Universal trend of the information entropy of a fermion in a mean field

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(Received 23 June 2000; published 3 May 2001)

We calculate the information entropy of single-particle states in position space S_r and momentum space S_k for a nucleon in a nucleus, a Λ particle in a hypernucleus, and an electron in an atomic cluster. It is seen that S_r and S_k obey the same approximate functional form as functions of the number of particles S_r (or S_k) $=a+bN^{1/3}$ in all of the above many-body systems in position and momentum space separately. The net information content S_r+S_k is a slowly varying function of N of the same form as above. The entropy sum S_r+S_k is invariant to a uniform scaling of coordinates, and is a characteristic of the single-particle states of a specific system. The order of single-particle states according to S_r+S_k is the same as their classification according to energy, keeping the quantum number n constant. The spin-orbit partners are ordered correctly. It is also seen that S_r+S_k is enhanced by the excitation of a fermion in a quantum-mechanical system. Finally, we obtain a relationship of S_r+S_k with the energy of the corresponding single-particle state, i.e., $S_r+S_k = k\ln(\mu E+\nu)$. This relation holds for all systems under consideration.

DOI: 10.1103/PhysRevC.63.064307 PACS number(s): 21.10.−k, 21.80.+a, 89.70.+c

I. INTRODUCTION

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

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

where $\int p(x)dx=1$. 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 the uncertainty of the corresponding state. We note that the information and thermodynamic entropy are different concepts, but can be connected by employing some assumptions.

An important step in the past was the discovery in Ref. [1] of an entropic uncertainty relation (EUR), which for a three-dimensional system has the form

$$S_r+S_k \geqslant 3(1+\ln\pi)\cong 6.434 \quad (\hbar=1), \tag{2}$$

where

$$S_r=-\int \rho(\mathbf{r})\ln\rho(\mathbf{r})d\mathbf{r} \tag{3}$$

is the information entropy in position space,

$$S_k=-\int n(\mathbf{k})\ln n(\mathbf{k})d\mathbf{k} \tag{4}$$

is the information entropy in momentum space, and $\rho(\mathbf{r})$ and $n(\mathbf{k})$ are the density distributions in position and momentum space, respectively, normalized to unity.

The lower bound in Eq. (2) is attained for Gaussian density distributions. The physical meaning of the above inequality is the following: an increase of S_k corresponds to a decrease of S_r and vice versa, which indicates that a diffuse density distribution $n(k)$ in momentum space is associated with a localized density distribution $\rho(r)$ in configuration space, and vice versa.

Relation (2) represents a strengthened version of Heisenberg's uncertainty principle for two reasons: first the EUR leads to Heisenberg's uncertainty relation, but the inverse is not true. Second, the right-hand side of the EUR does not depend on the state of the system, while in Heisenberg's relation it does depend. It is obvious from Eqs. (3) and (4) that S_r and S_k depend on the unit of length in measuring $\rho(\mathbf{r})$ and $n(\mathbf{k})$. However, the important quantity is the entropy sum S_r+S_k (the net information content of the state), which is invariant to a uniform scaling of coordinates.

Information entropy was employed in the past to study quantum-mechanical systems [1–9]. Recently [10] we studied the position- and momentum-space information entropies S_r and S_k respectively, for the total densities of various systems: the nuclear density distribution of nuclei, the electron density distribution of atoms, and the valence electron density distribution of atomic clusters. We showed that a similar functional form $S=a+b\ln N$ for the total entropy as a function of the number of particles N holds approximately for the above systems (in agreement with Refs. [2,3] for atomic systems). We conjectured that this is a universal property of a many-fermion system in a mean field.

The concept of information entropy also proved to be fruitful in a different context [9]. We used the formalism of Ghosh, Berkowitz, and Parr [11] within the ground-state density-functional framework, to define the concept of an information entropy associated with the density distribution of a nuclear system. It turned out that S increases with the quality of the wave function, and can serve as a criterion of the quality of a nuclear model. Another interesting result [12] is the fact that the entropy of an N-photon state subjected to Gaussian noise increases linearly with the logarithm of N.

Encouraged by previous works, we attempt in the present paper to calculate S_r and S_k for the wave functions of single-particle states (instead of the total densities as in Ref. [10])

for various systems, i.e., a nucleon in a nucleus, an electron in an atomic cluster and a Λ particle in a hypernucleus. For these systems we employ models existing in the literature.

