Quantum-Information Content of Fractional Occupation Probabilities in Nuclei

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Abstract

Three measures of the information content of a probability distribution are briefly reviewed. They are applied to fractional occupation probabilities in light nuclei, taking into account short-range correlations. The effect of short-range correlations is to increase the information entropy (or disorder) of nuclei, comparing with the independent particle model. It is also indicated that the information entropy can serve as a sensitive index of order and short-range correlations in nuclei. It is concluded that increasing \( Z \), the information entropy increases i.e. the disorder of the nucleus increases for all measures of information considered in the present work.

1 Introduction

The Boltzmann–Gibbs–Shannon information entropy\[1, 2\] of a discrete probability distribution \((p_1, p_2, \ldots, p_k)\) is defined as the quantity

\[ S = - \sum_{i=1}^{k} p_i \ln p_i \]  

(1)

with the constraint \( \sum_{i=1}^{k} p_i = 1 \). \( S \) is measured in bits if the base of the logarithm is 2 and in nats (natural units of information) if the logarithm
is natural. This quantity appears in different areas: information theory, ergodic theory and statistical mechanics. It is closely related to the entropy and disorder in thermodynamics. The maximum value of $S$ is $S_{\text{max}} = \ln k$ obtained if $p_1 = p_2 = \ldots = p_k$. The minimum value of $S$ is found when one of the $p_i$’s equals 1 and all the others are equal to 0. Then $S_{\text{min}} = 0$. Information entropy was first introduced by Shannon as a way to measure the information content or uncertainty in a distribution. It has been applied in many cases e.g. the quantum mechanical description of physical systems.[3–14]

For continuous probability distributions, $S$ is defined by the integrals

$$
S_r = - \int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r} \\
S_k = - \int n(\vec{k}) \ln n(\vec{k}) d\vec{k} \\
S_S = S_r + S_k
$$

where $\rho(\vec{r})$, $n(\vec{k})$ are the density distributions of the system in position-space and momentum-space respectively. $S_r$, $S_k$ depend on the unit of $r$ and $k$, but the important quantity is the sum $S_r + S_k$ which is invariant to a uniform scaling of coordinates.

The discrete case considered in this work corresponds to a discrete probability distribution $p_i$, which in the literature (atomic case) is $p_i = \frac{n_i}{Z}$, where $n_i$ is the occupation number of the i-th natural orbital of the electron, divided by $Z$ for normalization to 1. If $p_i$ is inserted into (1) gives

$$
S_J = - \sum \frac{n_i}{Z} \ln \frac{n_i}{Z} \tag{3}
$$

which is called Jaynes entropy (atomic case). We extend the above definition to nuclear fractional occupation probabilities by putting into (1)

$$
p_i = p_q \quad \text{(Table 1), where } q = 1s, 1p, 1d, \ldots \tag{4}
$$

We also call this Jaynes entropy and use the same symbol $S_J$.

In quantum information theory and its applications in chemistry,[25] there are two definitions of $S$ referred to as $S_{\text{Jaynes}} = S_J$ (discrete case) and $S_{\text{Shannon}} = S_S$ (continuous case). $S_{\text{Jaynes}} = S_J$ and $S_{\text{Shannon}} = S_S$ were calculated and compared in chemical systems.[25] A relationship between them was found as well as a connection with correlation energy $E_{\text{corr}}$ with considerable success.[10]

The aim of the present work is to extend the above calculations to nuclear physics evaluating $S_J$ in nuclei. $S_S$ was obtained previously,[10] where a universal property $S_S = a + b \ln N$ was proposed (N is the number of nucleons
in nuclei, valence electrons in atomic clusters and electrons in atoms). It is remarkable that this relation holds in various systems in spite of the fact that the interaction is different. We also employ two alternative information measures (discrete) for the sake of comparison i.e. Onicescu’s $S_E$ and Stotland’s $S_F$ described below (Section 2).

