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Information Entropies for Modified Hulthén Potential

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Abstract: Information entropies (Fisher, Shannon, and Rényi), with their associated quantities, are calculated and discussed for the Modified Hulthén Potential (MHP) in the position and momentum spaces using the J-matrix method. Interesting characteristic features of the entropy densities are shown, where the position and momentum space information entropies show scaling behavior and satisfy uncertainty relations. Many of our results are reported for the first time. The outcome is compared with the available literatures' results.

Keywords: Shannon entropy; Fisher information; Rényi entropy; J-matrix method; Modified Hulthén Potential.

1 Introduction

In [1], a modification for the simple Hulthén potential (MHP) [2,3,4,5], was proposed as:

$$V_{MHP}(r,Z,\mu,a,b) = -Z\mu\frac{1}{e^{\mu r}-1}\cos(b\mu r)+\frac{a}{r^2}, \quad (1)$$

with a, b, and μ are being parameters. The MHP (1), with $a=b=0$, has the Coulombic behavior for small values of r, but decreases exponentially for $r >> \frac{1}{\mu}$. Over the years, a simple potential $(a=0)$ has been widely used in chemical physics, plasma physics, and quantum chemistry. In general, the MHP does not have an exact analytic solution, except for the simple potential with zero angular momentum. Consequently, different computational methods have been employed to obtain their solutions. For a comprehensive review of the available computation methods in use to solve such potentials, we refer the reader to the recent work [1,5,6,7].

Due to the unavailability of the exact analytical solution of the MHP, accordingly, the present study presents the results of our numerical calculation on the information entropies (such as Shannon [8], Fisher [9], Rényi [10]) and their associated quantities [11,12,13] for the MHP. A sample calculation is done using the J-matrix method [5,6,7,14,15,16] for the exponential-cosine screened Coulomb potential with electron densities, and their gradients are manipulated in both r- and p-spaces. The J-matrix has been proven to be an essential numerical tool to calculate the bound and resonance state energies, the scaling behavior of atomic and molecular systems [5,6,7,14,15,16] , as well as the information entropies [14,15]. Accordingly, we briefly retrieve the required equations and definitions of the J-matrix that are needed to help us in our discussions in the theory section.

Before we begin our task in calculating the information entropy for MHP using the J-matrix method, we shed some light and retrieve the most recent publications in the related subject. This is mainly due to the vast number of publications on the subject. Dehesa and co-workers [17,18] applied the information theory to study the one and two-electron atoms, as well as the Rydberg states [19]. Aquino et. al..[20] calculated the Shannon entropy and Fisher information for hydrogen atoms under soft spherical confinement. Moreover, the calculation of the entropies in the information theory has been given for systems with different potentials rather than the Coulombic-potential [17-20]. For example, it has been applied for: the hyperbolic [21] and asymmetric double-well potential [22], the asymmetric trigonometric Rosen-Morse potential [23], and position-dependent mass Schrödinger problem with a hyperbolic well [24]. Ref. [25] discussed the Shannon-entropy-based uncertainty relation for D-dimensional central potentials. In Ref. [26], information-theoretic measures of hydrogen-like ions in weakly-coupled Debye plasmas.

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Regarding the Rényi entropy, the Fisher Rényi complexity measure and its applications are elegantly analytically discussed by Dehesa and his coworkers [27, 28,29] The Rényi and Tsallis entropies have been discussed for the hydrogenic Rydberg atoms [30]. Ref. [31] discussed the Fisher information, Rényi entropy power and quantum phase transition in the Dicke model. Ref. [32] used the finite-size scaling method to study the Shannon-Rényi entropy in two-dimensional systems with spontaneously broken continuous symmetry. The scaling behavior of the Rényi entropy for He-like atoms, using the exponential-cosine screened Coulomb potential, was discussed in Ref. [33].

The outline of this article is as follows: In Section II, we provide some general expressions corresponding to the information entropies, as well as a brief introduction to the J-matrix method [14,15,16] In Section III, we present our numerical results of the scaling, product, and uncertainty properties of the r- and p-space entropies derived for the MHP. Finally, a summary of the main results is accessible in Section IV. In the present study, we are using the atomic units throughout the manuscript, unless mentioned otherwise.

2 Theory

It is well known that the electron density in the r-space, $\rho(r)$, and its gradient, are the corner stones in calculating the information entropies. Thus, in applying the J-matrix method [14,15,16] in our study, we start with the particle's density of the stationary and nonrelativistic states, in 3-dimensional quantum systems, in the form:

$$\rho(r) = |\psi(r,Z,\mu,a,b)|^2, \tag{2}$$

that satisfies the normalization condition:

$$\int \rho(r)dr = 1, \tag{3}$$

where $dr = r^2 dr d\Omega$ and $d\Omega = \sin\theta d\theta d\phi$ is the solid angle. The wave functions in (2), $\psi(r,Z,\mu,a,b)$, are the bounded solutions of the Schrödinger equation:

$$[\hat{H}]|\psi\rangle = [\hat{H}_o + V(r,Z,\mu,a,b)]\psi(r,Z,\mu,a,b = E\psi(r,Z,\mu,a,b), \tag{4}$$

