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Fisher information and Shannon entropy calculations for two-electron systems

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Abstract: Fisher information is calculated for the ground state of He-isoelectronic series, in position (r) space. The results are given, and discussed, as a function of the nuclear charge (Z) and the screening parameter (λ) in the case study of Yukawa potential. Simple and explicit one, two and three-correlated terms of Hylleraas wave function are used to focus on extracting the most characteristic physical features of the results. The numerical values of Fisher information are given in 1- and 2-electron charge densities, and their ratio of 2- to 1-electron densities results are defined and analyzed. To enable a comparison with others, the Fisher-Shannon information products, that measure the electron-electron correlation's strength, are calculated in 1- electron density. The calculations of Fisher information, the ratio, and the Shannon-information products for two-electron systems in the presence of Yukawa potential are carried out for the first time in this literature.

Key words: Hylleraas coordinates, non-Coulombic helium, Yukawa potential, Fisher information, Shannon entropy, Helium-like ions, Shannon-information products.

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1. Introduction

Knowing the continuously charged electronic states' density $\rho(\vec{r})$, the Fisher information's value, F, is defined as [1] :

$$F \equiv \int \frac{\left(\vec{\nabla}\rho(\vec{r})\right)^2}{\rho(\vec{r})} d\vec{r},\tag{1}$$

where $d\vec{r}$ is the volume element in the respected coordinates. Fisher information, which is the gradient functional of $\rho(\vec{r})$, indicates a local measure of the intrinsic accuracy or localization of the electron density distribution. The larger the value of F is, the more concentrated the electronic states' density, i.e. more localized distribution. Moreover, the gradient term in F makes it quite sensitive to even small localized perturbations of $\rho(\vec{r})$.

Another important, and complementary, quantity with Fisher information, is Shannon entropy, defined as [2]:

$$S \equiv -\int \rho(\vec{r})\ln\left(\rho(\vec{r})\right) d\vec{r}.\tag{2}$$

S gives a global measure of the overall randomness, or delocalization, of the electron in the corresponding density distribution. Unlike F, S is not too sensitive to large localized perturbations in $\rho(\vec{r})$. The smaller the value of S is, the more concentrated the wave function of

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the state, i.e. more localized distribution. The complementary nature of Shannon entropy and Fisher information accounts for their observed variation with respect to Z, with the definition of Fisher-Shannon information product $"P"$ [3,4], in 3D as:

$$P = \frac{1}{3} F \frac{1}{2\pi e} e^{2S/3} > 1 \; . \tag{3}$$

The product, P , measures the spatial delocalization of the electron cloud and is considered as an appropriate measure of electron-electron (el-el) correlations. In the following study, we will use the abbreviation "el" for electron.

From the above two paragraphs, we conclude that: for larger values of Fisher information, the distribution is more localized. On the contrary, with a rise in Shannon entropy, the distribution becomes more diffused. In quantum mechanics, such a conclusion can only be drawn when the distribution is nodeless. But, there are cases where both Fisher information and Shannon entropy may rise simultaneously; see for example the application of Morse potential in diatomic molecules [5]. Actually, Fisher information is a local quantity and it measures the fluctuation in a given distribution, whereas Shannon entropy is an expectation value of uncertainty.

As an application of Fisher information, let us recall few articles that are related to one and two-electron systems. Recently Fisher information has been discussed and applied in different atomic systems [6-12], such as: confined hydrogen-like ions [6], confined isotropic harmonic oscillator [7], some central potentials [8], for elementary chemical reactions [9], in D-dimensional single-particle systems with central potentials [10], for dipole polarizability in atoms [11], and in quantum phase transition with the Dicke model [12]. Because Fisher information and Shannon entropy are considered as complementary quantities, they can give complete descriptions of the localization-delocalization characters of the atomic system. The literatures combining them are vast and wealthy [13-16]. For example, for parity-restricted harmonic oscillator [13], for a hydrogen atom under soft spherical confinement [14], for the exponential-cosine screened Coulomb potential [15] and Hulthén potential [16]. In addition to Shannon entropy and Fisher information, there are many other entropies such as Rényi [17] and Tsallis [18, 19]. For a comprehensive account of Rényi and Tsallis entropies, we refer the reader to the recent literatures [20-25].