It has been found that $S_S$ is important in chemical systems as a measure of basis set quality[6] and is related to various properties e.g. the kinetic energy, ionization potentials and can serve as a similarity index. A recent example of application of $S_J$ in organic chemistry is.[26] where the information entropy of Coulomb electron pairs (with antiparallel spins) and Fermi ones (with parallel spins) in a molecule was estimated. It was found that $S_J$ of Fermi pairs is less than that of Coulomb ones indicating that Fermi pairs are more ordered (or structured) than Coulomb ones. In nuclear physics a relation of $S_S$ with kinetic energy was obtained[11] while a universal trend[12] of $S_S$ for the single particle state of a fermion in a mean field was proposed for various systems i.e. a nucleon in a nucleus, a Λ particle in a hypernucleus and an electron in an atomic cluster. Also a relation $S_S = k \ln (\mu E + \nu)$ for the entropy of single particle states was proposed as function of the single particle energy $E$. The concept of information entropy also proved to be fruitful in a different context, i.e. the formalism of Ghosh, Berkowitz and Parr.[9] It turned out that employing their definition of information entropy, $S_S$ can serve as a criterion of the quality of a nuclear model by observing that $S_S$ increases with the quality of a nuclear model.

The outline of the paper is the following: In Section 2 two alternative measures of information are described (according to Onicescu and Stotland). In Section 3 a simple model for the estimation of fractional occupation probabilities is briefly reviewed. Section 4 contains a calculation of information entropies employing three measures of information, while our conclusions are briefly stated in Section 5.

2 Alternative measures of information

The information energy[15]-[17] of a single statistical variable $x$ with the normalized density $\rho(x)$ is defined by

$$E(\rho) = \int \rho^2(x)dx$$  \hspace{1cm} (5)
For a Gaussian distribution of mean value $\mu$, standard deviation $\sigma$ and normalized density $\rho(x)$, the probability density function is

$$\rho(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Relation (5) gives

$$E(\rho) = \frac{1}{2\pi\sigma^2} \int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{\sigma^2}} \, dx$$

Thus

$$E(\sigma) = \frac{1}{2\sigma\sqrt{\pi}}$$

Therefore, the greater the information energy $E$, the narrower is the Gaussian distribution.

Relation (5) was proposed by Onicescu[15, 16] who tried to define a finer measure of information. For a discrete probability distribution one has:

$$E = \sum_{i=1}^{k} p_i^2$$

The maximum value of $E$ is obtained if one of the $p_i$’s equals 1 and all the others are equal to zero i.e. $E_{\text{max}} = 1$ (total order), while $E$ is minimum when $p_1 = p_2 = \ldots = p_k = \frac{1}{k}$, hence $E_{\text{min}} = \frac{1}{k}$ (total disorder). Because $E$ reaches minimum for equal probabilities (total disorder), by analogy with thermodynamics, it has been called information energy, although it does not have the dimension of energy.[18] It has been connected with Planck’s constant appearing in Heisenberg’s uncertainty relation.[19]

So far only the mathematical aspects of this concept have been developed, while its physical aspects have been neglected. The greater the information energy, the more concentrated is the probability distribution, while the information content decreases. Thus the relation between $E$ and information content $S_E$ is reciprocal:

$$S_E = \frac{1}{E}$$

where $S_E$ is the information corresponding to $E$.

Very recently Stotland et al.[20] defined a new measure of information entropy by the relation:

$$F = -\sum_r \left[ \prod_{r' \neq r} \frac{p_r}{p_r - p_{r'}} \right] p_r \ln p_r$$
e.g. for $k = 2$ we get:

$$F = -\frac{1}{p_1 - p_2} (p_1^2 \ln (p_1) - p_2^2 \ln (p_2))$$

(12)

The expression of information content analogous to Shannon entropy is:

$$S_F = S_0(k) + F$$

(13)

where $S_0(k)$ is the minimum uncertainty entropy of a quantum system and the second term is called the excess statistical entropy. $S_0(k)$ is given by the relation:

$$S_0(k) = \sum_{i=2}^{k} \frac{1}{i}$$

(14)

$S_F$ in relation (3) of [19] is denoted by $S[\rho]$.