where $(\hat{H})$is the full Hamiltonian and $\{E\}$ is the associated eigenvalues. In the following discussion, and for simplicity, the parameters Z,μ,a and b are suppressed from the labels of the wave function and the potential. In (4),

$$H_o = -\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2}, \tag{5}$$

is the reference Hamiltonian of the system, with orbital quantum number l. In spherical polar coordinates (r,θ,ϕ) , the eigenfunction $\Psi(r)$ has the form:

$$\psi(r) = R_n^l(r)Y_{l,m}(\theta,\phi), \tag{6}$$

where $R_n^l(r)$ is the solution of the radial non-relativistic Schrödinger equation:

$$[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r)]R_n^l(r) = E_n^l(r)R_n^l(r), \tag{7}$$

and $Y_{l,m}(\theta,\phi)$ is the spherical Harmonics which satisfies the non-radial operator $\hat{\Lambda}^2$:

$$\hat{\Lambda}^2 Y_{l,m}(\theta,\phi) = l(l+1)Y_{l,m}(\theta,\phi), \tag{8}$$

where

$$\hat{\Lambda}^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin^2\theta\frac{\partial}{\partial\phi^2}), \tag{9}$$

with $l = 0,1,2,3,...$ and $m = -l,-l+1,...,0,...,l-1,l$. In (7), E_n^l represents the eigenvalues of the full Hamiltonian $\hat{H}$, and $R_n^l(r)$ are the corresponding eigenfunctions.

In the J-matrix method, to find the radial function $R_n^l(r)$ and the corresponding eigenvalues E_n^l, we diagonalize the full Hamiltonian $(\hat{H})$ in a suitable L^2 basis set, $\{\phi_n^l(\lambda r)\}_{n=0}^{N-1}$. To do so, we are using

$$\phi_n^l(\lambda r) = a_n^l(\lambda r)^{l+1}e^{\frac{-\lambda r}{2}}L_n^{2l+1}(\lambda r);\ \ n = 0,1,2,...,N-1 \tag{10}$$

where $L_n^{2l+1}(\lambda r)$ is the associated Laguerre polynomial, $a_n^l = \sqrt{\frac{\lambda\Gamma(n+1)}{\Gamma(n+2l+2)}}$is the normalization constant, N is the dimension of the J-matrix, and the parameter λ is introduced to be the positive length scale of the basis that allows for more computational freedom. The wavefunction $\phi_n^l(r)$, the basis of the J-matrix, tridiagonalizes H_o in the form

$$(H_o)_{n,n'} = \frac{\lambda^2}{8}[2(n+l+1)\delta_{n,n'} + \sqrt{n(n+2l+1)}\delta_{n,n'+1} + \sqrt{(n+1)(n+2l+2)}\delta_{n,n'-1}]. \tag{11}$$

In the manipulation of (11), we use the differential equation, differential formula, three-term recursion relation, and orthogonality formula of the $L_n^{2l+1}(\lambda r)$. In the J-matrix method, the reference Hamiltonian of the system H_o is fully accounted for, while the potential $V(r)$ is approximated by its representation in a subset of the basis, such that:

$$(H)_{n,m} = \langle n|H|m\rangle \cong \begin{cases} (H_o)_{n,m} + V_{nm}(r); & n,m \le N-1 \\ (H_o)_{n,m}; & n,m > N-1 \end{cases} \tag{12}$$

The integer N in (12) is chosen large enough to ensure a good sampling of the potential.

Returning back to the matrix elements of the potential $V(r)$, which is obtained by evaluating the integral:

$$V_{n,m}(r) = \int_0^\infty \phi_n(\lambda r)V(r)\phi_m(\lambda r)dr = \lambda^{-1}a_n a_m \int_0^\infty x^\nu e^{-x}L_n^\nu(x)L_m^\nu(x)[xV(\frac{x}{\lambda})]dx. \tag{13}$$

The evaluation of such an integral for a general effective potential is almost always done numerically. We use the Gauss quadrature approximation [16], which gives

$$V_{nm} \cong \sum_{k=0}^{N-1} \Lambda_{nk}\Lambda_{mk}[\varepsilon_k V(\frac{\varepsilon_k}{\lambda})] \tag{14}$$

for an adequately large integer N. ε_k and $\{\Lambda_{nk}\}_{n=0}^{N-1}$ are the N eigenvalues and corresponding eigenvectors of the NxN tridiagonal basis overlap matrix $\langle\phi_n|\phi_m\rangle$, whose elements are:

$$K_{n,n} = 2n+2l+2, \quad K_{n,n+1} = -\sqrt{(n+1)(n+2l+2)} \tag{15}$$

The output of the diagonalization of (7) in the associated Laguerre basis is a set of the eigenvaluesE_n^l and the corresponding eigenvectors $\{\Omega_{n0}^l, \Omega_{n1}^l, ..., \Omega_{nN-1}^l\}$. Then, the radial function$R_n^l(r)$is calculated by the expansion:

$$R_{n,n}^l(r) = \sum_{m=0}^{N-1} \Omega_{nm}^l \phi_m^l(r), \tag{16}$$

Thus, the electron density functions of the nlm-state can be written as:

$$\rho(r) = |\Psi(r)|^2 = \rho_{n,l}(r)\rho_{l,m}(\theta,\phi) = |R_n^l(r)|^2|Y_{l,m}(\theta,\phi)|^2, \tag{17}$$

