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Rényi and Tsallis Entropies of $2p$ Orbital Helium Atom

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Abstract

In this paper, an analytical model of $2p$ orbital helium atom has been considered to quantify the values of the Rényi and Tsallis entropies along with their theoretical aspects. The normalized radial wave function used here (in atomic units) is obtained by solving the Schrödinger equation. The complete form of the coordinate space wave function is obtained by the use of the spherical harmonics. The momentum space wave function is obtained by taking the Fourier transform of the coordinate space wave function. The probability densities constituted with the respective coordinate and momentum space wave functions have been used to compute the numerical values of the Rényi and Tsallis entropies in the coordinate and momentum space for different values of the order β varying from 2 to 10. The computed values are presented in a tabular form. Further, it is mathematically demonstrated that in the limit of order $\beta \to 1$, both the Rényi and Tsallis entropies lead to the Shannon entropy. Finally, an outlook of the present work has been summarized with some concluding remarks.

Keywords: Entropic moment; Helium atom; Rényi entropy; Shannon entropy; Tsallis entropy.

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1.Introduction

It is an important fact that the accurate values of the physical quantities obtained from the experiments or theoretical calculations could serve as the stepping stone in the area of research. Nowadays, the information theory of quantum mechanical systems is of great scientific challenge because (i) it provides a deeper insight into the internal structure of the systems [1] and (ii) it offers the strongest support to the modern quantum computation and information [2] which is regarded as the basic need for the numerous technological developments [3]. Actually, even for the one-dimensional single-particle systems with an analytically solvable Schrödinger equation where the wave functions of their physical states are controlled by special functions of mathematical physics such as classical orthogonal polynomials, spherical harmonics, Bessel functions, Macdonald functions, etc. [4], the basic information-theoretic quantities remain to be computed. This is because of the lack of knowledge relating to the application of the information-theoretic properties of special

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functions despite the so many results provided by the theory of orthogonal polynomials and potential theory [5]. The determination of these information-theoretic quantities is one of the main goals of the information theory of the finite quantum systems, which is the strongest support of the modern information and computation. Moreover, these measures and the ideas related to disorder, randomness, localization and uncertainty are the basic ingredients that perform a relevant role for the identification and description of numerous quantum phenomena in physical systems and chemical processes. This was initially pointed out by Bialynicki-Birula and Mycielski [6], Sears *et al.* [7], Levine [8], Fisher [9], Frieden [10], Jaynes [11-15], Rényi [16], Shannon [17], Tsallis [18,19], Stam [20] and others, through various aspects of research in the fields of statistical mechanics, communication theory and classical information theory. The information-theoretic quantities play various significant roles in physical systems and chemical processes. Rényi $[R_{\rho,\gamma}(\beta)]$ and Tsallis $[T_{\rho,\gamma}(\beta)]$ entropies find numerous applications in science, technology, engineering, medicine, and economics, among others. Rényi entropy which was proposed by the Hungarian mathematician bearing his name [21] was successfully applied in coding theory [22]. Besides applications in physics and information theory, Rényi measure was used in the investigation of spatial distribution of earthquake epicenters [23], for the analysis of the landscape diversity and integrity [24,25], for predicting the behaviour of the stock markets [26], exploration and modification of the brain activity [27], digital image analysis [28], etc. Tsallis entropies are widely utilized in non-extensive systems including the structures and processes characterized by non-ergodicity, long-range correlations and space-time (multi) fractal geometry [29]. It should be noted that the subscripts ρ and γ (or ρ, γ) used in different expressions throughout our works are representing the coordinate space and momentum (or combining the both) spaces respectively.

A few years ago, attempts were made by Ou *et al.* [30] to calculate the Rényi entropy, Tsallis entropy and Onicescu information energy for helium atom using highly correlated Hylleraas wave function. Later, Martinez-Flores [31] also worked on the same track using the screened Coulomb potential for helium atom. There are literatures where the numerical calculations for the Shannon and Fisher entropies were made using the correlated wave function for helium atom [32]. The similar calculations have been done for the free particles also [33,34]. An analytic correlated wave function was studied in detail to analyze the effect of electron correlation on the Rényi entropy, Tsallis entropy and Onicescu information energy for the neutral atoms helium to beryllium by Sarkar [35].