Our aim is to investigate the dependence of S_r and S_k on the excitation of a fermion in a quantum-mechanical system, as well as its dependence on the system under consideration and the number of particles N. We also attempt to connect the information entropy with the energy of the single-particle state. The study of the dependence of S on the quantum state of a system is also interesting (as stated in Ref. [7]) for two reasons: (i) The information-theoretical and physical entropy are connected via Boltzmann's constant k_B by Jayne's relation $S_{phys}=k_B S_{inf}$. Thus one can ascribe to any quantum object a certain value of its physical entropy S_{phys} if one calculates S_{inf}. (ii) It is interesting to know the value of the information entropy which is a measure of the spatial ''spreading out'' of the wave function for various states of various systems.

The present paper is organized as follows. In Sec. II we calculate S_r and S_k for single-particle states of a nucleon in a nucleus as function of the number of nucleons N using the simplest model available, i.e., the harmonic-oscillator potential and a more realistic one (Skyrme). In Sec. III we calculate S_r and S_k for a Λ particle in a hypernucleus employing a simple and a (semi) analytical relativistic model. In Sec. IV we determine S_r and S_k for the single-particle states of an electron in atomic (metallic) clusters using the Woods-Saxon potential. In Sec. V we present a relationship of S_r+S_k with the energy. Finally, Sec. VI contains a discussion of our results (comparison of Secs. II, III, and IV) and our conclusions.

II. INFORMATION ENTROPY FOR A NUCLEON IN A NUCLEUS

The information entropy S_r in position space for a single-particle wave function $\psi_{nlj}(r)$, normalized as

$$4\pi\int_0^\infty |\psi_{nlj}(r)|^2 r^2 dr = 1,$$

is defined by

$$S_r = -4\pi\int_0^\infty |\psi_{nlj}(r)|^2 \ln|\psi_{nlj}(r)|^2 r^2 dr \tag{5}$$

while the entropy S_k in momentum space is

$$S_k = -4\pi\int_0^\infty |\phi_{nlj}(k)|^2 \ln|\phi_{nlj}(k)|^2 k^2 dk, \tag{6}$$

where $\phi_{nlj}(\mathbf{k})$ is the Fourier transform of $\psi_{nlj}(\mathbf{r})$ and $\phi_{nlj}(k)$ is normalized as

$$4\pi\int_0^\infty |\phi_{nlj}(k)|^2 k^2 dk = 1.$$

In this section we calculate S_r and S_k for the single-particle states $1s,\ 1p,\ 1d,\ldots$ of a nucleon in a nucleus in the framework of the harmonic-oscillator (HO) model. For the HO parameter we use the well-known expression $\hbar\omega = 41N^{-1/3}$ MeV ($N=A$ is the mass number).

We find that the value of $\hbar\omega$ is important only for S_r and S_k, while the net information content $S=S_r+S_k$ is independent of $\hbar\omega$ and consequently of A. It depends only on the state under consideration, and characterizes it. These values for the states $1s$, $1p$, $1d$, and $2s$ are 6.4341, 7.8388, 8.6651, and 8.3015, respectively.

However, the HO model is a simplification. Thus, we employed a more realistic parametrization of the nuclear mean field i.e., the Skyrme (SkIII) interaction [13]. In this model protons and neutrons move in different potentials. We choose to work with protons. However, similar results can be obtained for neutrons. We found that the values for S_r and S_k obtained from the wave functions of single-particle states calculated according to SkIII are well represented by the expression

$$S_r \ (\text{or}\ S_k) = a + bN^{1/3} \tag{7}$$

while S_r+S_k is a slowly varying function of N of the same form as Eq. (7). The values of the parameters are shown in Table I.

In Fig. 1(a) we plot our fitted expressions (SkIII) $S_r\ (\text{or}\ S_k)=a+bN^{1/3}$ for the entropies S_r, S_k, S_r+S_k of $1s$ states as functions of $N^{1/3}$. The lines correspond to our fitted expressions, while the corresponding values of our numerical calculations are denoted by squares for S_r, circles for S_k, and triangles for S_r+S_k. Similar graphs can be plotted for the higher states $1p, 1d, 2s, \ldots$. From Fig. 1(a) we see that the values of the entropies are represented well by our fitted expressions. In Fig. 1(b) we compare the sum $S_r+S_k=a+bN^{1/3}$ for various single-particle states. We observe that the entropy sum S_r+S_k is enhanced with the excitation of the single-particle states. We see that S_r+S_k is a slowly varying function of N. We also note that the spin-orbit partners are ordered correctly, i.e., the state $1p_{3/2}$ is lower than $1p_{1/2}$, etc. (as for the energy), although their difference is small and cannot be shown in the figure. To support this argument we present Table II, where the entropies and energies of various partners are compared for the nuclei ^{16}O, ^{40}Ca, and ^{208}Pb.