With the knowledge of the electron state density,$\rho(r)$, and following the recent references [11,12] one can express the following quantities in the r-space:

1.The Shannon entropy [8]:

$$S_r \equiv -\int \rho(r) ln[\rho(r)]dr, \tag{18}$$

2.The Fisher information [9]:

$$I_r \equiv \int \frac{[\nabla\rho(r)]^2}{\rho(r)}dr, \tag{19}$$

3.The Rényi entropy, R_β [10]:

$$R_{\beta,r} \equiv \frac{1}{1-\beta} ln[\int [\rho(r)]^\beta dr]; \ \beta \neq 1, \tag{20}$$

It is known that S_r is a gauge that provides the information about the localization, extent, spread, shape and uncertainty of the electronic density distribution of states in the respective spaces. In other words, a more localized distribution, $\rho(r)$ corresponds to the smaller value of the S_r, and vice versa. The Rényi entropy can be argued to be a generalization of Shannon's concepts and definitions. In general, S_r is a limited value of the R_β as $\beta \to 1$.

4.Moreover the expectation expressions for r^2 and P^2 are:

$$\langle r^2\rangle = \int r^2\rho(r)dr, \tag{21}$$

$$\langle p^2\rangle = -\int \Psi(r)\frac{1}{r}\frac{\partial^2}{\partial r}[r\Psi(r)]dr, \tag{22}$$

With the above definitions, one can also define: the Shannon entropy power [17-19], $J_r = \frac{1}{2\pi e}e^{\frac{2S_r}{3}}$, the Fisher-Shannon information product $P_r = \frac{I_r J_r}{3}$, which should satisfy the relation $P_r > 1$.

In the p-space, to calculate the density $\gamma(p)$ one has to apply the Fourier transformation to $\Psi(r)$, in (6), in the spherical coordinates, i.e.

$$\Psi(p) = \int e^{ip.r}\Psi(r)dr, \quad \gamma(p) = |\Psi(p)|^2. \tag{23}$$

Consequently, one can replace, in Eqs. (17-21), the subscript r by p, $\rho(r)$ by $\gamma(p) = |\Psi(p)|^2$, and integrate with respect to dp with the normalization condition $\int\gamma(p)dp = 1$. In addition, we have to check the Shannon entropy sum $S_T = S_r + S_p$ that contains the net information and obeys the well-known lower bound Bialynicki-Birula and Mycielski BBM-condition [13] in the form:

$$S_T \geq 3(1+\ln(\pi)). \tag{24}$$

In the end, we introduce the definition that used for the M-moment of r [14], in the form:

$$(r^M)_{nl,n'l'} = \langle nl|r^M|n'l'\rangle \equiv \int_0^\infty R_n^l(r)R_{n'}^{l'}(r)r^{2+M}dr, \tag{25}$$

where M is an integer number. The analytical expression for the Buckingham static polarizability, $\alpha_{nl,l'}^\beta$, of hydrogen 1s-state is [34,35]:

$$\alpha_{ls,p}^\beta = \frac{2}{3}[\frac{6(r^2)_{1s,1s}^3 + 3(r^3)_{1s,1s}^2 - 8(r)_{1s,1s}(r^2)_{1s,1s}(r^3)_{1s,1s}}{9(r^2)_{1s,1s} - 8(r)_{1s,1s}^2}], \tag{26}$$

and the expressions for the excited states $2p$ and $3d$ are [36]:

$$\alpha_{2p,d}^\beta = \frac{16}{5}(r^2)_{2p,2p} + \frac{8}{15}(r^3)_{2p,2p}, \tag{27}$$

$$\alpha_{3d,f}^\beta = \frac{324}{35}(r^2)_{3d,3d} + \frac{27}{35}(r^3)_{3d,3d}, \tag{28}$$

3 Results and discussions

It is our main objective in this section to demonstrate and discuss our numerical results. In other words, we numerically investigate the dependence of the Rényi entropy $R_{\beta,r}$, and other informatics properties, on the quantum number n and the order parameter β. But before we do so, we have to mention that; by including the screening parameter in (1), the number of states are reduced tremendously. This is opposite to the Coulombic case where we have an infinite number of states.

Our study starts with Table 1 that displays the numerical values of the nine information-theoretic quantities. The quantities are: the Shannon entropies S_r, S_p, S_T, the Rényi entropies $R_{1,r}$, $R_{1,p}$, the Fisher

Table 1: Numerical values for the MHP, corresponding to with different values of (Z,μ,a,b), which illustrate its independence on $[\mu,Z]$ values if the ratio $\frac{\mu}{Z}$, a, and b are held fixed.The literature references are given as superscript.