In this paper, an analytical model consisting of $2p$ orbital helium atom (two one-electron system) will be studied. Here, a two one-electron system has been considered, where '$1s$' electron is under the influence of full nuclear charge '$2e$' but the other 'n, l' electron is under the influence of the screened charge 'e'. The coordinate space wave function $\psi(\vec{r})$ is obtained by the product of the normalized radial wave function R_{nl} [36] and the spherical harmonics $Y_l^{m_l}$. The momentum space wave function $\phi(\vec{p})$ is obtained by taking the Fourier transform [37] of that coordinate space wave function $\psi(\vec{r})$. The coordinate and momentum space probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ constructed by these wave functions are then used to compute the numerical values of the Rényi and Tsallis entropies both in the coordinate

and momentum space for the different values of the order β (a non-negative parameter) varying from 2 to 10. It is shown that in the limit of the order $\beta \to 1$, both the Rényi and Tsallis entropies lead to the values of the Shannon entropy for this system. Further, the expressions obtained for the probability densities are used to study and analyze the variation of the probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ in the coordinate and momentum space as functions of the coordinate $(\vec{r})$ and momentum $(\vec{p})$through their graphical representations.

The physical and chemical properties of a system in a given quantum-mechanical state described by three integer quantum numbers (n, l, m) are controlled by the spread of the of the coordinate and momentum space densities $[\rho_n(\vec{r})$ and$\gamma_n(\vec{p})]$. The location and motion of a quantum mechanical particle in information theory is described with the help of densities $\rho_n(\vec{r})$ and $\gamma_n(\vec{p})$. These densities which are constituted by the squared amplitudes of the corresponding one-particle wave functions$\psi_n(\vec{r})$ and $\phi_n(\vec{p})$ are described as follows:

$$\rho_n(\vec{r}) = |\psi_n(\vec{r})|^2 \quad \text{and} \quad \gamma_n(\vec{p}) = |\phi_n(\vec{p})|^2 \tag{1}$$

where a discrete index 'n' counts all possible bound quantum states. In general, d-dimensional space, $\psi_n(\vec{r})$ and $\phi_n(\vec{p})$ are related with the Fourier transform as follows:

$$\psi_n(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} \phi_n(\vec{p})\, e^{i\vec{p}\cdot\vec{r}} d^3p \text{ where, } \phi_n(\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} \psi_n(\vec{r})\, e^{-i\vec{p}\cdot\vec{r}} d^3r \tag{2}$$

with integrations carried out over the whole available region.

Among the prevailing information-theoretic quantities, a very special role is played by the Rényi and Tsallis entropies whose expressions in the coordinate and momentum spaces are defined as follows where the order $\beta \neq 1$:

$$R_{\rho_n}(\beta) = \frac{1}{1-\beta} ln\left(\iiint_{-\infty}^{\infty} \rho_n^{\beta}(\vec{r}) d^3r\right), \tag{3}$$

$$R_{\gamma_n}(\beta) = \frac{1}{1-\beta} ln\left(\iiint_{-\infty}^{\infty} \gamma_n^{\beta}(\vec{p}) d^3p\right), \tag{4}$$

and

$$T_{\rho_n}(\beta) = \frac{1}{\beta-1}\left(1 - \iiint_{-\infty}^{\infty} \rho_n^{\beta}(\vec{r}) d^3r\right), \tag{5}$$

$$T_{\gamma_n}(\beta) = \frac{1}{\beta-1}\left(1 - \iiint_{-\infty}^{\infty} \gamma_n^{\beta}(\vec{p}) d^3p\right). \tag{6}$$

Here, the non-negative parameter β is the 'Order' of the Rényi and Tsallis entropies associated with the probability densities$\rho_n^{\beta}(\vec{r})$ and $\gamma_n^{\beta}(\vec{p})$ respectively in the coordinate and momentum spaces.