It was noticeable that most of the Fisher information's published literatures are for one electron with different potentials. Unfortunately, due to the presence of the gradient in F , the Fisher information literatures for He-isoelectronic series are scarce [3,4,26-29]. This shortage of literatures for Fisher information has motivated us to study and use it for 2-electron systems. Accordingly, in this article, our objectives are the following: 1- Calculate numerically the values of F and S in r-space, and in 1- and 2-el densities; 2- Discuss the behavior of F and S as a function of the nuclear charge Z and the screening parameter λ using the effective screened Coulomb potential, Yukawa potential, in the form [30]:

$$V_{YP}(r) = -Z \frac{e^{-\lambda r}}{r} \; . \tag{4}$$

Eq. (4) arises, for instance, from a Thomas-Fermi approximation to the electron gas; in plasma physics it is known as the Debye-Hückel potential [31]. In $V_{YP}(r)$, λ is given a different

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expression, depending on the problem considered. 3- Define and examine the ratio of 2- to 1- electron densities of Fisher information, and product P, that measure the el-el correlation's strength. The procedure will be done using the Ritz's variational principle [20-22] for different values of λ, where $\lambda << \lambda_c$. λ_c is defined as the critical value of λ above which only one-electron bound state exists. For example, it was found that for helium, $\lambda_c \approx 2.06$, for Yukawa potential. To the best of our knowledge there is no previous attempt to evaluate the F integrals for these systems using Yukawa potential.

The outline of this article is as follows. In Section 2, we present the basic equations for computing F for 2-el systems. Also, we explain 1- and 2-el charge density approaches for calculating F and S, and define their corresponding ratio R_F and R_S. We devote Section 3 to present our numerical results of Fisher information for the 1s²- state of atoms from helium to neon and thus try to shed some light regarding the effect of el-el correlation on F, P and R_F. The dependent behavior of F, P and R with Z, and λ, is discussed. Finally, concluding remarks of our outcomes are accessible in Section 4. All results in this paper are expressed in atomic units (a.u.).

2. Theoretical Background

The Hylleraas coordinates (s,t,u) are expressed in terms of the two electrons, defined by 1 and 2, interparticle coordinates (r_1,r_2,r_{12}) relative to an infinitely heavy nucleus as: $s = r_1 + r_2$, $t = r_1 - r_2$ and $u = r_{12}$, with the conditions that $-u \le t \le u$, $0 \le u \le s \le \infty$ and $d\tau = \pi^2 (s^2 - t^2) u \, du \, ds \, dt$ is the volume element. Accordingly, in Hylleraas coordinates, the non-relativistic Hamiltonian of He-like sequence with a given potential V, is written as:

$$\hat{H} = -\left(\frac{\partial^2}{\partial s^2} + \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial u^2} \right) - 2\frac{s(u^2 - t^2)}{u(s^2 - t^2)}\frac{\partial^2}{\partial s \partial u} - 2\frac{t(s^2 - u^2)}{u(s^2 - t^2)}\frac{\partial^2}{\partial t \partial u} - \frac{4s}{(s^2 - t^2)}\frac{\partial}{\partial s} + \frac{4t}{(s^2 - t^2)}\frac{\partial}{\partial t}$$

$$-\frac{2}{u}\frac{\partial}{\partial u} + \left[V((s-t)/2) + V((s+t)/2) \right] - \frac{V(u)}{Z} \quad (5)$$

and the used 3-parameter wave function is:

$$\phi(s,u,t,a,b,c) = A\left[e^{-as}(1 + bu + ct^2) \right] \quad (6)$$

where A is the normalization constant, and a, b, and c are the variational parameters. Substituting ϕ into Eq. (5), and searching for the minimum energy expectation value, $\langle E \rangle$, one finds the optimal values of a, b, and c.

To study the effect of the el-el correlation, and for the sake of comparative study, we will use the following wave functions [20]:

$$\phi_1(s,a) = A_1 e^{-as}, \quad (7)$$

and

$$\phi_2(s,u,a,b) = A_2\left[e^{-as}(1+bu)\right]. \tag{8}$$

Note that, ϕ_1 allows us to calculate F and S in both spherical and Hylleraas coordinates.

The present calculations have been done using two distinctive approaches. The first is done by means of the 2-el density:

$$\rho(s,u,t,\mathsf{L}) = |\phi(s,u,t,\mathsf{L})|^2 , \tag{9}$$

and its unity-normalized:

$$\int \rho(s,u,t,\mathsf{L}) \, d\tau = 1; \tag{10}$$

then we can calculate F with the help of the gradient in Hylleraas coordinates (See Appendix A):

$$\nabla = \sqrt{2}\frac{\partial}{\partial s}\hat{s} + \sqrt{2}\frac{\partial}{\partial t}\hat{t} + \frac{\partial}{\partial u}\hat{u} . \tag{11}$$

The second approach is done by means of the 1-el density. In this method we start by marginalizing (integrating out) some degrees of freedom. For example r_2 , according to [32] as:

$$\rho(r_1) = \frac{2\pi}{r_1}\int_0^\infty\int_{|r_1-r_2|}^{r_1+r_2}|\phi|^2 r_2 dr_2 r_{12}dr_{12} = \frac{2\pi}{r_1}\left(\int_0^{r_1}\int_{r_1-r_2}^{r_1+r_2}|\phi|^2 r_2 dr_2 r_{12}dr_{12} + \int_{r_1}^\infty\int_{r_2-r_1}^{r_1+r_2}|\phi|^2 r_2 dr_2 r_{12}dr_{12}\right) \tag{12}$$

$$\equiv \rho(r)$$

with testing the normalization condition:

$$4\pi\int r^2\rho(r)dr = 1 . \tag{13}$$

Then, using the gradient $\frac{\partial}{\partial r}$ in spherical coordinates, Fisher's integral in Eq. 1 could be solved numerically. This method of integrating out some degrees of freedom is important in discussing the quantum entanglement [31, 33-37].