(Z,μ,a,b)	n	-E	$\langle r^2\rangle$	$\langle p^2\rangle$	S_r	$R_{1,r}$	J_r	I_r	P_r	S_p	$R_{1,p}$	I_p	P_p	S_T	P_rP_p	I_rI_p
	1	0.1666978	14.598	0.1700	6.6017	6.5918	4.7452	0.6802	1.0759	-0.1258	-0.1248	58.407	1.0482	6.4759	1.1277	39.728
		0.166700[1]	14.59115[1]	0.17009[1]	6.601715[1]			0.680353[1]		−0.125927[1]		58.3646[1]		6.47578[1]		39.7085[1]
$(1,0.05,0.5,0)$	2	0.0499884	113.65	0.0932	9.5679	9.5677	34.505	0.3729	4.2887	-1.8439	-1.8442	454.62	2.5954	7.7240	11.131	169.52
		0.049989[1]	113.655[1]	0.09323[1]												
	3	0.0171888	456.68	0.0513	11.589	11.588	132.64	0.2053	9.0774	-3.0810	-3.0814	1826.7	4.5715	8.5081	41.497	375.05
	4	0.0050215	1458.5	0.0270	13.302	13.302	416.00	0.1081	14.986	-4.2533	-4.2537	5694.1	6.5219	9.0490	97.737	615.36
	1	0.3750701	6.4880	0.3826	5.3853	5.3874	2.1260	1.5304	1.0846	1.0906	1.0904	25.959	1.0482	6.4759	1.1368	39.728
		0.375075[1]	6.48496[1]	0.3827[1]	5.385321[1]			1.530794[1]		1.090467[1]		25.9398[1]		6.475781[1]		39.7085[1]
$(1.5,0.075,0.5,0)$	2	0.1124739	50.513	0.2097	8.3515	8.3520	15.343	0.8390	4.2907	-0.6275	-0.6280	202.05	2.5954	7.7240	11.136	169.52
		0.112475[1]	50.51334[1]	0.20977[1]												
	3	0.038675	202.97	0.1155	10.373	10.373	59.005	0.4620	9.0859	-1.8646	-1.8650	811.89	4.5715	8.5081	41.536	375.05
	4	0.011299	648.23	0.0608	12.086	12.086	184.93	0.2432	14.989	-3.0369	-3.0373	2530.7	6.5219	9.0490	97.756	615.35
	1	0.162877	14.269	0.1735	6.5690	6.5587	4.6417	0.6939	1.0735	-0.0946	-0.0935	57.093	1.0462	6.4744	1.1231	39.614
		0.16287[1]	14.26236[1]	0.1735[1]	6.568969[1]			0.694011[1]		-0.094702[1]		57.0494[1]		6.47426[1]		39.5929[1]
$(1.5,0.075,0.5,2)$	2	0.041142	105.70	0.10128	9.4526	9.4524	31.953	0.4047	4.3107	-1.6918	-1.7267	422.80	2.6712	7.7607	11.515	171.12
		0.04114[1]	105.6998[1]	0.10119[1]												
	3	0.004943	430.81	0.0552	11.510	11.510	125.95	0.2210	9.2775	-3.0135	-3.0139	1723.1	4.510	8.4965	41.845	380.77
	1	0.151779	13.461	0.1828	6.4844	6.4734	4.3851	0.7310	1.0685	-0.0133	-0.0138	53.861	1.0419	6.4711	1.1132	39.372
		0.15178	13.4536[1]	0.18279[1]	6.484443[1]			0.731167[1]		−0.01345[1]		53.8143[1]		6.47099[1]		39.3472[1]
$(1,0.05,0.5,2)$	2	0.017901	93.953	0.1161	9.2697	9.2696	28.286	0.4643	4.3774	-1.4657	-1.4656	375.82	2.7606	7.8040	12.084	174.48
		0.0179[1]	93.95266[1]	0.11608[1]												
	1	0.341502	5.9826	0.4112	5.2680	5.2703	1.9663	1.6447	1.0780	1.2031	1.2028	23.938	1.0419	6.4711	1.1232	39.372
		0.3415[1]	5.97938[1]	0.41128[1]	5.2680481[1]			1.645125[1]		1.202944[1]		23.9175[1]		6.47099[1]		39.3472[1]
$(1.5,0.075,0.5,2)$	2	0.040278	41.757	0.2612	8.0533	8.0540	12.579	1.0446	4.3798	-0.2493	-0.2497	167.03	2.7606	7.8040	12.091	174.48
		0.04028[1]	41.75674[1]	0.26118[1]												
	1	0.244264	8.7285	0.2821	5.8441	5.8440	2.8824	1.1285	1.0843	0.6224	0.6223	34.914	1.0319	6.4665	1.1188	39.401
		0.24426[1]	8.72829[1]	0.282131[1]												
$(1.5,0.075,0.75,2)$	2	0.013195	54.960	0.2040	8.4624	8.4623	16.513	0.8159	4.4908	-0.5876	-0.5879	219.838	2.8999	7.8748	13.023	179.36
		0.0132[1]	54.95997[1]	0.20396[1]												

information measures, I_r, I_p , the powers P_r and P_p, as well as the bound state energies, the expectation values $\langle r^2\rangle$ and $\langle p^2\rangle$, for the s-wave of the MHP. The quantities given in Table 1 present the following observations:

1.Our numerical values are in excellent agreement, up to 5 digits, with the only published literature [1].
2.In all cases, the BBM-definition, Eq. (24), the sum $S_T > 6.43419$, is satisfied for all the given parameters. The S_T values shows scaling behavior in which they are independent of the $[Z,\mu]$ when the ratio $\frac{\mu}{Z}$, b, and a are fixed.
3.The Fisher-Shannon information products of P_r, P_p and their multiplication are all greater than 1.
4.In regards to the Rényi entropy, $R_{\beta,r}(R_{\beta,p})$, it is known that the Shannon entropies $S_{1,r}(S_{1,p})$ are limited values of the Rényi entropies as $\beta \to 1$, which is proven numerically in our cases. Note that, because of the indeterminate form of R_1, one can use L′Hospital′s rule to calculate R_1 analytically, which gives the Shannon expression, or calculate it numerically by choosing β close to 1. In our calculations, we chose $\beta = 1.0001$.
5.According to the definition of the Shannon entropy, more localized distributions, $\rho(r)$, correspond to the smaller value of the S_r. This means the delocalization $\rho(r)$ increases with increasing μ and n.
6.In the r-space, the results support the scaling property that the MHP is independent of the set of values $[Z,\mu]$ when the ratio μ/Z, b, and a are fixed.
7.For the nth-state, with fixed n, the product P_rP_p and the Fisher information measure I_rI_p are independent on all the parameters (Z,μ,a,b). As an example, for the 1s-state $P_rP_p \approx 1.1$ and $I_rI_p \approx 39$.
8.For the fixed parameters (Z,μ,a,b), the product P_rP_p and I_rI_p increase with increasing n.

Table 2: Numerical values of Rényi entropies for the MHP, corresponding to different values of (l,Z,μ,a,b).

		r-space				p-space			
(l,Z,μ,a,b)	n	R_2	R_3	R_4	R_5	R_2	R_3	R_4	R_5
$(0,1,0.05,0.5,0)$	1	5.9731	5.7099	5.5620	5.4662	-0.7653	-1.0395	-1.1993	-1.3063
	2	8.8135	8.0878	7.6329	7.3713	-3.2760	-3.6292	-3.8045	-3.9159
	3	10.803	9.7160	9.0593	8.7000	-4.8869	-5.3395	-5.5482	-5.6753
	4	12.541	11.164	10.339	9.8977	-6.1695	-6.6716	-6.8982	-7.0334
$(0,1.5,0.75,0.5,0)$	1	4.7567	4.4935	4.3456	4.2498	0.4511	0.1769	0.0171	-0.0899
	2	7.5971	6.8714	6.4165	6.1549	-2.0596	-2.4128	-2.5881	-2.6995
	3	9.5872	8.4996	7.8429	7.4836	-3.6705	-4.1231	-4.3318	-4.4589
	4	11.325	9.9479	9.1228	8.6813	-4.9531	-5.4552	-5.6818	-5.8170
$(1,1,0.05,0.5,0)$	1	7.3853	7.0987	6.9303	6.8174	-0.7290	-1.0014	-1.1603	-1.2667
	2	9.6378	9.0130	8.5964	8.3391	-3.1354	-3.4956	-3.6733	-3.7857
	3	10.513	10.513	9.9064	9.5548	-4.8688	-5.3232	-5.5332	-5.6615
$(1,1.5,0.075,0.5,0)$	1	6.1689	5.8823	5.7139	5.6010	0.4874	0.2150	0.0561	-0.0503
	2	8.4214	7.7966	7.3800	7.1227	-1.9190	-2.2792	-2.4569	-2.5693
	3	10.211	9.2968	8.6900	8.3383	-3.6525	-4.1068	-4.3168	-4.4451
$(0,1,0.05,0.5,2)$	1	5.8730	5.6161	5.4714	5.3777	-0.6368	-0.9055	-1.0626	-1.1680
	2	8.4943	7.7799	7.3443	7.0945	-2.9398	-3.3149	-3.4989	-3.6149
$(0,1.5,0.075,0.5,2)$	1	4.6566	4.3997	4.2551	4.1613	0.5796	0.3109	0.1538	0.0484
	2	7.2779	6.5635	6.1279	5.8781	-1.7234	-2.0985	-2.2825	-2.3985
$(0,1.5,0.075,0.5,2)$	1	6.5047	6.2742	6.1452	6.0617	-1.1832	-1.4404	-1.5922	-1.6944
	2	8.9404	8.2951	7.8923	7.6584	-3.3106	-3.7108	-3.9061	-4.0291
$(0,1,0.05,0.75,2)$	1	5.2883	5.0578	4.9288	4.8453	0.0332	-0.2240	-0.3758	-0.4780
	2	7.7240	7.0787	6.6759	6.4420	-2.0942	-2.4944	-2.6897	-2.8127

Table 3: Scaling laws of Rényi entropies in the form $R_\beta = c\ln(n)+d$ for the MHP in r- and p-spaces.

	r-space				p-space			
(Z,μ,a,b)	$R_{\beta,r}$	c	d	R^2	$R_{\beta,p}$	c	d	R^2
$(1,0.05,0.5,0)$	$R_{1,r}$	4.779	6.468	0.995	$R_{1,p}$	-2.922	- 0.004	0.999
	$R_{2,r}$	4.675	5.819	0.993	$R_{2,p}$	-3.871	- 0.699	0.998
	$R_{3,r}$	3.879	5.588	0.993	$R_{3,p}$	-4.038	- 0.962	0.998
	$R_{4,r}$	5.573	5.451	0.993	$R_{4,p}$	-4.087	- 1.116	0.998
	$R_{5,r}$	5.469	5.358	0.992	$R_{5,p}$	-4.107	- 1.219	0.997