The following comment is appropriate. A relation of S_r and S_k with N can be extracted from Eqs. (12) and (13) of Ref. [7] and the relation $\hbar\omega=41N^{-1/3}$, or equivalently the size parameter of the HO, $b\simeq N^{1/6}$ fm [14]

$$S_r = f(n) + \ln\sigma_r, \quad \sigma_r = b = \sqrt{\hbar/m\omega},$$

$$S_k = f(n) + \ln\sigma_k, \quad \sigma_k = \sqrt{m\omega/\hbar},$$

where $f(n)$ depends on the quantum number n:

$$f(n) = -C_n^2\int_{-\infty}^{\infty} H_n^2(\xi)e^{-\xi^2}\ln[C_n^2 H_n^2(\xi)e^{-\xi^2}]d\xi.$$

Thus we obtain

$$S_r = f(n) + \tfrac{1}{6}\ln N, \tag{8}$$

TABLE I. Values of the parameters a and b which appear in the expressions S_r (or S_k)$=a+bN^{1/3}$ for a nucleon (proton) in nuclei according to the SkIII interaction, a Λ in hypernuclei according to a relativistic model, and an electron in atomic clusters with a Woods-Saxon potential.

Case	State	S_r		S_k		S_r+S_k	
		a	b	a	b	a	b
Nucleus	$1s_{1/2}$	3.0831	0.8652	3.2353	-0.8140	6.3217	0.0501
	$1p_{3/2}$	4.2824	0.6368	3.6256	-0.6688	7.9084	-0.0322
	$1p_{1/2}$	4.2724	0.6235	3.6799	-0.6675	7.9521	-0.0439
	$1d_{5/2}$	4.7500	0.5743	4.0980	-0.6513	8.8480	-0.0771
	$1d_{3/2}$	4.9553	0.5042	4.0080	-0.6071	8.9618	-0.1024
	$2s_{1/2}$	5.2456	0.3364	3.4355	-0.4641	8.6756	-0.1260
Hypernucleus	$1s_{1/2}$	3.5817	0.4967	2.8303	-0.4756	6.4120	0.0214
	$1p_{3/2}$	4.4347	0.3789	3.5123	-0.4021	7.9475	-0.0232
	$1p_{1/2}$	4.3764	0.3835	3.6575	-0.4199	8.0342	-0.0364
	$1d_{5/2}$	5.2553	0.2462	3.6249	-0.2938	8.8803	-0.0475
	$1d_{3/2}$	4.9910	0.2819	4.0503	-0.3543	9.0414	-0.0724
Cluster	$1s$	4.3038	0.7113	2.0923	-0.6883	6.3960	0.0232
	$1p$	5.1114	0.6135	2.7700	-0.6299	7.8816	-0.0163
	$1d$	5.5191	0.5636	3.1420	-0.5842	8.6611	-0.0205
	$2s$	5.3858	0.4918	2.9672	-0.5301	8.3536	-0.0383

$$S_k=f(n)-\tfrac{1}{6}\ln N. \tag{9}$$

Adding Eqs. (8) and (9), we see that the two N-dependent terms cancel each other, so that S_r+S_k becomes exactly independent of N for the HO. However, for more realistic cases this cancellation is not exact, and S_r+S_k is a slowly varying function of N. Equations (8) and (9) suggest a linear dependence of S_r and S_k on $\ln N$. However, for more realistic systems, our numerical calculations show that a linear dependence on $N^{1/3}$ is more accurate than one on $\ln N$.

III. INFORMATION ENTROPY FOR A Λ IN A HYPERNUCLEUS

We construct a simple and (semi) analytical relativistic model of a hypernucleus from Refs. [15,16], where a Dirac equation with a scalar potential $U_S(r)$ and the fourth component of a vector potential $U_V(r)$ was considered in the case of rectangular shapes of these potentials with the same radius:

$$R=r_0A_{core}^{1/3}.$$

In Ref. [15] the Dirac equation was solved, and gave the wave functions $G(r)$ and $F(r)$ for the large and small components for a Λ particle in a hypernucleus. These components can be found in relations (12) and (13) of Ref. [15].