In the following sections, we are going to use the subscript 1 or 2 on F or S to differentiate between 1-el and 2-el values of the entropy, respectively. The superscript "co" or "uc" on F or S will be used to differentiate between correlated and uncorrelated F- and S- values, respectively. Also, we use the superadditivity of Fisher information [3] to define the ratio of 2-el to 1-el of Fisher information calculations as:

$$R_F = \frac{F_2}{F_1}, \tag{14}$$

that can be used to measure the el-el correlation's strength. In our case, the ratio R_F fulfills the inequality:

$$R_F \geq 2 . \tag{15}$$

The inequality condition (15) is opposite to subadditivity of Shannon's criteria [3] $R_S \leq N$, where N is the number of electrons [3,24,40]. The equality, in both cases, holds if the wave function is a Hartree product; that is, if the electrons are assumed to be independent and uncorrelated [3, 37]. Using the simple wave functions in Eqs. (6-8) allows us to calculate F and S in 1- and 2-el densities.

3. Results and discussion

Before we start extracting the most characteristic physical features of our results, we would like to stress on the following points: 1- Although the energies, and Shannon entropy in 2-el density, are discussed in details in our previous work [20-22], we are going to retrieve few of them here for completeness. 2- To reach our objectives, and to enable the comparison of the published results [3,23, 32-37, 42-45], we are going to use one, two and three-correlated terms wave functions given by Eqs. (6-8) rather than an extensive electronic wave function [3,23, 32-37, 42-45]. 1

The wave functions, Eq. (6-8) are used to calculate: F and S in 1- and 2- electron charge densities. We present in Table 1 the average energy, Fisher information's results of $1s^2$-state for helium and 8 members of its isoelectronic ions, from lithium to neon. For uncorrelated Slater's type wave function, $\phi_1(s, a = Z)$, one can find $F_1^{uc}(a = Z) = 4Z^2$ and $F_2^{uc}(a = Z) = 8Z^2$, with the exact ratio of $R_F = 2$. In Table 1, the following comments were found: 1- Compared to the available literatures [40, 42,43], our energies are in good agreement up to three digits at $Z = 2$, and increases to 4 digits as Z increases. To facilitate comparison with the available literature, the results in [40, 42,43] have been truncated to six digits; 2- For He, due to the el-el interaction, it was found that the difference in the average energy between ϕ_1 and ϕ_2 is less than 1.5%, but the difference in F ($F_2^{co}(\phi_2) > F_2^{uc}(\phi_1)$) increases by more than 15%. As the el-el interaction decreases with increasing Z, the difference in F decreases too; 3- All F values are positive and smaller than the Slater type values; 4- F increases as Z increases. This implies that the electronic density will be more localized with increasing Z ; 5- The criteria $R_F \geq 2$ is fulfilled in all cases and decreases with increasing Z , i.e. it is Z dependent. The equality holds if the electrons are assumed to be uncorrelated, which is the case of ϕ_1. As Z increases, the ratio R_F decreases, which means that as Z increases the el-el interaction decreases and can be neglected, which is a known fact; 6- At fixed Z , the F_1 values are the same, up to three digits, for the three wave functions. This means that the el-el interaction is not significant in 1-el density calculated values; 7- The effect of the el-el interaction is responsible for the increase in F_2 ($F_2^{co}(\phi_2) > F_2^{uc}(\phi_1)$) by a factor more than 20% in 2-el density calculation; 8- The effect of the variational parameter "c", in Eq. 6, is responsible for the decrease in F_2^{co} , since $F_2^{co}(\phi) < F_2^{co}(\phi_2)$, by a factor less than 5%.

The last row in Table 1 provides the fitting equations of F as a function of Z and its associated correlation coefficient R^2 [39]. The values of $R^2 \approx 1$ show the strong correlation between F and Z . Due to the variational calculation it is found that $F \propto Z^\beta$, where the exponent $\beta > 2$. The results of Ref. [28] are given for comparison, although they do not use any type of Hylleraas wave function.

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Table1: The mean energy, Fisher information results and R_F for 1s²-state of helium and 8 members of its isoelectronic ions using Coulomb potential.