Rényi and Tsallis attempted to quantify 'information' with the help of a non-negative parameter, $0 < \beta < \infty$, which can be considered as a factor describing the reaction of the system to its deviation from the equilibrium. Eqs. (3) to (6) were used to study the variations of entropy with the varying β values. If the limit of the integration in Eqs. (3) to (6) are taken as infinite then the corresponding values of the entropy lead to divergence. Special case $\beta = 1$ with the help of the L'Hospital's rule leads both the Rényi and Tsallis entropies to the celebrated Shannon entropies:

$$S_{\rho_n} = -\iiint_{-\infty}^{\infty} \rho_n(\vec{r}) ln\rho_n(\vec{r})\, d^3r \tag{7}$$

$$S_{\gamma_n} = -\iiint_{-\infty}^{\infty} \gamma_n(\vec{p}) ln\gamma_n(\vec{p})\, d^3p. \tag{8}$$

The dependence on S_{ρ_n} or S_{γ_n} was introduced in 1948 by C.E. Shannon during the mathematical analysis of communication [38] for the random discrete distribution of a given sample of probabilities p_i. From a quantum informational point of view, S_{ρ_n} or S_{γ_n}

quantitatively describes the lack of our knowledge about the corresponding property of the system. The smaller (greater) the value of this entropy is the more (less) information we have about a quantum mechanical object. Accordingly, the physical meaning of the Rényi entropy and the parameter 'β' can be construed as follows; the equilibrium distribution corresponds to $\beta = 1$, and any value of $\beta \neq 1$ is a deviation from it. The Rényi entropy is a measure of the sensitivity of the system to its deviation from the equilibrium. If the parameter $\beta > 1$, then the corresponding entropy decreases, which means that such a configuration provides more information about the object than its equilibrium counterpart. On the other hand, the values of $\beta < 1$, increases the entropy with the corresponding decrease of the available information. In the extreme case $\beta \to 0$, it reaches to its maximum value which for the infinite interval leads to a logarithmic divergence. Within this limit the integrals in Eqs. (3) to (6) are just a flat unit line; in such cases the Rényi entropy in the coordinate space does not provide any information about the location of the particle in space. Thus, the rate of change of the entropy with the order β just shows the sensitivity of the system to the degree of non-equilibrium.

Further, it can be noted that the Rényi and Tsallis entropies are interrelated as follows:

$$R = \frac{1}{1-\beta} ln[1 + (1-\beta)T] \text{ and } T = \frac{1}{\beta-1}\left[1 - e^{(1-\beta)R}\right]. \quad (9)$$

And both the entropies are decreasing functions of the order β. One important difference between them lies in the fact that the Rényi entropy is additive (or extensive) whereas the Tsallis entropy is non-additive (or non-extensive).

The aim of our present work is to derive an analytical model to quantify the values of the Rényi and Tsallis entropies of the $2p$ orbital helium atom (two one-electron systems) using its normalized wave function. The analytical model will be used to study the variations of the coordinate and momentum space probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ as functions of the coordinate $(\vec{r})$ and momentum $(\vec{p})$ graphically. Further, it will be used to compute the numerical values of the Rényi and Tsallis entropies and also demonstrate that in the limit of the non-negative parameter $\beta \to 1$ both the Rényi and Tsallis entropies lead to the Shannon entropy. The values of the entropies are to be computed both in the coordinate and momentum space with respect to varying values of the order β. In applicative context it will, therefore, be quite interesting to examine how the computed values of the Rényi and Tsallis entropies respond both in the coordinate and momentum space. Until now research has been focused mainly on Shannon entropy involving hydrogen-like systems [39,40]. To the best of our knowledge, the Rényi and Tsallis entropies using the wave function of the $2p$ orbital helium atom (two one-electron system) has not been reported before in the literature.

The structure of the paper is as follows. The necessary mathematical elements to find the probability densities and their variations with graphical representation in the coordinate and momentum space for arbitrary $2p$ orbital using the complete form of the normalized wave function of the helium atom are summarized in Section 2. Then, in Section 3, it has been explicitly demonstrated hat in a closed and simple mathematical form how both the Rényi and Tsallis entropies in the limit of the order $\beta \to 1$ lead to the Shannon entropy. In Section 4, the numerical values of the Rényi and Tsallis entropies have been computed using

their corresponding probability densities $\rho_n(\vec{r})$ and $\gamma_n(\vec{p})$ for different values of the order β both in the coordinate and momentum space. The computed values are presented in a tabular form. Finally, Section 5 has been devoted to present an outlook of the work done with some concluding remarks.

2. Materials and Method

In this Section, the necessary mathematical treatments have been described to find the probability densities of arbitrary $2p$ orbital states of helium atom employing the normalized radial wave function with the help of corresponding spherical harmonics. The exact solutions of the Schrödinger differential equation are very important in understanding the main recipe of the problems in Physics that can only be brought by such solutions [41,42]. These solutions are not only treated as valuable tools in checking and improving models but can be introduced in numerical methods for solving some complicated physical problems at least in some limiting cases also [43,44].One of such method is the analytical solution of the radial Schrödinger equation which is of high importance in non-relativistic quantum mechanics; because the wave function contains all necessary information for full description of a quantum mechanical system [45,46]. However, an alternative method known as the Nikiforov-Uvarov (NU) method [47] was also proposed for solving Schrödinger wave equation.