The Dirac spinors in terms of large (G) and small (F) components can be expressed

$$\psi_{nlj}=\begin{pmatrix} iG_{nlj}(r)/r \\ F_{nlj}(r)/r \end{pmatrix}. \tag{10}$$

The density distribution of a Λ in position space is

$$\rho_{nlj}(r)=\frac{1}{4\pi}[G_{nlj}^2(r)/r^2+F_{nlj}^2(r)/r^2], \tag{11}$$

and the normalization is

$$4\pi\int_0^\infty \rho_{nlj}(r)r^2dr=1.$$

In momentum space we have

$$\phi_{nlj}(k)=\begin{pmatrix} iX_{nlj}(k) \\ Y_{nlj}(k) \end{pmatrix}, \tag{12}$$

where $X_{nlj}(k)$ and $Y_{nlj}(k)$ are the Fourier transforms of $G_{nlj}(r)/r$ and $F_{nlj}(r)/r$, respectively. Thus the density distribution in momentum space is given by

$$n_{nlj}(k)=\frac{1}{4\pi}[X_{nlj}^2(k)+Y_{nlj}^2(k)], \tag{13}$$

and the normalization is

$$4\pi\int_0^\infty n_{nlj}(k)k^2dk=1.$$

The information entropies of the Λ particle are calculated according to the relations

$$S_r=-4\pi\int_0^\infty \rho_{nlj}(r)\ln\rho_{nlj}(r)r^2dr, \tag{14}$$

$$S_k=-4\pi\int_0^\infty n_{nlj}(k)\ln n_{nlj}(k)k^2dk, \tag{15}$$

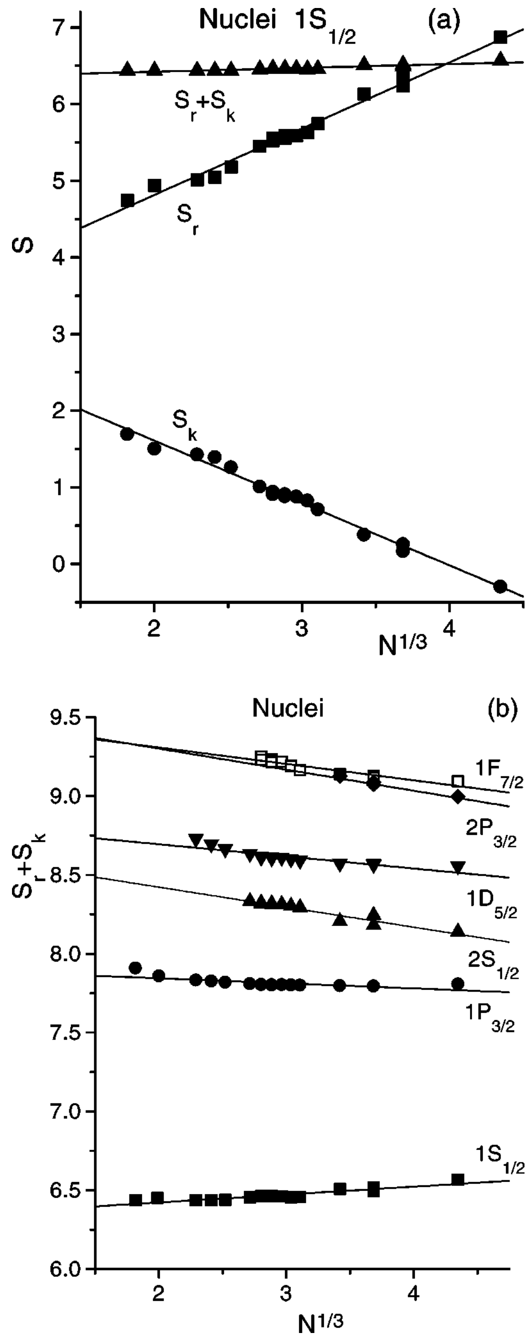

FIG. 1. (a) Values of the information entropies S_r (squares), S_k (circles), and S_r+S_k (triangles), calculated numerically, vs the number of particles N. These values correspond to the single-particle states of a proton in various nuclei, according to the SkIII interaction. The lines correspond to our fitted expressions S_r (or S_k) $= a + bN^{1/3}$. (b) Comparison of the sum S_r+S_k for various proton single-particle states.

where $\rho_{nlj}(r)$ and $n_{nlj}(k)$ are given by Eqs. (11) and (13) respectively.