Z	ϕ_1				ϕ_2				ϕ			
	$\langle -E \rangle$	F_2^{uc}	F_1^{uc}	R_F	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F
2	2.8477	22.7812	11.3906 13.3096[a]	2	2.8911	27.6255	11.4189 12.1287[a]	2.4193	2.9024 2.90337[b,c] 2.90372[a]	26.6721	11.4552	2.3284
3	7.2227	57.7812	28.8906 31.7643[a]	2	7.2682	65.5555	28.9121 28.4294[a]	2.2674	7.2780 7.27948 7.27991[b,c]	64.2324	28.9476	2.2189
4	7.2227	57.7812	54.3906 58.0412[a]	2	13.6441	119.4399	54.4091 53.8456[27]	2.1952	13.653 13.6556[d]	117.7414	54.4446	2.1626
5	21.9727	175.7812	87.8906 92.8915[a]	2	22.0195	189.3011	87.9075 86.5378[a]	2.1534	22.028 22.0309[d]	187.2251	87.9430	2.1289
6	13.5977	108.7812	129.3906 135.1810[a]	2	32.3949	275.1496	129.4065 126.2190[a]	2.1262	32.403 32.4062[d]	272.6951	129.4421	2.1067
7	44.7227	357.7812	178.8906 185.3460[a]	2	44.7701	376.9905	178.9059 173.4250[a]	2.1072	44.778 44.7814[d]	374.1568	178.9415	2.0909
8	21.9727	175.7812	236.3906 243.3420[a]	2	50.7686	494.8265	236.4054 227.8750[a]	2.0931	59.153 59.1566[d]	491.6134	236.4411	2.0792
9	75.4727	603.7812	301.8906 309.2030[a]	2	75.5203	628.6591	301.9051 264.5170[a]	2.0823	75.528 75.5317[d]	625.0663	301.9408	2.0702
10	32.3477	258.7812	375.3906 382.9400[a]	2	93.8954	778.4894	375.4048 359.2810[a]	2.0737	93.904 93.9068[d]	774.5168	375.4406	2.0630

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Fitting	$F_2^{uc} = 5.2931\ Z^{2.1624}(0.9996)$	$F_2^{co} = 6.6979\ Z^{2.07}\ \ (0.9999)$	$F_2^{co} = 6.4251\ Z^{2.0872}(0.9999)$
	$F_1^{uc} = 2.6466\ Z^{2.1624}(0.9996)$	$F_1^{co} = 2.6533\ Z^{2.1624}(0.9996)$	$F_1^{co} = 2.6625\ Z^{2.1624}(0.9997)$
[a]Ref. [28], [b]Ref. [40], [c]Ref. [42], [d]Ref. [43]			

For completeness and to facilitate comparison with others [3, 24,2 8, 40], we have to compute the Fisher-Shannon information product, P. Table 2, shows the Shannon entropy of 1-el density results of $1s^2$- state for helium and 8 members of its isoelectronic ions for Coulomb potential using our three wave functions. In table 2, our products are in good agreement with the published literatures [3,22], up to 5 digits at $Z = 10$. The small differences in the results are mainly due to the different wave functions that we used. The criteria in Eq. 3 is fulfilled for each wave function. For non-correlated wave function, ϕ_1, the value of P is constant and has the asymptotic value $(Z \to \infty)$ 1.237333 [3]. For the other two wave functions, P decreases monotonically with increasing Z to reach the asymptotic value. Note that, the wave functions in Refs. [3, 24, 40] have more than 200 terms, compared to ours, which are 1-, 2- and 3-term.

Table2: Shannon entropy and Fisher-Shannon information product for $1s^2$- state for helium and 8 members of its isoelectronic ions with Coulomb potential.

Z	ϕ_1		ϕ_2		ϕ	
	S	P	S	P	S	P
2	2.5750	1.2373	2.6016	1.2626	2.6946	1.3476
	2.4323[a]		2.6004[a]		2.705102 85[b]	1.35866[d]
3	1.1789	1.2373	1.2014	1.2570	1.2518	1.3015
	1.0989 [a]		1.2391[a]		1.2552726[c]	1.30511[d]
4	0.2299	1.2373	0.2483	1.2531	0.2824	1.2827
	0.1812 [a]		0.3099[a]			1.28441[d]
5	-0.4900	1.2373	-0.4745	1.2504	-0.4489	1.2724
	-0.5361[a]		-0.4165[a]			1.27341[d]
6	-1.0701	1.2373	-1.0569	1.2484	-1.0364	1.2659
	-1.1041[a]		-0.9892[a]			
7	-1.5560	1.2373	-1.5444	1.2470	-1.5274	1.2615
	-1.5812[a]		-1.4702[a]			
8	-1.9741	1.2373	-1.9638	1.2459	-1.9493	1.2582
	-1.9922 [a]		-1.8833[a]			
9	-2.3409	1.2373	-2.3310	1.2455	-2.3190	1.2557
	-2.2534[a]		-2.2467[a]			
10	-2.6678	1.2373	-2.6595	1.2443	-2.6482	1.2538
	-2.6758[a]		-2.5748[a]			1.25398[d]
[a]Ref. [28], [b]Ref. [24], [c]Ref. [40], [d]Ref. [3]						