3 Fractional occupation probabilities

In [21]-[23] a simple method was proposed for the introduction of short range correlations (SRC) in the ground state nuclear wave function for nuclei in the region $4 \leq A \leq 40$. The correlations were of the Jastrow type and the correlation parameters were determined by fitting the charge form factor experimental data. The above method gives the correlated proton density distribution $\rho_{\text{cor}}(r)$. In [21] $\rho_{\text{cor}}(r)$ was used as input in a method for the determination of fractional occupation probabilities, where the natural orbital representation (NOR) is employed, by imposing the condition $\rho_{\text{cor}}(r) = \rho_{n.o}(r)$ where $\rho_{n.o}(r)$ is the density distribution constructed by natural orbitals. This provides a systematic study of the effect of SRC on the occupation numbers of the shell model orbits and the depletion of the nuclear Fermi sea in light nuclei.

The "natural orbitals" $\phi_q$ are defined [24] as the orthogonal basis which diagonalizes the one-body density matrix

$$\rho(\vec{r}, \vec{r'}) = \sum_q a_q \phi_q^*(\vec{r}) \phi_q(\vec{r'})$$

(15)

where $a_q$ is the occupation number of the state $q \equiv nlj$. Thus the density distribution takes the simple form:

$$\rho(\vec{r}) = \frac{1}{4\pi} \sum_{nl} (2j + 1) n_q |\phi_q(\vec{r})|^2$$

(16)
where \( n_q = \frac{a_q}{2j+1} \) is the occupation probability of the \( q (\equiv nlj) \) state.

In \cite{21} we used occupation probabilities \( n_{nl} \) related to \( n_{nlj} \) as follows:

\[
n_{nl} = \frac{l + 1}{2l + 1} n_{nl, l+1/2} + \frac{l}{2l + 1} n_{nl, l-1/2}
\] (17)

Values of \( n_{nl} \) for various states and nuclei can be found in Table IV of \cite{21} (case A in the present work) and Table I of \cite{22} (case B). In case B a sort of state dependence of the single particle wave functions in the "natural orbital" representation was taken into account.

4 Calculation of information entropies and discussion

In the present work we employ the probabilities \( p_q = \frac{n_{nl} 2^{2l+1}}{Z} \) which sum up to 1 (\( \sum_q p_q = 1 \)). Probabilities \( p_q \) are shown in Table 1. Using these values we calculate the information entropies of light nuclei according to Jaynes (\( S_J \)), Onicescu (\( S_E \)) and Stotland (\( S_F \)) as functions of the atomic number \( Z \).

It is seen that the above information entropies show a similar behaviour i.e. they are increasing functions of \( Z \) for all cases A, B, C considered in the present work (case C corresponds to IPM–Independent Particle Model). IPM is a starting point for the nuclear many body problem. In Table 1 we show \( p_q \) for \( ^{16}\text{O} \) and \( ^{40}\text{Ca} \) for IPM. However, due to the interaction between nucleons including short-range correlations (SRC), nucleons are excited to higher levels and the Fermi surface is depleted giving fractional occupation probabilities of energy levels, which deviate from the standard values of IPM.

It is concluded that increasing \( Z \) the information entropy increases i.e. the disorder of a nucleus increases for three measures of information.

In the present work we look at the information content (\( S_J \)) of nuclei by employing the occupation probabilities of protons distributed to energy levels. The corresponding probability distribution \( (p_1, p_2, \ldots, p_k) \) is discrete. In previous work \cite{10} we calculated the information entropy for a continuous density distribution \( \rho(r) \) (position space) and \( n(k) \) (momentum space) of nucleons in nuclei (and other systems as well i.e. atoms and atomic clusters).

We proposed the universal relation \( S_S = a + b \ln N \) described above.

The two ways of looking at information entropy give at least the same qualitative behaviour, i.e. the information entropy increases (disorder in-
creases) as $Z$ increases. However, the depletion of the Fermi sea due to short-range correlations is in our model about 32% i.e. about constant, at least for the region of $Z$ considered ($4 \leq Z \leq 40$). This indicates that the information entropy is a sensitive index of disorder of a nucleus.