A neutral helium atom has been considered here, where one electron is in the '$1s$' ground state and the other electron is in an 'n,l' excited state ($n \geq 2, l \geq 1$). The non-relativistic Hamiltonian (in atomic units) of helium atom can be written in the following form:

$$\widehat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \tag{10}$$

where the subscript 1 and 2 represents the electron 1 and 2, respectively, and r_{12} is the distance between the two electrons.

If the '$1s$'electron is under the influence of full nuclear charge $2e$, but the 'n,l' electron only to the screened charge e, then the two one-electron states can be described by the solution of the following differential equations

$$\left(-\frac{1}{2}\nabla^2 - \frac{2}{r}\right)u = E_1 u \; ; \left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right)v_{nl} = E_n v_{nl} \tag{11}$$

$$\text{with,} u \equiv |1\rangle = \sqrt{\frac{8}{\pi}}e^{-2r} \; ; E_1 = -2 \; ; v_{nl} \equiv |n\rangle = R_{nl}(r)Y_{l,m}(\theta,\varphi); E_n = -\frac{1}{2n^2}, \tag{12}$$

where, $R_{nl}(r)$ belongs to the radial wave functions of the hydrogen atom.

Now, the Schrödinger equation of the two-electron problem can be written as follows:

$$\left\{-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}\right\}\psi = E\psi. \tag{13}$$

The approximate solution of this problem has been solved and discussed in detail in Flügge [36] by the symmetrized product wave function represented as follows:

$$\psi = u(1)v_n(2) + \varepsilon v_n(1)u(2) = |1n\rangle + \varepsilon|n1\rangle \tag{14}$$

with $\varepsilon = +1$ for para-helium (spins anti-parallel) and $\varepsilon = -1$ for ortho-helium (spins parallel).

The wave function ψ is normalized according to $\langle\psi|\psi\rangle = 2$ and the expression for the normalized radial wave function R_{nl} for the states $n = 2, l = 1$ has been obtained (in atomic units) after some cumbersome mathematical workout as:

$$R_{2,1} = \frac{1}{\sqrt{24}}\, re^{-\frac{r}{2}}. \tag{15}$$

2.1. *Calculation of the complete wave functions $\psi(\vec{r})$ and $\phi(\vec{p})$ in the coordinate and momentum space*

In order to find the complete form of the wave function in the coordinate space for the state corresponding to $n = 2$ and $l = 1$, we take recourse of the expression for the normalized radial wave function $R_{2,1} = \frac{1}{\sqrt{24}}\, re^{-\frac{r}{2}}$; and the values of spherical harmonics ($Y_l^{m_l}$) with $Y_1^0 = \frac{\sqrt{3}}{2\sqrt{\pi}}\cos\theta$, $Y_1^{+1} = \frac{\sqrt{3}}{2\sqrt{2\pi}} sin\,\theta\, e^{i\varphi}$ and $Y_1^{-1} = \frac{\sqrt{3}}{2\sqrt{2\pi}} sin\,\theta \cdot e^{-i\varphi}$. When, $n = 2$ and $l = 1$ the corresponding values for 'm_l' are taken as $-1, 0, +1$.

In terms of the corresponding radial parts of the normalized radial wave function $R_{2,1}$ and spherical harmonics Y_1^0, Y_1^{+1}, Y_1^{-1}, the expression of the coordinate space wave function $\psi(\vec{r})$ can be written as below:

$$\psi(\vec{r}) = \{\psi_{2,1,0} + \psi_{2,1,+1} + \psi_{2,1,-1}\} = R_{2,1} \cdot Y_1^0 + R_{2,1} \cdot Y_1^{+1} + R_{2,1} \cdot Y_1^{-1}$$

Thus, we get the expression for the coordinate space wave function:

$$\psi(\vec{r}) = re^{-\frac{r}{2}}\left(\frac{1}{\sqrt{32\pi}}\cos\theta + \frac{1}{8\sqrt{\pi}}\sin\theta\, e^{i\varphi} + \frac{1}{8\sqrt{\pi}}\sin\theta\, e^{-i\varphi}\right). \tag{16}$$