For the depths of the potential we used the values [15] $D_+ = 30.55$ MeV, $D_- = 300$ MeV, and $r_0 = 1.01$ fm, and the radius parameter $R = r_0 A_{core}^{1/3}$ obtained by fitting the experimental binding energies of the ground state of the Λ particle. In the following we put $A_{core} = N$ =number of particles.

TABLE II. Values of the sp energy (E) in MeV and entropy sum (S) for ^{16}O, ^{40}Ca, and ^{208}Pb and for the higher states of ^{208}Pb for protons and neutrons.

		Protons		Neutrons	
Nucleus	State	E	S	E	S
^{16}O					
	$1p_{1/2}$	-9.72	7.901	-13.00	7.892
	$1p_{3/2}$	-15.09	7.859	-18.47	7.854
^{40}Ca					
	$1p_{1/2}$	-22.47	7.818	-29.71	7.816
	$1p_{3/2}$	-25.71	7.809	-33.00	7.807
	$1d_{3/2}$	-7.91	8.693	-14.82	8.678
	$1d_{5/2}$	-13.91	8.633	-20.95	8.626
^{208}Pb					
	$3p_{1/2}$			-6.96	9.949
	$3p_{3/2}$			-7.98	9.942
	$2f_{5/2}$			-8.27	10.138
	$2f_{7/2}$			-11.04	10.131
	$1h_{9/2}$			-12.48	9.981
	$1h_{11/2}$	-9.49	9.871	-18.03	9.901
	$2d_{3/2}$	-8.41	9.636	-17.48	9.660
	$2d_{5/2}$	-10.16	9.607	-19.45	9.626
	$1g_{7/2}$	-13.49	9.551	-21.97	9.577
	$1g_{9/2}$	-17.23	9.516	-25.77	9.536
	$2p_{1/2}$	-17.56	9.011	-26.71	9.026
	$2p_{3/2}$	-18.55	8.997	-27.79	9.009

Next we fitted the expressions S_r (or S_k) $= a + bN^{1/3}$ to the values of S_r and S_k calculated from Eqs. (14) and (15), and found that these values are represented well. The values of the parameters a and b for various states are shown in Table I.

In Fig. 2(a) we plot our fitted expressions for S_r, S_k, and S_r+S_k as functions of $N^{1/3}$ for the $1s$ state. This is done for a Λ in a hypernucleus in a similar way as for a nucleon in a nucleus [Fig. 1(a)]. Similar graphs can be plotted for the higher states. In Fig. 2(b) we compare the sum S_r+S_k for various single-particle states of a Λ [similarly to Fig. 1(b)]. The spin-orbit ordering is reproduced correctly as in nuclei (Sec. II). A comparison of various states for some hypernuclei is shown in Table III.

IV. INFORMATION ENTROPY FOR AN ELECTRON IN AN ATOMIC CLUSTER

We consider atomic (metallic) clusters composed of neutral sodium atoms, where the electrons move in an effective radial electronic potential parametrized by a Woods-Saxon potential of the form

$$V_{WS}(r) = \frac{-V_0}{1+\exp[(r-R)/a]}, \tag{16}$$

with $V_0 = 6$ eV, $R = r_0 N^{1/3}$, $r_0 = 2.25$ Å, and $a = 0.74$ Å. For a detailed study regarding the parametrization of Ekardt's potentials, see Ref. [17].