We may also calculate $S_J$, $S_E$, $S_F$ for the IPM occupation probabilities of the shell model orbits (case C) and compare with the values of entropy corresponding to fractional occupation probabilities due to short-range correlations (case A and B). Thus the effect of SRC can be assessed by looking at the differences of the corresponding values of entropy. It is seen that SRC increase $S_J$, $S_E$, $S_F$ comparing with the corresponding values calculated according to IPM. A similar trend was found in[8] for $S_S$ calculated with correlated and uncorrelated continuous density distributions $p(r)$ and $n(k)$.

It is noted that for $^{40}\text{Ca}$ (Case C) we do not present any value for $S_F$ (Table 1) because in this case the probabilities $p_q$ for $n_{1s}$, $n_{2s}$ are equal and thus $S_F$ diverges. It is also seen that the information entropies in case B are smaller than those in case A, indicating that the inclusion of state dependence decreases the values of entropy i.e. increases the order of nuclei.

A final comment seems appropriate. Information entropy for a discrete probability distribution (denoted as $S_{Jaynes} = S_J$ in[25]) is minimal for IPM and maximal for an unbound system and also for an extreme wave function i.e. the natural orbitals are equally occupied with $p_q < 1$. In a similar sense, information entropy for a continuous probability distribution (denoted as $S_{Shannon} = S_S$ in[25]) is maximal for a uniform distribution e.g. that of an unbound system and is minimal e.g. a delta-like distribution. In fact, the two types of $S$ were compared[25] for chemical systems. In our nuclear case the two measures of information are shown as functions of $Z$ in Fig. 1, where the values of information in the continuous case are obtained using a linear relation $S_S = a + b \ln Z$ derived in[10] and in the discrete one from $S_J$ of Table 1. Fig. 1 is analogous to the atomic case seen in Fig. 5.[25]

It is seen that $S_S$, $S_J$ increase as $Z$ increases. This is expected for distributions normalized to 1. However, the case of $S_S = S_r + S_k$ which increases with $Z$ is not completely evident, because as $Z$ increases, $S_r$ increases, $S_k$ decreases and $S_S = S_r + S_k$ increases due to a delicate balance between $S_r$ and $S_k$ (as seen in our previous work). This is the case with the entropic quantity $S_S$ calculated with density distributions normalized to 1, while entropic-like quantities $S$ calculated with density distributions normalized to the number of particles are not monotonic functions of $Z$.[8] However, one considers entropic quantities more desirable than entropic-like ones, because entropic
quantities are in the spirit of Shannon’s definition using the relation \( \sum p_i = 1 \) (normalized to one).

There is no obvious relation between \( S_S \) and \( S_J \) due to the non-linear nature of the logarithm. However, an attempt to compare various entropies was made for atoms in,\(^{25}\) where the following properties were reported and are summarized below.

The Jaynes entropy per electron \( \frac{S_J}{N} \) is the difference between the ensemble average of the Shannon entropy \textit{per electron} \( \frac{S_u}{u} \) and the ensemble average of the Shannon entropy of \textit{one electron} \( \bar{S}_u \) (see\(^{25}\) relations (2.5) and (2.9)) which may be interpreted as a measure of the difference in the average shape of the square of a natural orbital per electron, and the shape of the square of a natural orbital of one electron. This property is expressed in the following relationship

\[
\frac{S_J}{N} = \left( \frac{\bar{S}_u}{u} \right) - \bar{S}_u = \ln \mu - \ln \varepsilon \tag{18}
\]

Here \( S_u \) corresponds to a probability distribution normalized to 1, where the ensemble average of the quantity \( \bar{F} \) is defined as:

\[
\bar{F} = \sum_j \frac{\nu_j}{N} F_j
\]

\( \varepsilon_j \) is the single particle energy in state \( j \) and \( \mu \) is the chemical potential.

Relation (18) is interesting, since it equates the differences from a density perspective (the orbital entropies) to energetic differences.