The momentum space wave function $\phi(\vec{p})$ is obtained by performing the Fourier transform of each component of the momentum space wave function $\phi_{2,1,0}$, $\phi_{2,1,+1}$ and $\phi_{2,1,-1}$ in terms of the components of the coordinate space wave function $\psi_{2,1,0}$, $\psi_{2,1,+1}$ and $\psi_{2,1,-1}$ using the Fourier transform relation of the Eq. (2) which is rewritten as:

$$\phi(\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\iiint_{-\infty}^{\infty} \psi(\vec{r})\, e^{-i\,\vec{p}\,.\vec{r}}\, d^3r \text{ where, } \psi(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\iiint_{-\infty}^{\infty} \phi(\vec{p})\, e^{+i\,\vec{p}\,.\vec{r}}\, d^3p.$$

And the expression of the momentum space wave function $\phi(\vec{p})$ is written as:

$$\phi(\vec{p}) = \{\phi_{2,1,0} + \phi_{2,1,+1} + \phi_{2,1,-1}\} = \frac{1}{(2\pi)^{\frac{3}{2}}}\iiint_{-\infty}^{\infty}\{\psi_{2,1,0} + \psi_{2,1,+1} + \psi_{2,1,-1}\}e^{-i\,\vec{p}\,.\vec{r}}\, d^3r.$$

Thus, finally the expression for the momentum space wave function $\phi(\vec{p})$ is as follows:

$$\phi(\vec{p}) = -\frac{64ip}{\pi(1+4p^2)^3}\ . \tag{17}$$

2.2. *Calculation of the probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ in the coordinate and momentum space*

The probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ associated with the coordinate and momentum space wave functions $\psi(\vec{r})$ and $\phi(\vec{p})$ are obtained as the sum of the square of the modulus values of each component of the coordinate space wave function ($\left|\psi_{2,1,0}\right|^2 + \left|\psi_{2,1,+1}\right|^2 + \left|\psi_{2,1,-1}\right|^2$) and the momentum space wave function ($\left|\phi_{2,1,0}\right|^2 + \left|\phi_{2,1,+1}\right|^2 + \left|\phi_{2,1,-1}\right|^2$).

And the expression for the coordinate space probability density $\rho(\vec{r})$ is as follows:

$$\rho(\vec{r}) = \psi^*(\vec{r})\psi(\vec{r}) = \frac{1}{32\pi} r^2 e^{-r}. \tag{18}$$

Similarly, the probability density $\gamma(\vec{p})$ associated in the momentum space for the wave function $\phi(\vec{p})$ can be obtained as the following:

$$\gamma(\vec{p}) = \phi^*(\vec{p})\phi(\vec{p}) = \frac{4096p^2}{\pi^2(1+4p^2)^6}. \quad (19)$$

2.3. *Graphical representation of the probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ in the coordinate and momentum space*

The following graphs labelled as Fig. 1A,B have been plotted with the help of the expressions obtained for the coordinate and momentum space probability densities which are varying against their coordinate and momentum.

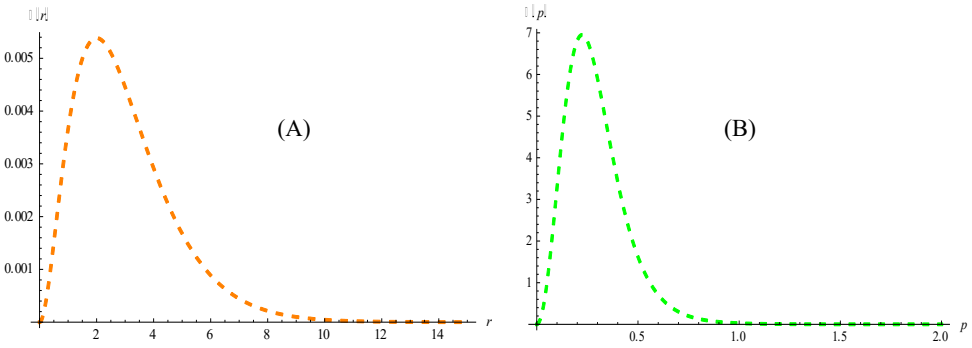

Fig. 1. (A) Coordinate space probability density $\rho(\vec{r})$ versus the coordinate $(\vec{r})$. (B) Momentum space probability density $\gamma(\vec{p})$ versus the momentum $((\vec{p}))$.