Table 4: Scaling laws of Rényi entropies in the form $R_{\beta,r} = cn^\nu$ for the MHP.

	r-space			
(Z,μ,a,b)	$R_{\beta,r}$	c	ν	R^2
(1,0.05,0.5,0)	$R_{1,r}$	6.6477	0.5055	0.999
	$R_{2,r}$	6.0091	0.5347	0.999
	$R_{3,r}$	5.7338	0.4825	0.999
	$R_{4,r}$	5.5732	0.4456	0.999
	$R_{5,r}$	5.4692	0.4265	0.999

Table 5: The bound states energy, the squares of the M-moment $(r^M)_{nl,n'l'}$, and Buckingham static polarizabilities, $\alpha^B_{nl,l'}$, of the 1s-state as well as the excited states 2p and 3d of MHP, at 10 selected μ-values of the MHP $(Z=1, b=1, a=0)$. All values are in a.u. The compared references numbers are given in the superscript square bracket..

Initial state	μ	0.0	0.05	0.1	0.2	0.3	0.4	0.5	0.55	0.6	0.65	0.7	0.75
	$-E_{1s}$	0.5	0.47353	0.44451	0.38095	0.313176	0.244276	0.176869	0.144503	0.113473	0.084173	0.05710	0.03301
	$\langle r\rangle_{1s,1s}$	1.5	1.49731	1.49097	1.47626	1.46917	1.47885	1.51681	1.55333	1.60956	1.69896	1.8526	2.1604
$1s$	$\langle r^2\rangle_{1s,1s}$	3.0	2.98803	2.96043	2.90012	2.87927	2.93983	3.14493	3.34596	3.66984	4.22355	5.28487	7.8030
	$\langle r^3\rangle_{1s,1s}$	7.5	7.45069	7.33967	7.11265	7.06972	7.39296	8.41778	9.46358	11.2545	14.6045	21.9166	45.0362
	$\alpha^B_{1s,p}$	4.5	4.46079	4.3727	4.19313	4.15726	4.40972	5.25109	6.1634	7.8414	11.3291	20.2255	52.7651
		4.5[4,14]											
	μ	0.0	0.05	0.1	0.105	0.11	0.115	0.12	0.125	0.13	0.14	0.15	0.16
	$-E_{2p}$	0.125	0.095742	0.0614403	0.057904	0.054364	0.050824	0.0472874	0.043756	0.0402362	0.03324	0.02632	0.01953
	$\langle r\rangle_{1s,1s}$	5.0	4.92522	4.85837	4.85854	4.86053	4.86451	4.87069	4.87929	4.89059	4.9227	4.97103	5.04214
$2p$	$\langle r^2\rangle_{2p,2p}$	30.0	29.0597	28.3264	28.347	28.3923	28.4649	28.5679	28.7047	28.8799	29.3685	30.1056	31.2137
	$\langle r^3\rangle_{2p,2p}$	210.0	199.733	192.921	193.353	194.08	195.135	196.559	198.402	200.728	207.174	217.083	232.526
	$\alpha^B_{2p,d}$	208.0	199.515	193.537	193.833	194.367	195.163	196.253	197.677	199.482	204.506	212.115	223.898
		208.0[36]											
	μ	0.0	0.01	0.02	0.03	0.035	0.04	0.045	0.05	0.055	0.06	0.062	0.07
	$-E_{3d}$	0.05555	0.050140	0.0440552	0.037472	0.034046	0.030555	0.0270183	0.023449	0.019866	0.016282	0.01485	0.00919
	$\langle r\rangle_{3d,3d}$	10.2255	10.4378	10.353	10.2581	10.2158	10.1806	10.1549	10.1411	10.1414	10.1585	10.1707	10.3059
$3d$	$\langle r^2\rangle_{3d,3d}$	118.25	124.226	122.155	119.89	118.907	118.113	117.566	117.319	117.432	117.97	118.323	122.396
	$\langle r^3\rangle_{3d,3d}$	1513.37	1657.39	1615.21	1570.16	1551.14	1536.25	1526.62	1523.34	1527.63	1540.91	1549.14	1653.26
	$\alpha^B_{3d,f}$	2478.6	2452.89	2397.28	2338.79	2314.42	2295.64	2283.97	2281.02	2288.63	2309.41	2322.19	2408.41
		2478.6[36]											

Table 6: The scaled energies for 1s, 2p, 3d states in Table 5, with the corresponding R^2 and μ_c.