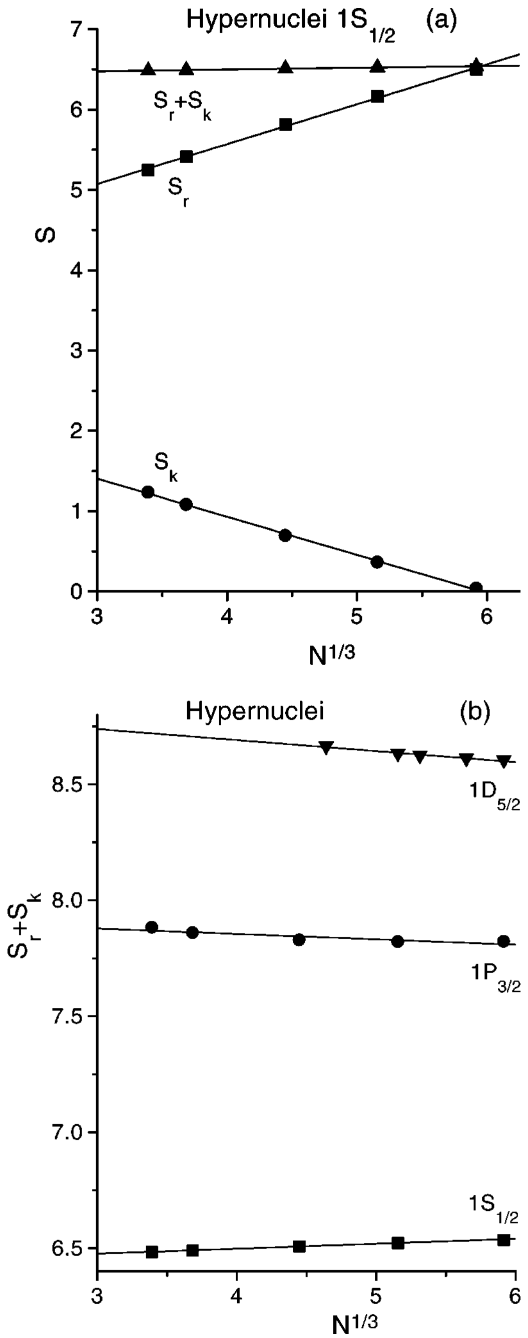

FIG. 2. The same as in Fig. 1, for a Λ in hypernuclei employing a relativistic model.

We found the wave functions of the single-particle states in configuration space numerically solving the Schrödinger equation for atomic clusters for various values of the number of valence electrons N. The wave functions in momentum space were found by Fourier transforming the corresponding ones in configuration space. Using the above wave functions, we calculated the information entropies S_r and S_k [relations (5) and (6)] for single-particle states instead of the total density distributions as in Ref. [10]. Then we fitted the form S_r (or S_k) $= a + bN^{1/3}$ to these values, and found that these expressions well represent the values of S_r and S_k. In Fig. 3(a) we plot S_r, S_k, and $S_r + S_k$ as functions of $N^{1/3}$ [similarly as in Figs. 1(a) and 2(a)] and in Fig. 3(b) we compare $S_r + S_k$ for various states [similarly as in Figs. 1(b) and 2(b)]. In Table I we present the values of the parameters a and b which were obtained from the fitting.

V. RELATIONSHIP OF THE INFORMATION ENTROPY WITH THE ENERGY OF SINGLE-PARTICLE STATES

In Fig. 4 we plot $S_r + S_k$, obtained with the HO model of the nucleus, versus the energy of the single-particle states. We use $\hbar\omega = 41N^{-1/3}$ with $N = 208$ (Pb), and keep the quantum number n equal to 1. A fitting procedure gives, for $n = 1$, the relation

$$S = k \ln(\mu E + \nu), \tag{17}$$

where $k = 2.0206$, $\mu = 3.5373$ MeV^{-1}, and $\nu = -12.5320$. Similar relations hold for $n > 1$.

Next we plot the sum $S_r + S_k$ as a function of the energy E of single-particle states for a proton in a nucleus according to SkIII interaction for ^{208}Pb (Fig. 5) and an electron in an atomic cluster with $N = 198$ (Fig. 6) for $n = 1$. Similar curves hold for larger values of $n > 1$. In both cases the dependence of $S_r + S_k$ on E can be represented well by the functional form [Eq. (17)]. The values of the constants are the following:

$k = 1.5262$, $\mu = 17.3043$ MeV^{-1},

$\nu = 793.109$ for a proton in a nucleus

$k = 1.2386$, $\mu = 1481.48$ eV^{-1},

$\nu = 8730.52$ for an electron in a cluster.

TABLE III. Values of the sp energy (E) in MeV and entropy sum (S) for various states of Λ hypernuclei.

State	A_{core}	E	S	A_{core}	E	S	A_{core}	E	S
$1p_{1/2}$	39	-7.737	7.932	50	-10.079	7.894	88	-15.167	7.850
$1p_{3/2}$	39	-9.040	7.883	50	-10.903	7.859	88	-15.576	7.828
$1p_{1/2}$	137	-18.462	7.837	207	-20.973	7.835			
$1p_{3/2}$	137	-18.705	7.821	207	-21.123	7.822			
$1d_{3/2}$	137	-9.713	8.659	207	-13.820	8.623			
$1d_{5/2}$	137	-10.477	8.633	207	-14.264	8.603			