To study the screening effect on Fisher information of Helium atom, we displayed the F results for $1s^2$-state of helium as a function of λ in Table 3. The following observations were noticed: 1- Compared to Ref. [42], our energies are in good agreement up to four digits at small values of λ, and decrease to 2 digits as we approach the continuum. 2- $R_F \geq 2$, and it is λ independent. R_F stays constant up to three digits for all values of λ ; 3- The values of F are a decreasing function of λ, which implies that the electronic density will be more delocalized (more spreading) with increasing λ. 4- The F_1 values are the not affected by the el-el interaction. The values are constant, up to three digits, for the three wave functions. 5- The effect

of the el-el interaction is more pronounced in 2-el density calculations, since $F_2^{co} > F_2^{uc}$. 5- The effect of the variational parameter "c", in Eq. 6, is responsible for a small decrease in F_2^{co}, since $F_2^{co}(\phi) < F_2^{co}(\phi_2)$. 6- The last row provides the fitting equations and their associated correlation R^2 as a function of λ and correlation coefficient R^2. The values of $R^2 \approx 1$ show the strong correlation between F and λ.

To complete our goals of the present study, we showed F results for 1s² of three elements of He-like ions, as a function of λ using the correlated wave function ϕ in Table 4. The following notes were found: 1- An analysis of the results shows that for the values of λ considered, our energies are in good agreement, up to three digits, with the published literatures Refs. [42-46], even though the number of terms in our wave functions are 3-term. 2- For fixed λ, $R_F > 2$ and decreases with increasing Z, which means that as Z increases the el-el interaction decreases and could be neglected, as we have mentioned earlier. 3- For each ion, R_F is λ independent and stays constant up to two digits. 4- The values of F decrease as λ increases, which implies that the electronic density will be more delocalized (more spreading) with increasing λ. 5- For fixed λ, the values of F increase as Z increases, which implies that the electronic density will be more localized with increasing Z.

Conclusion:

We have conveyed our numerical outcomes, of our Fisher information's studies, for the 1s²-state of helium and helium-like ions that interrelate with Yukawa potential, in *r*-space. Fisher information's calculations have been done by employing the Hylleraas wave functions with 1-, 2-, and 3-parameter, and in 1- and 2-el densities. It was found that Fisher information is an increasing function of Z, at fixed λ, and a decreasing function of λ, at fixed Z. This means that the electronic density will be more localized with increasing Z and decreasing λ. For our system, the el-el interaction becomes appreciable only for 2-el density calculations. The Fisher information's 1-el density calculations are not sensitive to the el-el interaction, and this is mainly due to the gradient in the F expression. We have also defined the el-el correlation ratio R_F and found that the ratio satisfies the inequality $R_F \geq 2$, which is opposite to the Shannon's criteria $R_S \leq 2$. The equality, in both cases, holds if the electrons are assumed to be independent and uncorrelated. It is found that R_F is Z dependent, but not λ. So, not only is the Fisher-Shannon information product an appropriate measure of el-el correlations, but also R_F too. We believe the presented data for Fisher information studied using Yukawa potential will be of valuable reference and will inspire further research on information-theoretic quantities of atomic and molecular systems.

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Table3

Fisher information results $1s^2$- state of He atom as a function of λ using the three wave functions.

λ	ϕ_1				ϕ_2				ϕ			
	$\langle -E \rangle$	F_2^{uc}	F_1^{uc}	R_F	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F
0.2	2.2903	22.4583	11.2291	2	2.3330	27.2333	11.2627	2.4180	2.3455 2.34666[a]	26.2252	11.2932	2.3222
0.4	1.8099	21.6063	10.8031	2	1.8508	26.2027	10.8484	2.4154	1.8662	25.0738	10.8644	2.3079
0.6	1.3967	20.3466	10.1733	2	1.4351	24.6867	10.2333	2.4124	1.4549 1.45816[a]	23.4126	10.2275	2.2892
0.8	1.0434	18.7573	9.3786	2	1.0788	22.7839	9.4550	2.4097	1.1042 1.10973[a]	21.3720	9.4216	2.2684
1.0	0.7444	16.8903	8.4452	2	0.7766	20.5603	8.5391	2.4078	0.8085 0.81599[b]	19.0499	8.4769	2.2473
1.2	0.4953	14.7778	7.3889	2	0.5239	18.0574	7.5021	2.4070	0.5629 0.57487[a]	16.5258	7.4189	2.2275
1.4	0.2928	12.4304	6.2152	2	0.3175	15.2916	6.3508	2.4078	0.3634	13.8678	6.2713	2.2113
1.6	0.1345	9.8197	4.9099	2	0.1549	12.2386	5.0758	2.4112	0.2060	11.1318	5.0571	2.2012
1.8	0.0198	6.7863	3.3932	2	0.0352	8.7533	3.6183	2.4192	0.0878	8.3410	3.7903	2.2006
Fitting	$F_2^{uc} = -3.9394\lambda^2 - 1.8343\lambda + 22.781$ (0.9995) $F_1^{uc} = -1.9697\lambda^2 - 0.9171\lambda + 11.391$ (0.9995)				$F_2^{co} = -4.5456\lambda^2 - 2.3727\lambda + 27.626$ (0.9994) $F_1^{co} = -1.9326\lambda^2 - 0.9015\lambda + 11.419$ (0.9995)				$F_2^{co} = -3.3990\lambda^2 - 4.0806\lambda + 26.672$ (0.9974) $F_1^{co} = -1.6558\lambda^2 - 1.2810\lambda + 11.455$ (0.9984)			
[a]Ref. [42], [b]Ref. [45]												