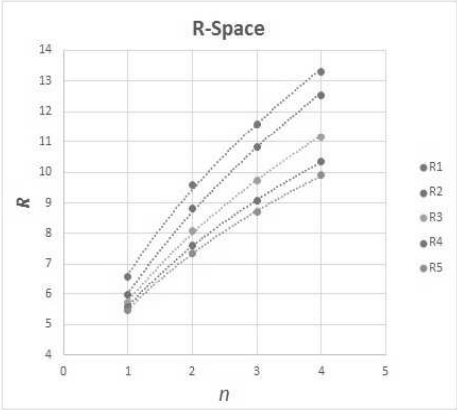
$nl-state$	E_{nl}	R^2	μ_c
1s	$-0.4847\mu^3+0.5117\mu^2+0.511\mu-0.5$	1.0	0.830
2p	$-5.591\mu^3+1.8416\mu^2+0.5072\mu-0.125$	1.0	0.191
3d	$-26.689\mu^3+4.1732\mu^2+0.4993\mu-0.0555$	1.0	0.084

9.The values with different signs for the entropy in respective space, at different parameters, are mainly due to the flipping of the electronic densities.

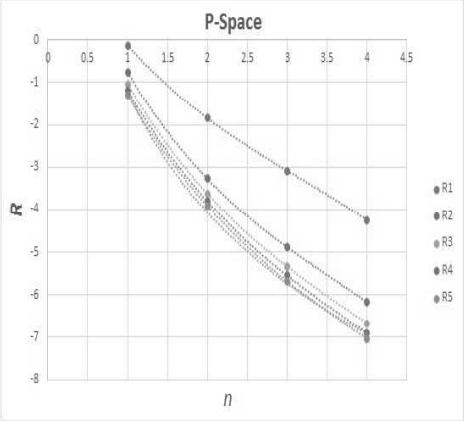
To facilitate satisfying our purpose, i.e. to study the variation of the $\beta-th$ order Rényi entropy in terms of β and n, we assembled Table 2. Table 2 displays the numerical values of Rényi entropies R_β, $\beta=2,3,4$and 5 in $r-$ and $p-spaces$, for the MHP that corresponds to different values of (l,Z,μ,a,b). The numerical values in Table 2 are used to plot Figure 1. With the parameters $(Z=1,\ \mu=0.05,\ a=0.5,\ b=0)$, Figure 1 shows the plotting of the quantities R_β, where $\beta=1,2,3,4,$ and 5 for MHP in r- and p-spaces, as a function of n.

In the r-space, Figure 1 shows the following behavior: i- as n increases, $R_{\beta,r}$ increases for all values of β. According to the definition of the Shannon entropy, more localized distributions, $\rho(r)$, correspond to the smaller value of the $R_{1,r}$, which means the delocalization $\rho(r)$ increases with increasing n; ii- the quantities with the lowest orders (particularly the cases $\beta=1,2,$ and $\beta=3$, which correspond to the Shannon entropy, the second-order, and the third-order of Rényi entropy, respectively) are most significant for the quantification of the electron distribution spreading of the system; iii- the slope of the curves decreases as β increases; iv- For $\beta>3$, the curves start to be very close to each other. In fact, such behavior has been realized for all the D-dimensional states in case of hydrogen Rydberg states [37], and should be expected since the Rényi entropy is defined by (20) as a continuous and non-increasing function in β.

In the p-space, Figure 1 shows that: i- as n increases, $R_{\beta,p}$ increases in the negative value for all values of β. It is important to realize that the conjugate position and momentum space information entropies have an inverse relationship with each other. A strongly-localized distribution in the position space corresponds to widely-delocalized distribution in the momentum space.



(a)



(b)

Fig. 1: The quantities R_β, where $\beta = 1,2,3,4$ and 5 with the parameters $(Z = 1, \mu = 0.05, a = 0.5, b = 0)$ for MHP as a function of n in R- and P-spaces. For guidance purposes only, we've used the dotted line.

When one entropy increases, the other entropy decreases, but only to the extent that their sum stays above the stipulated lower bound of $3(1+\ln(\pi))$; ii- the quantities with the lowest orders (particularly the cases $\beta = 1$, and 2, are the most significant for the quantification of the electron distribution spreading of the system; iii- the slope of the curves increases as β increases. iv- For $\beta > 3$, the curves start to be very close to each other.

Due to the scarcity of analytical study, we attempt to propose a kind of relationship between R_β and n in a logarithmic law form as follows:

$$R_\beta = c\, ln(n) + d, \tag{29}$$

where c and d are fitting parameters. With the help of Tables 1 and 2 with the parameters $(Z = 1, \mu = 0.05, a = 0.5, b = 0)$, one can find the values of the parameters

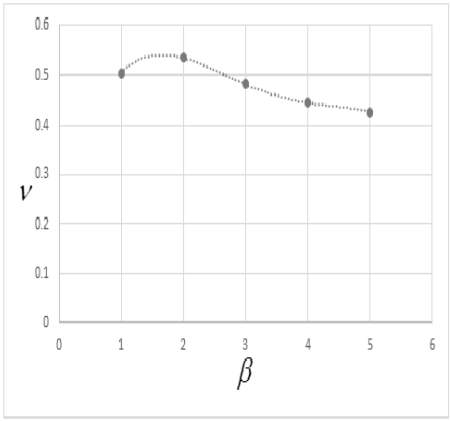


Fig. 2: Scaling laws of the exponent ν in terms of β for the MHP with $(Z = 1, \mu = 0.05, a = 0.5, b = 0)$.

c, d and the associated correlation coefficient R^2 that are calculated in r- and p- spaces and given in Table 3. The values of $R^2 > 0.99$, in Table 3, indicate the strong correlation between R_β and the parameters c, d and n.