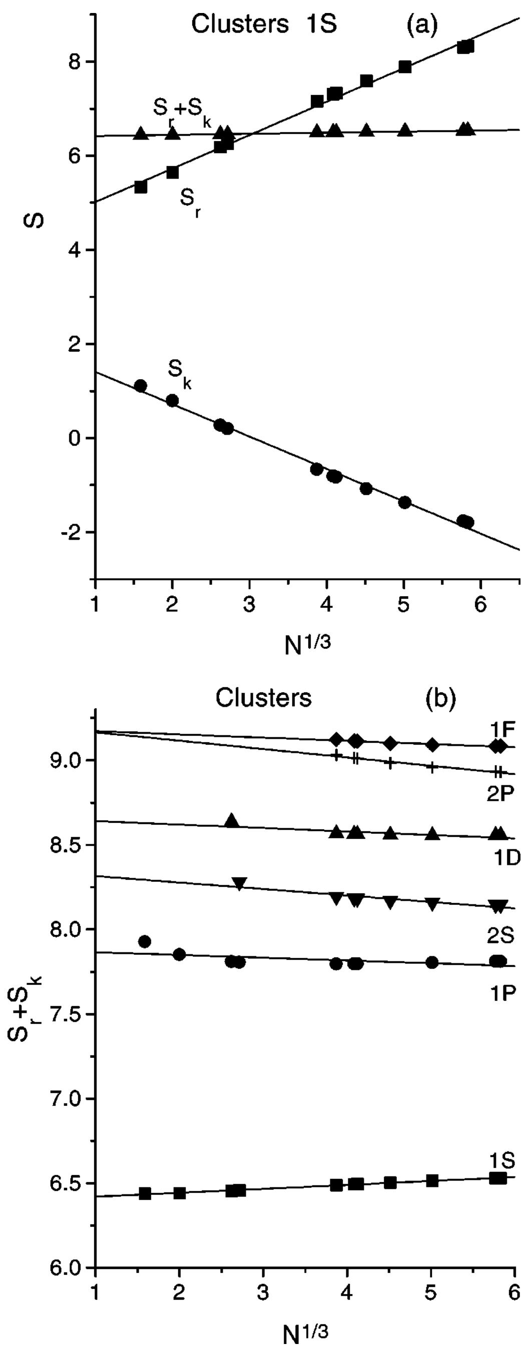

FIG. 3. The same as in Fig. 1, for an electron in atomic clusters with a Woods-Saxon potential.

A similar relation may be obtained for a Λ in a hypernucleus, but the number of values of S_r+S_k available is small. Relation (17) can be extracted from the asymptotic form for the one-dimensional HO given in Eq. (31) of Ref. [7]. However, in the present work we extend the calculations to more realistic three-dimensional systems, and we obtain relation (17).

VI. DISCUSSION AND CONCLUSIONS

Comparing our results in Secs. II, III, and IV, we see that a similar functional form S_r (or S_k)$=a+bN^{1/3}$ describes well the information entropies S_r and S_k of the single-particle states for a nucleon in a nucleus, a Λ in a hypernucleus, and a valence electron in an atomic cluster, although the single-particle potentials are different. We conjecture that this is a universal trend of the information entropies S_r and S_k for a fermion in a mean field, while the net information

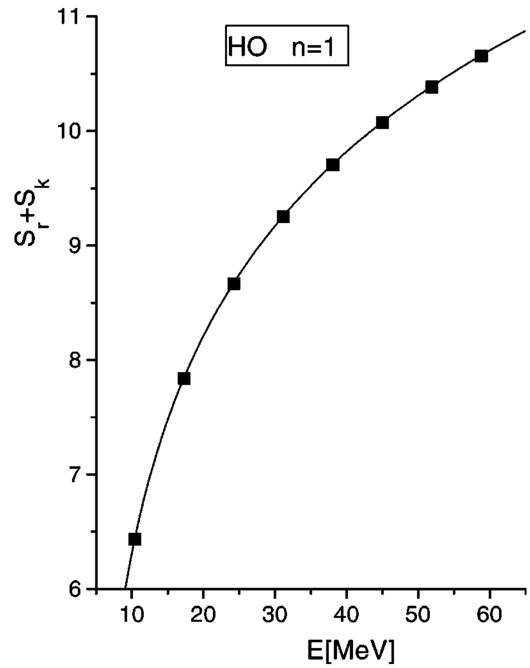

FIG. 4. The values of the entropy sum S_r+S_k (squares) of single-particle states for a nucleon in Pb^{208} according to the HO model for $n=1$. The line corresponds to our fitted expression $S=k\ln(\mu E+\nu)$.