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Table4: The mean energy and Fisher information results for 1s²- state of Li^+, Be^{2+} and B^{3+} as a function of λ using ϕ.

λ	Li+				Be²⁺				B³⁺			
	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F	$\langle -E \rangle$	F_2^{co}	F_1^{co}	R_F
0.2	6.3273 6.3292677[b]	63.7622	28.7583	2.2172	12.3054	117.2648	54.2419	2.1619	20.2821	186.7462	87.7326	2.1286
0.4	5.4677 5.4700821[44]	62.4959	28.2424	2.2128	11.0556	115.9495	53.6789	2.1601	18.6383	185.4039	87.1401	2.1277
0.6	4.6903 3.66896[a]	60.5947	27.458	2.2068	9.8963	113.9303	52.8084	2.1574	17.0901	183.3135	86.2131	2.1263
0.8	3.9881	58.173	26.4462	2.1997	8.8208	111.3087	51.6702	2.1542	15.6317	180.5656	84.989	2.1246
1.0	3.3553 3.3626607[b] 3.36127[45]	55.3175	25.2380	2.1918	7.8239 7.82958[c]	108.1642	50.2952	2.1506	14.2582 14.26312[c]	177.2336	83.4977	2.1226
1.2	2.7871 2.79753[a]	52.0969	23.8577	2.1837	6.9008	104.5613	48.7085	2.1467	12.9651	173.378	81.7643	2.1205
1.4	2.2792	48.5675	22.3255	2.1754	6.0476	100.5534	46.9309	2.1426	11.7486	169.0501	79.8096	2.1182
1.6	1.8282	44.7772	20.6584	2.1675	5.2606	96.1857	44.9798	2.1384	10.6052	164.2935	77.6515	2.1158
1.8	1.4307 1.45791[a]	40.7674	18.8716	2.1603	4.5367	91.4973	42.8702	2.1343	9.5318	159.1464	75.3055	2.1133
2.0	1.0840 1.1230701[b] 1.09117[c]	36.5749	16.9787	2.1542	3.8729 3.89558[c]	86.5222	40.6153	2.1303	8.5256 8.54251[c]	153.6423	72.7851	2.1109
2.4	0.5325	27.7687	12.9264	2.1482	2.7157	75.8288	35.7141	2.1232	6.7047	141.6780	67.2678	2.1062
2.8	0.1557	18.5173	8.5803	2.1581	1.7707	64.3094	30.3557	2.1185	5.1240	128.6024	61.1807	2.1020
3.0	0.0289 0.01946[d]	13.5834	6.2475	2.1742	1.3728	58.2922	27.5262	2.1177	4.4187 4.44331[d]	121.7002	57.9444	2.1003
3.4					0.7181	45.8190	21.6014	2.1211	3.1698	107.2549	51.1217	2.0980
3.8					0.2419	32.7429	15.3299	2.1359	2.1258	92.0511	43.8718	2.0982
4.0					0.0684 0.05425[d]	25.7962	11.9942	2.1507	1.6773	84.1928	40.0991	2.0996
4.4									0.9210	67.9868	32.2728	2.1066
4.8									0.3462	51.0214	24.0404	2.1223
5									0.1256 0.10753[d]	42.0473	19.6896	2.1355

[a]Ref. [42], [b]Ref. [44], [c]Ref. [45], [d]Ref. [46]

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Disclosure statement

No potential conflict of interest was reported by the authors.

References

[1] R. A. Fisher, "Theory of Statistical Estimation", Math. Proc. Cambridge Philos. Soc. **22** (1925) 700-725.

[2] C. Shannon, "A mathematical theory of communication", Bell Syst. Tech. J. **27** (1948) 379–423.

[3] E. Romera, J. S. Dehesa, "The Fisher-Shannon information plane, an electron correlation tool", J. Chem. Phys. **120** (2004) 8906–8912.

[4] R. López-Ruiz, J. Sañudo, E. Romera, X. Calbet, "Statistical Complexity and Fisher-Shannon Information: Applications. In Statistical Complexity", K. D. Sen, Ed.; Springer, Dordrecht: Dordrecht, 2011; pp 65–127.

[5] M. S. Abdelmonem, Afaf Abdel-Hady, I. Nasser, "Information entropies for the Morse potential using the J-matrix method", Results in Physics **7** (2017) 1778–1780.