From the Fig. 1A,B it can be seen that the shape of the coordinate space probability density $\rho(\vec{r})$ indicated by the red dotted curve is flattened as compared to the momentum space probability density $\gamma(\vec{p})$; whereas the momentum space probability density $\gamma(\vec{p})$ indicated by the green dotted curve is observed as squeezed significantly as compared to the coordinate space probability density $\rho(\vec{r})$. Thus, it can be realized clearly from the above figure that the probability densities are playing a complementary role in respect of their shapes respectively in the coordinate and momentum space.

3. Shannon Entropy as a Limiting Case of Rényi and Tsallis Entropy

In this section, we shall discuss how the Rényi and Tsallis entropies as a limiting case turn in to the Shannon entropies.

Given a sample of probabilities p_i, the sum of 'p_i' can be written as $\sum_{i=1}^{N} p_i = 1$. The Shannon entropy for the probability density p_i is expressed as follows:

$$S = -\sum_{i=1}^{N} p_i \, ln \, p_i. \quad (20)$$

3.1. *Rényi entropy as Shannon entropy*

The Rényi entropy of the sample for a fixed distribution P of order β is given by

$R_\beta(P) = \frac{1}{1-\beta} ln \sum_{i=1}^{N} p_i^\beta$. (21)

At $\beta = 1$, the value of this quantity is potentially undefined as it generates the $\frac{0}{0}\left(\frac{\text{Zero}}{\text{Zero}}\right)$ form. In order to find the limit of the Rényi entropy, the L'Hospital's Theorem is applied to obtain

$$\lim_{\beta \to a} \frac{f(\beta)}{g(\beta)} = \lim_{\beta \to a} \frac{f'(\beta)}{g'(\beta)}.$$

Where in this case, $a = 1$. Let, $f(\beta) = ln \sum_{i=1}^{N} p_i^\beta$ and $g(\beta) = 1 - \beta$. (22)

Then $\frac{d}{d\beta} g(\beta) = -1$ and, applying the chain rule $\frac{d}{d\beta} f(\beta) = \frac{1}{\sum_{i=1}^{N} p_i^\beta} \sum_{i=1}^{N} \frac{d}{d\beta} p_i^\beta$. (23)

The form a^x can be differentiated w.r.t. 'x' by putting $\frac{d}{dx} a^x = \frac{d}{dx} e^{xlna} = e^{xlna} \frac{d}{dx} xlna = a^x lna$.

Therefore, $\frac{d}{d\beta} f(\beta) = \frac{1}{\sum_{i=1}^{N} p_i^\beta} \sum_{i=1}^{N} p_i^\beta \; lnp_i$. (24)

Letting $\beta \to 1$, the above quantity becomes $\frac{d}{d\beta} f(\beta) = \frac{1}{\sum_{i=1}^{N} p_i} \sum_{i=1}^{N} p_i \; lnp_i$.

Since the p_i sum to unity, this gives $\lim_{\beta \to 1} \frac{1}{1-\beta} ln \sum_{i=1}^{N} p_i^\beta = -\sum_{i=1}^{N} p_i \; lnp_i$ (25)

which is the Shannon entropy.

3.2. *Tsallis entropy as Shannon entropy*

The Tsallis entropy for a fixed distribution$P$ of order β is defined as

$T_\beta(P) = \frac{1}{\beta-1}\left(1 - \sum_{i=1}^{N} p_i^\beta\right)$. (26)

Let, the above quantity be expressed as$T_\beta(P) = \frac{f(\beta)}{g(\beta)}$ (27)

with $f(\beta) = \left(1 - \sum_{i=1}^{N} p_i^\beta\right)$, and $g(\beta) = \beta - 1$ which leads to $g'(\beta) = 1$ [The prime sign indicating the derivative of the quantity concerned w.r.t. 'β'].