Another kind of approach to study the dependence of $R_{\beta,r}$ on the principle quantum number n and β is by using the scaling in a form of power law:

$$R_{\beta,r} = cn^\nu, \tag{30}$$

where the values of the fitting parameters c, ν and the correlation coefficient R^2 are given in Table 4 for the state with the values $(Z = 1, \mu = 0.05, a = 0.5, b = 0)$. The values of $R^2 = 0.999$ indicate the strong correlation between $R_{\beta,r}$ and the parameters c, ν and n. The behavior of the exponent ν versus β is plotted in Figure 2, and the polynomial relation between them is given by:

$$\nu = -0.0039\beta^4 + 0.0554\beta^3 - 0.2748\beta^2 + 0.5248\beta + 0.204. \tag{31}$$

It was found that in (31) the correlation coefficients $R^2 = 1$, where it indicates the strong relation between the exponent ν and the parameter β.

Using (31), ν versus β is plotted in Figure 2. Figure 2 shows that the exponent ν starts with 0.5 at $\beta = 1$ and increases to a maximum at $\beta = 2$. After $\beta = 2$, it is found that ν starts to decrease gradually until reaching a constant value of 0.4 at $\beta > 5$. The observation that the ν decreases monotonically as the integer order β is increases indicates that the Rényi entropy, at fixed n, with the lowest orders (particularly the cases $\beta = 1,2$, and $\beta = 3$) is the most significant for the quantification of the electron distribution spreading of the system. Again, such behavior is realized for all the D-dimensional states in the case of hydrogen Rydberg states [37].

For more data that could be used in future comparison, we have Table 5 to offer calculated results for the bound

states energy, the squares of the M-moment $(r^M)_{nl,n'l'}$, and Buckingham static polarizabilities, $\alpha^{\beta}_{nl,l'}$, of the 1s-state as well as the excited states 2p and 3d of MHP $(Z=1,\ b=1)$, at 10 selected μ-values. For $\mu=0$, our values for all the calculated quantities are in excellent agreement with the published literatures [4, 14, 36]. Note that, for the case $\mu=0$, we have had indeterminate values for all the calculated variables in Table 5. In that case, we had to use $\mu=10^{-6}$.

Unfortunately, for $\mu>0$ there is no literature to compare with. The closest potential that we can use, and compare with, is the exponential-cosine screened Coulomb potential (ECSCP), in the form [14, Table 7]:

$$V_{ECSCP}(r)=-Z\frac{e^{-\mu r}}{r}cos(\mu r) \tag{32}$$

A comparative study between the two potentials (1) and (32) shows the following: i- the eigenvalues in MHP, $E_{nl}(MHP)$, are more bound than eigenvalues in ECSCP, $E_{nl}(ECSCP)$. Consequently one finds the critical value $\mu_c(MHP)>\mu_c(ECSCP)$. The critical value μ_c is defined as the value of μ after which no bound state exists. ; ii- The calculated quantities, $(r^M)_{nl,n'l'}$ and $\alpha^{\beta}_{nl,l'}$, almost stay constant, up to two or three digits, for a wide range of μ, $0<\mu<\mu_c$. Close to the critical value μ_c, $\mu\simeq\mu_c$, the quantities start to increase. This is different than the behavior of the quantities in ECSCP, as the quantities increase with increasing μ.

To close the discussion, we end with the scaling laws, which fits the data in Table 6, for the Buckingham static polarizabilities, $\alpha^{B}_{nl,l'}$, which are given by:

$$\begin{aligned}
\alpha^{B}_{1s,p} &= 20077\mu^6-38647\mu^5+27720\mu^4-8990.9\mu^3\\
&\quad +1265.3\mu^2-58.41\mu+4.5,\\
\alpha^{B}_{2p,d} &= 6.0x10^7\mu^6-3.0x10^7\mu^5+6.0x10^6\mu^4\\
&\quad -567925\mu^3+24755\mu^2-576.91\mu+208\\
\alpha^{B}_{3d,f} &= 6.0x10^9\mu^6-7.0x10^8\mu^5-6.0x10^6\mu^4\\
&\quad -6.0x10^6\mu^3-315956\mu^2+1.4951\mu+2478.6
\end{aligned} \tag{33}$$

and all have correlation coefficient $R^2=1$.

4 Perspective

In summary, we have reported the results of our numerical studies of some information-theoretical entropies for the MHP. The J-matrix method has been implemented for the MHP in spherical polar coordinates. The wave functions and their corresponding electron densities are calculated in r- and p- spaces. Many characteristic features have been realized in the case of this study. For example, it is found that the summation S_T satisfies the BBM sum. The scaling laws for the calculated informatics entropies and three other quantities are given as a function of the quantum number n. The scaling laws clearly show the correlation between the calculated quantities and the parameters n, μ and β. It is believed that this initial entropy study of the non-analytic potential will stimulate interesting studies, theoretically and experimentally, with other potentials, and inspire the investigation of entropies, such as the Tsallis, or non additive entropies [37,38,39].

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