[6] N. Mukherjee, S. Majumdar, A. K. Roy, "Fisher information in confined hydrogen-like ions", Chem. Phys. Lett. **691** (2018) 449-455.

[7] N. Mukherjee, A. K. Roy, "Fisher information in confined isotropic harmonic oscillator", Int. J. Quant. Chem. 2018; e25727.

[8] N. Mukherjee, A. K. Roy, "Relative Fisher information in some central potentials", Ann. Phys. (N.Y.) **398** (2018) 190-202.

[9] S. López-Rosa, R. O. Esquievel, J. C. Angulo, J. Antolín, J. S. Dehesa, N. Flores-Gallegos, "Fisher information study in position and momentum spaces for elementary chemical reactions", J. Chem. Theor. Comput. **6** (2010) 145–154.

[10]   E. Romera, P. Sánchez-Moreno, J. S. Dehesa, J.S. "Uncertainty relation for Fisher information of D-dimensional single-particle systems with central potentials", J. Math. Phys. **47** (2006) 103504-11.

[11]   K. D. Sen, C. P. Panos, K. C. Chatzisavvas, C. C. Moustakidis, "Net Fisher information measure versus ionization potential and dipole polarizability in atoms", Phys. Lett. A **364** (2007) 286–290.

[12]   Á. Nagy, E. Romera, "Fisher information, Rényi entropy power and quantum phase transition in the Dicke model", Physica A **391** (2012) 3650-3655.

[13]   Y.J. Shi, G.H. Sun, J. Jing, S.H. Dong, "Shannon and Fisher entropy measures for a parity-restricted harmonic oscillator" Laser Physics **27** (12) (2017) 125201-125210.

12/10/2019

[14]   N. Aquino, A. Flores-Riveros, J. F. Rivas-Silva, "Shannon and Fisher entropies for a hydrogen atom under soft spherical confinement", Phys. Lett. A **377** (2013) 2062-2068.

[15]   M. S. Abdelmonem, A. Abdel-Hady, I. Nasser, "Scaling behavior of Fisher and Shannon entropies for the exponential-cosine screened Coulomb potential", Mol. Phys. **115**, 13, (2017) 1480–1492.

[16]   A. Abdel-Hady, I. Nasser, "Information entropies for Modified Hulthén Potential", Appl. Math. Inf. Sci. **12**, 4, (2018) 717-725.

[17]   A. Rényi In: Proc. Fourth Berkeley Symp. Math. Stat. and Probability. Berkeley, CA: University of California Press; (1961) 547–61.

[18]   C. Tsallis, "Possible generalization of Boltzmann-Gibbs statistics", J. Stat. Phys. **52** (1988) 479–487.

[19]   C. Tsallis, "The nonadditive entropy S_q and its applications in physics and elsewhere: Some remarks", Entropy **13**(12) (2011) 1765-1804.

[20]   I. Nasser, M. Zeama, A. Abdel-Hady, "The Rényi entropy, a comparative study for He-like atoms using the exponential-cosine screened Coulomb potential", Results Phys. **7** (2017) 3892–3900.

[21]   I. Nasser, M. Zeama, A. Abdel-Hady, "The nonadditive entropy for the ground state of helium-like atoms using Hellmann potential", 2019 Molecular Physics https://doi.org/10.1080/00268976.2019.1612105.

[22]   M. Zeama, I. Nasser, "Tsallis entropy calculation for non-Coulombic helium", 2019 Physica A https://doi.org/10.1016/j.physa.2019.121468.

[23]   J. H. Ou, Y. K. Ho, "Benchmark Calculations of Rényi, Tsallis Entropies and Onicescu Information Energy for Ground State Helium Using Correlated Hylleraas Wave Functions", Int. J. Quantum Chem. **119** (2019), 119, e25928., and the references there in.

[24]   S. López-Rosa, A. L. Martín, J. Antolín, J. C. Angulo, "electron-pair entropic and complexity measures in atomic system", 2018 Int. J. Quantum Chem. e25861. doi:10.1002/qua.25861.

[25]   J. Bolívar, Á. Nagy, E. Romera, "Rényi-Fisher entropy product as a marker of topological phase transitions", Physica A **498** (2018) 66–73.

[26]   J. P. Restrepo Cuartas, J. L. Sanz-Vicario, "Information and entanglement measures applied to the analysis of complexity in doubly excited states of Helium" Phys. Rev. A **91** (2015) 052301-15.

[27]   A. Saha, B. Talukdar, P. Sarkar, "Fisher information of two-electron systems", Eur. Phys. J. Plus **133** (2018) 20-28.

[28]   G. A. Sekh, A. Saha, B. Talukdar, "Shannon entropies and Fisher information of K-shell electrons of neutral atoms", Physics Letters A (2018) https://doi.org/10.1016/j.physleta.2017.12.005

[29]   J. C. Angulo, J. Antolín, J.; K. D. Sen, "Fisher-Shannon plane and statistical complexity of atoms. Phys. Lett. A **372** (2008) 670–674.