Further, it can be written as

$f(\beta) = \left(1 - \sum_{i=1}^{N} p_i^\beta\right)$ and $f'(\beta) = -\sum_{i=1}^{N} p_i^\beta \; ln \, p_i$ [since, $(p_i^\beta)' = (e^{\beta \, ln \; p_i})' = p_i^\beta \; ln \, p_i$]. (28)

As both limits of $f(\beta)$ and $g(\beta)$tend to 0 as $\beta \to 1$, then after applying the L'Hospital's Theorem, the expression for $T_\beta(P)$ can be obtained as the following:

$\lim_{\beta \to 1} T_\beta(P) = \lim_{\beta \to 1} \frac{f(\beta)}{g(\beta)} = \lim_{\beta \to 1} \frac{f'(\beta)}{g'(\beta)} = -\sum_{i=1}^{N} p_i \; ln \, p_i$. (29)

which is namely the Shannon entropy. That is, the Tsallis entropy tends to the Shannon entropy as $\beta \to 1$.

4. Results and Discussion

In this Section, the numerical values of the Rényi $[R_{\rho_2}(\beta), R_{\gamma_2}(\beta)]$ and Tsallis $[T_{\rho_2}(\beta), T_{\gamma_2}(\beta)]$ entropies are calculated for the states $n = 2, l = 1$, varying the order β from 2 to 10 considering $\beta \neq 1$ for a continuous one-normalized one-electron probability densities $\rho_n(\vec{r})$ and $\gamma_n(\vec{p})$ in the coordinate and momentum space. In order to perform the calculations, we have introduced a change in the limits of the integration of Eqs. (3) to (6) from $(-\infty$ to $\infty)$ to (0 to $\infty)$ and carried out all the integrals after expressing the Eqs. (3) to (6) exactly in the similar forms as shown below:

$R_{\rho_n}(\beta) = \frac{1}{1-\beta} ln \left(\iiint_0^\infty \rho_n^\beta (\vec{r}) \, 4\pi r^2 dr\right)$ and $T_{\gamma_n}(\beta) = \frac{1}{\beta-1}\left(1 - \iiint_0^\infty \gamma_n^\beta (\vec{p}) 4\pi p^2 dp\right)$.(30)

To make it understand the changes made in Eqs. (3) to (6) only two expressions; one relating to the Rényi entropy and the other relating to the Tsallis entropy have been illustrated here in Eq. (30).

It is important to note that the expressions of the Rényi and Tsallis entropy contain the terms $\int \rho_n^{\beta}(\vec{r})\, dr$ or $\int \gamma_n^{\beta}(\vec{p})\, dp$ which are called the entropic moment or β-order frequency moment [48] of the one-normalized one-electron probability densities $\rho_n(\vec{r})$ and $\gamma_n(\vec{p})$[49,50]. In fact, it relates to several physical quantities such as the normalization of electron density for $\beta = 1$, Thomas-Fermi kinetic energy for $\beta = {}^{5}/_{3}$, Dirac exchange energy for $\beta = {}^{4}/_{3}$ and so on. For a continuous one-normalized one-electron probability densities, the numerical values of the Rényi $[R_{\rho_2}(\beta), R_{\gamma_2}(\beta)]$ and Tsallis $[T_{\rho_2}(\beta), T_{\gamma_2}(\beta)]$ entropies have been computed both in the coordinate and momentum space using different values of the order β varying from 2 to 10 and put them in a tabular form as following:

Table 1. The numerical values of Rényi $[R_{\rho_2}(\beta), R_{\gamma_2}(\beta)]$ and Tsallis $[T_{\rho_2}(\beta), T_{\gamma_2}(\beta)]$ entropies in coordinate and momentum space.

Order (β)	$R_{\rho_2}(\beta)$	$R_{\gamma_2}(\beta)$	$T_{\rho_2}(\beta)$	$T_{\gamma_2}(\beta)$
$\beta = 2$	4.96269	-2.29039	0.99301	-8.87882
$\beta = 3$	5.29164	-1.94661	0.49999	-24.03410
$\beta = 4$	5.35189	-1.87365	0.33333	-91.71610
$\beta = 5$	5.36420	-1.85188	0.25000	-411.83000
$\beta = 6$	5.36339	-1.84557	0.20000	-2035.17000
$\beta = 7$	5.35847	-1.84500	0.16667	-10702.40000
$\beta = 8$	5.35238	-1.84675	0.14286	-58767.60000
$\beta = 9$	5.34616	-1.84945	0.12500	-333092.00000
$\beta = 10$	5.34021	-1.85249	0.11111	-19342330.86000

From the above table, it can be observed that for the order $\beta \geq 4$, the values of the Rényi entropies tend to decrease very slowly in the coordinate space while a slowly increasing tendency for the same can be observed in the momentum space. However, a gradual decrease in the values of the Tsallis entropy is observed in the coordinate space but a rapid and strong decrease for the same can be observed in the momentum space with the increasing values of the order $\beta \geq 4$.

