should be noted that in the above analysis, the open shell nuclei, except ^{12}C, have been treated as $1d$ shell nuclei. However, the same analysis could be made if they were considered as $1d$-$2s$ shell nuclei, provided that the corresponding occupation probabilities of the various states are known. That analysis was made, as an example, for ^{36}Ar, assuming that the occupation probabilities of the various states are: $\eta_{1s} = \eta_{1p} = \eta_{2s} = 1$ and $\eta_{1d} = 0.8$. The values of the parameters b_0 and y which were found are: $b_0 = 1.7861$ fm and $y = 7.7658$. Thus, the value of the parameter y now becomes larger (less correlations) than that of the closed shell nucleus ^{40}Ca and closer to the values of the open shell nuclei ^{24}Mg and ^{28}Si (see Table 2).

Finally, comparing the values of the information entropy sum, which were calculated with and without SRC and are displayed in Table 2, it is seen that the introduction of SRC increases the information entropy sum by 3% to 5% in agreement with the simple model of SRC used in Ref. [11].

4 Summary

In the present work a systematic study of Shannon's information entropy sum S has been made for various $N = Z$, s-p and s-d shell nuclei using correlated

one-body density matrix which depends on the HO size b_0 and the correlation parameter y. It is found that, for all the nuclei we have examined, S depends only on y through a simple two-parameter relation.

From the dependence of S on y and its linear dependence on the logarithm of the number of nucleons of the nucleus, the correlation parameter y for a nucleus can be determined, provided that there are enough experimental data for two neighboring nuclei. It is mentioned that, usually, the two parameters of the correlated one-body density matrix are determined for each nucleus by least-squares fit of the theoretical $F_{ch}(q)$ to the experimental. Within the present method, those parameters are determined even in those cases where there are not any experimental data for the charge form factor as this has been made for the nucleus ^{36}Ar. The only experimental data which are used are the experimental charge RMS radius of the nucleus, as well as the experimental charge form factors and RMS radii of only two nuclei, those of ^{4}He and ^{40}Ca. It is noted also that, using the sum of the information entropies S_r and S_k, the short range correlation parameter has been determined indirectly, from the density distribution, as well as from the momentum distribution. This appears to be an interesting feature of the present method, since that parameter is usually determined only from the density distribution. We would like to mention that "experimental data" for the momentum distribution are not directly measured but are obtained by means of y-scaling analysis [32] and are only known for ^{4}He and ^{12}C.

It would be interesting if the dependence of the information entropy sum on the various parameters could be examined with more sophisticated models, such as the density dependent interactions, and if the present method could be applied for the determination of a parameter of those models.

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