[30]   H. Yukawa, "On the interaction of elementary particles", Proc. Phys. Math. Soc. Japan **17** (1935) 48-57.

[31]   Y. C. Lin, T. K. Fang, Y. K. Ho, "Quantum entanglement for helium atom in the Debye plasmas", Phys. Plasmas **22** (2015) 032113-8.

[32]   J. -L. Calais, P. -O. Löwdin, "A simple method of treating atomic integrals containing functions of r_{12}", J. Mol. Spectrosc. **8** (1962) 203-211.

12/10/2019

[33]   Z. Huang, S. Kais, "Entanglement as measure of electron–electron correlation in quantum chemistry calculations", Chem. Phys. Lett. **413** (2005) 1-5.

[34]   Y. C. Lin, C. Y. Lin, Y. K. Ho, "Spatial entanglement in two-electron atomic systems", Phys. Rev. A **87** (2013) 022316 –5.

[35]   J.S. Dehesa, T. Koga, R. J. Yanez, A.R. Plastino, R. O. Esquivel, "Quantum entanglement in helium", J. Phys. B At. Mol. Opt. Phys. **45** (2012) 015504-015511.

[36]   P. Kościk, A. Okopińska, Entanglement Entropies in the Ground States of Helium-Like Atoms. Few-Body Syst. **55** (2014) 1151–1157.

[37]   R.J. Yáñez, A.R. Plastino, J.S. Dehesa, "Quantum entanglement in a soluble two-electron model atom", Eur. Phys. J. D **56** (2010) 141–150.

[38]   N. L. Guevara, R. P. Sagar, R. O. Esquivel, "Information uncertainty-type inequalities in atomic systems", J. Chem. Phys. **119** (2003) 7030 –7036.

[39]   C.P. Panos, N.S. Nikolaidisb, K.ch. Chatzisavvas, C.C. Tsouros, "A simple method for the evaluation of the information content and complexity in atoms A proposal for scalability", Phys. Lett. A **373** (2009) 2343-2350.

[40]   C.H. Lin, Y.K. Ho, Shannon Information Entropy in Position Space for Two-Electron Atomic Systems. Chem. Phys. Lett. 633 (2015), 261–264.

[41]   G. Arfken, H. Weber, "*Mathematical Methods for Physicists*". 6th Edition (2005) (ALSEVIER Academic Press).

[42]   L. U. Ancarani, Rodriguez, "Correlated expansions of n^1S and n^3S states for two-electron atoms in exponential cosine screened potentials", Phys. Rev. A **89** (2014) 012507-9.

[43]   H. Nakashima, H. Nakatsuji, "Solving the electron-nuclear Schrödinger equation of helium atom and its isoelectronic ions with the free iterative-complement-interaction method", J. Chem. Phys. **128** (2008) 154107-7.

[44]   S. Kar, Y. K. Ho, "The ground state and doubly-excited 1,3P° states of hot-dense plasma-embedded Li+ ions." Eur. Phys. J. D **44** (2007) 1-8.

[45]   B. Saha, T. K. Mukherjee, P. K. Mukherjee, G. H. F. Diercksen, " Variational calculations for the energy levels of confined two-electron atomic systems ", Theor Chem Acc **108** (2002) 305-310.

[46]   L. C. Santos, M. G. R. Martins, J. D. M. Vianna, "Analytical solutions for Yukawa potential applied to atomic systems embedded in Debye plasmas", Int. J. Quantum Chem. 111(7-8) (2011) 1671–1679.

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Appendix A

The gradient in Hylleraas coordinates

This appendix is devoted to derive the gradient expression in Hylleraas coordinates. In tensor notations [41], using:

$$u^1 = s, u^2 = t, u^3 = u; \text{ and } x^1 = (s+t)/2, x^2 = (s-t)/2, x^3 = u;$$

one can determine the scale factors as follows:

$$g_{11} = \sum_{k=1}^{3}\left(\frac{\partial x^k}{\partial u^1}\right) = \frac{1}{2}, g_{22} = \sum_{k=1}^{3}\left(\frac{\partial x^k}{\partial u^2}\right) = \frac{1}{2}, g_{33} = \sum_{k=1}^{3}\left(\frac{\partial x^k}{\partial u^3}\right) = 1,$$

then the gradient in Hylleraas coordinates is:

$$\nabla = \frac{1}{\sqrt{g_{11}}}\frac{\partial}{\partial s}\hat{s} + \frac{1}{\sqrt{g_{22}}}\frac{\partial}{\partial t}\hat{t} + \frac{1}{\sqrt{g_{33}}}\frac{\partial}{\partial u}\hat{u} = \sqrt{2}\frac{\partial}{\partial s}\hat{s} + \sqrt{2}\frac{\partial}{\partial t}\hat{t} + \frac{\partial}{\partial u}\hat{u} .$$

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