5. Conclusion

In the present work we have considered an analytical model to quantify the values of the Rényi and Tsallis entropies of the$2p$ orbital helium atom (two one-electron systems). The normalized radial wave function R_{nl} has been used to obtain the complete form of the wave function $\psi(\vec{r})$ with the help of corresponding spherical harmonics (Y_1^0, Y_1^{+1} and Y_1^{-1}) for the state $n = 2$, $l = 1$ and for the corresponding values of '$m_l = -1, 0, +1$'. The radial wave function for the two one-electron system is obtained by solving the Schrödinger equation by the symmetrized product wave function. The wave function $\psi(\vec{r})$ is normalized according to $\langle\psi|\psi\rangle = 2$. The momentum space representation $\phi(\vec{p})$ is obtained by taking the Fourier transform of the coordinate space wave function$\psi(\vec{r})$. The coordinate and momentum space densities [$\rho(\vec{r})$ and$\gamma(\vec{p})$] are constituted by the squared amplitudes of the

corresponding one-electron wave functions $\psi(\vec{r})$and $\phi(\vec{p})$. Interestingly, it can be noted that the momentum space wave function $\phi(\vec{p})$ as obtained through the Fourier transform of the coordinate space wave function$\psi(\vec{r})$ is an imaginary quantity; however the square of the modulus value of $\phi(\vec{p})$ i.e. the probability density $\gamma(\vec{p})$is a real quantity and is independent of both the angles θ and φ. The variation of shapes of the probability densities as functions of coordinate$(\vec{r})$ and momentum$(\vec{p})$ has been observed graphically in Sub-section 2.3 revealing the complementary nature of the probability densities in the coordinate and momentum space. Here, in one hand, the coordinate space probability density $\rho(\vec{r})$ is seen to be flattened significantly in the coordinate space as compared to the momentum space probability density $\gamma(\vec{p})$ and on the other hand, the momentum space probability density $\gamma(\vec{p})$ gets squeezed a lot showing the opposite behaviour of the coordinate space probability density $\rho(\vec{r})$ in the momentum space. Further, the numerical values for the coordinate and momentum space Rényi and Tsallis entropies (for $\beta \neq 1$) have been computed for different values of the order β varying from 2 to 10 and the obtained values are put into a tabular form accordingly. It has been demonstrated in Sub-sections 3.1 and 3.2 by applying L'Hospital's Theorem in a closed and simple mathematical form that in the limit of the order $\beta \to 1$, both the Rényi and Tsallis entropies lead to the values of the Shannon entropy i.e. $S = -\sum_{i=1}^{N} p_i \, ln p_i$. From the Table 1, it can be observed that for the order $\beta \geq 4$, the values of the Rényi entropies tend to decrease very slowly in coordinate space while a slowly increasing tendency for the same can be observed in the momentum space. However, a gradual decrease in the values of the Tsallis entropy is observed in the coordinate space but a rapid and strong decrease for the same can be observed in the momentum space with the increasing values of the order $\beta \geq 4$.Meanwhile, the positive values of the coordinate space Rényi and Tsallis entropy signify the spreading (delocalization) of the wave functions whereas the negative values for both the entropies in the momentum space indicate the gathering (localization) of the wave functions and these phenomena are showing some of the important aspects of the wave packet dynamics as well. The indications can also be predicted and analyzed from the graphical representation of the variations of the probability densities in both the coordinate and momentum space. It is important to mention that all the numerically computed quantities are expressed in atomic units ($m = 1,\ \hbar = 1$ and $e = 1$). It can further be noted that the calculated numerical values reported in this work for the Rényi and Tsallis entropies against the varying order β not only qualitatively agree, but are also more accurate than the trends those are presented in the contemporary literature. Moreover, a self-consistency in the numerical values has been found fulfilling the analytical relations of the Rényi and Tsallis entropies for the increasing order β. To the best of our knowledge, it is believed that the numerical results presented in this work would serve as a useful and reliable reference for the various applications involving the Rényi and Tsallis entropies. This research has got further scopes for analyzing the information-theoretic quantities of other atomic and molecular systems in excited states. Such systems will be tried to investigate further in our future works.

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