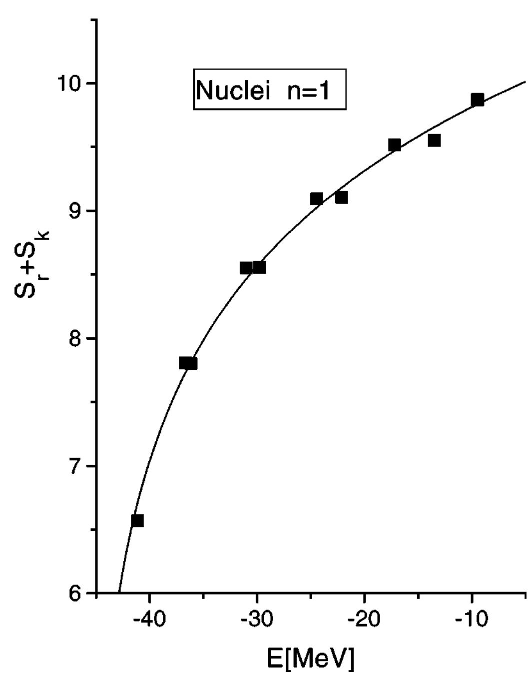

FIG. 5. The same as in Fig. 4, but for a proton in Pb^{208} according to the SkIII interaction for $n=1$.

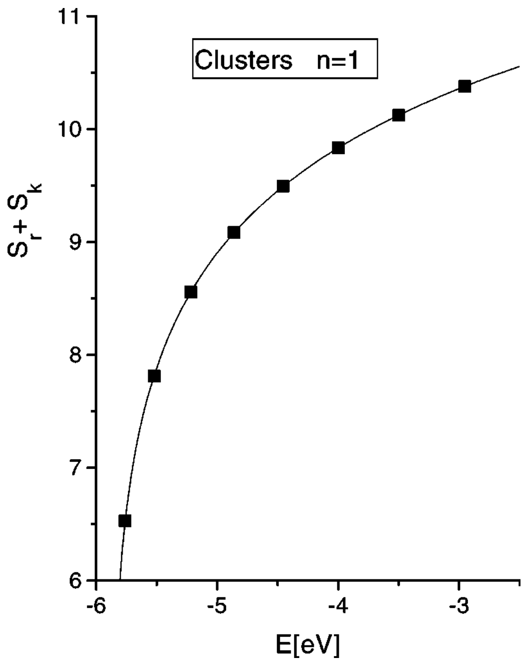

FIG. 6. The same as in Fig. 4, but for an electron in atomic clusters ($N=198$) using the Woods-Saxon potential for $n=1$.

content S_r+S_k of the single-particle states of a fermion in a mean field is a slowly varying function of N of the form $S=a+bN^{1/3}$ for the systems considered above. For nuclei and a simple HO potential, S_r+S_k is exactly a constant independent of N, i.e., $b=0$. We note that in Ref. [10] we found the universal property $S=a+b\ln N$ for the total density distributions of various systems.

In both cases it is not clear why S depends linearly on $\ln N$ (total densities) or linearly on $N^{1/3}$ (single-particle states), but we note that in atomic physics there is already a connection of the information entropy with experiment, i.e., with fundamental and/or experimental quantities, e.g., the kinetic energy or the magnetic susceptibility. Both characteristics have been used in a study of the dynamics of atomic and molecular systems [18]. This connection established the information entropy as an interesting entity for atomic physics. In the present paper we obtained a relationship of S_r+S_k with a fundamental quantity as the energy of the single-particle states, i.e., $S=k\ln(\mu E+\nu)$. It is remarkable that the same functional form holds for various systems.

S is a monotonic (increasing) function of the sp energy (for quantum number $n=$const), e.g., $1p_{1/2}$ has an energy larger than $1p_{3/2}$. Thus $1p_{1/2}$ has a value of S larger than $1p_{3/2}$. This gives the correct ordering. This rule is verified by our numerical calculations, as can be seen in Table II for nuclei and Table III for hypernuclei.

In Table I we observe a change of sign of the parameter b from a $1s$ state to other sp states. For the HO S_r+S_k does not depend on N, as can be seen by adding Eqs. (8) and (9). However, for more realistic cases (examined in the present work) this cancellation is not exact. The change of sign of the parameter b from the $1s$ state to other single-particle states is due to an interplay of the two terms. It is remarkable that the same sign change occurs for all the cases under consideration.

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