We conclude by giving an interesting relation\(^{25}\) between \( I \) (the orbital mean excitation of an atom) and \( \frac{S_v}{v} \):

\[
\ln I = -\frac{1}{2} \left( \frac{S_v}{v} \right) + \ln \gamma + \frac{\ln 4\pi}{2} \tag{19}
\]

Here \( S_v \) corresponds to distributions normalized to \( N \) \( (\gamma \) is a correction term for the shift in the plasma frequency due to the chemical environment). The above properties represent a considerable progress in chemistry for understanding the concept of information entropy. Although we have found interesting relationships as described in\(^{12}\) we hope that more progress will be made in similar matters in nuclear physics.

Finally, it is noted that a study of \( S_S \) and \( S_J \) for correlated bosons in a trap is carried out in\(^{27}\) with results analogous to Fig. 1.
5 Conclusions

A simple model of fractional occupation probabilities in light nuclei is employed to calculate the information entropy $S$ as function of the atomic number $Z$. For the sake of comparison, three different definitions of information content of a quantum system are used i.e. according to Jaynes, Onicescu and Stotland. It is concluded that $S$ is an increasing function of $Z$ in all cases. It is seen that short-range correlations increase $S$ (or disorder) of nuclei. Also the inclusion of state dependent correlations decrease $S$ (increase order). Finally, the information entropy is proposed as a sensitive index of order and short-range correlations in nuclei.

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| Nuclei | $n_{1s}$ | $n_{1p}$ | $n_{1d}$ | $n_{2s}$ | $n_{1f}$ | $n_{2p}$ | $S$   | $S_E$ | $S_F$ |
|--------|--------|--------|--------|--------|--------|--------|------|------|------|
| $^4$He(A) | 0.485 | 0.515 | | | | | 0.693 | 1.998 | 0.693 |
| $^{12}$C(A) | 0.223 | 0.528 | 0.249 | | | | 1.018 | 2.561 | 1.077 |
| $^{12}$C(B) | 0.265 | 0.584 | 0.151 | | | | 0.956 | 2.304 | 1.061 |
| $^{16}$O(A) | 0.172 | 0.509 | 0.299 | 0.020 | | | 1.086 | 2.642 | 1.333 |
| $^{16}$O(B) | 0.216 | 0.596 | 0.174 | 0.015 | | | 1.007 | 2.313 | 1.313 |
| $^{16}$O(C) | 0.250 | 0.750 | | | | | 0.562 | 1.600 | 0.650 |
| $^{24}$Mg(A) | 0.120 | 0.350 | 0.383 | 0.055 | 0.082 | 0.010 | 1.400 | 3.408 | 1.575 |
| $^{26}$Si(A) | 0.100 | 0.296 | 0.364 | 0.060 | 0.160 | | 1.490 | 3.852 | 1.753 |
| $^{28}$Si(B) | 0.141 | 0.420 | 0.186 | | 0.043 | 0.210 | | 1.416 | 3.612 | 1.578 |
| $^{32}$S(A) | 0.088 | 0.259 | 0.350 | 0.062 | 0.219 | | 0.022 | | 1.520 | 4.006 | 1.756 |
| $^{32}$S(B) | 0.107 | 0.305 | 0.351 | 0.065 | 0.158 | | 0.015 | | 1.501 | 3.890 | 1.752 |
| $^{40}$Ca(A) | 0.068 | 0.201 | 0.325 | 0.064 | 0.301 | 0.042 | | 1.541 | 4.047 | 1.756 |
| $^{40}$Ca(B) | 0.093 | 0.224 | 0.359 | 0.060 | 0.237 | | 0.027 | | 1.531 | 4.029 | 1.756 |
| $^{40}$Ca(C) | 0.100 | 0.300 | 0.500 | | 0.100 | | | | 1.168 | 2.778 | 1.575 |

Table 1: Probabilities $p_q$ and values of information entropy ($Shannon-S$, $Onicescu-S_E$ and $Stotland-S_F$) for various nuclei. For cases A, B and C see text
Figure 1: Discrete $S_J$ (present work) and Continuous $S_S$ Shannon information entropies as functions of $\ln Z$
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