J-matrix calculation of Tsallis entropy for Hellmann potential

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Abstract: The Tsallis entropy for a system that interrelates with the Hellmann potential is calculated and discussed. The calculation is done in the position and momentum spaces using the J-matrix method. Most of our outcomes are reported for the first time. The results are compared with the available literature results.

1. Introduction.

About thirty years ago, nonadditive entropy known as “Tsallis entropy $S_q$” was first proposed by Tsallis himself [1]. Accordingly, the concept that related with nonadditive statistical mechanics has found applications in a variety of disciplines including physics, fluids, informatics, linguistics, among others [2,3]. We refer to Ref [4] for recent, more historical details, and applications. The Tsallis entropy is useful in cases where there are strong correlations between different microstates in a system. It is defined as the $q$-generalized entropy, in the form:

$$S_q = \frac{1}{q-1} \left(1 - \int \rho^q(r) dr\right); \quad q > 0$$

(1)

where $q$ and $\rho(r)$ are the Tsallis index and the electron states’ density, respectively. $dr = r^2 dr d\Omega$ is the infinitesimal volume element and $d\Omega = (\sin \theta d\theta d\phi)$ is the solid angle. The entropy $S_q$ satisfies the following property: if $A$ and $B$ are two probabilistically independent systems, then

$$S_q(A + B) = S_q(A) + S_q(B) + (1 - q)S_q(A)S_q(B)$$

(2)

The Tsallis index $q$ plays crucial rules in nonadditive entropy since it is considered a way of characterizing a system’s correlations – particularly how strong they are. It is either more or less than one in such systems. When the correlations in a system are weak or non-existent, $q$ approaches 1 and $S_q$ becomes additive and reduces to the usual Shannon entropy $S$ [5]:

$$S = -\int \rho(r) \ln [\rho(r)] dr.$$  

(3)

The index $q$ is usually used as a fitting parameter in case of systems that are not well enough understood.

It is known that $S_q$, as $S$, is a basic quantity measuring the expected amount of information contained in the probability distribution in respected space. In other words, it gives a complete description of the
localization-delocalization characters of the atomic system. In Ref [6] the Tsallis entropies, of the Rydberg quantum states of hydrogenic systems in the $D$-dimensional ($D > 1$), are elegantly analytically determined in the $r$ - space. The solution includes the lower terms of $q$ .

In addition to the application of nonadditive entropy in different fields [2-4], we are going to apply it in atomic systems. In doing so, let us consider two probabilistically independent and isolated systems $A$ and $B$ System $A$ has the Coulombic potential (CP), $-Z/r$, and system $B$ has the Yukawa potential (YP) [7, 8], $-Z e^{-\mu r}/r$. In the case when the two systems are merged with each other, they form a new combined system $C$, which interacts with the Hellmann potential (HP) [9-11]. The Hellmann potential (HP) consists of a summation of CP and YP as:

$$V(r) = -Z \left( \frac{e^{-\mu r}}{r} + \frac{1}{r} \right),$$  

where $Z$ is the nuclear charge and $\mu$ is the screening parameter.

It is our aim to numerically calculate $S_q$, in position ($r$ -) and momentum ($p$ -) spaces, and consequently calculate the $q$ - values that satisfies the nonadditive relation, Eq. (2). The numerical calculation will be done using the J-matrix method [12-14] for different values of $\mu$, where $\mu << \mu_c$. $\mu_c$ is defined as the critical value of the screening parameter, and above which no bound states exist. For example, for YP it was found that $\mu_c (YP) = 1.18$.

The structure of our work is the following: First, in Section 2, we briefly review the constructing of the implemented wavefunctions using J-matrix method. The wavefunctions and their squares, $|\Psi(r)|^2$, are calculated in the position and momentum spaces. Second, our numerical results of the scaling and the uncertainty properties of the $r$ - and $p$ - space for the Tsallis entropy are presented in Section 3. Finally, some concluding remarks of our results are accessible in Section 4.

2. Background theory

It is understood that $\rho(r)$ is important in calculating the information entropies. Thus, in incorporating the J-matrix method to calculate $\rho(r)$, we start with $\rho(r)$ of the stationary and nonrelativistic quantum systems as:

$$\rho(r) = |\Psi(r)|^2,$$

that fulfill the normalization condition,

$$\int \rho(r) d\mathbf{r} = 1.$$  

The wave functions $\{\Psi(r)\}$ in (5) are the bounded solutions of the Schrödinger equation.

Symbolically, the nonrelativistic Schrödinger wave equation (in atomic units) is written in the form:

$$\hat{H} \Psi(r) = \left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{2r^2} + \frac{Z}{r} + \hat{V}(r, A, \cdots) \right] \Psi(r) = E \Psi(r)$$

where $\hat{H}$ is the full Hamiltonian, $\{E\}$ are the associated eigenvalues, and $\hat{V}(r, A, \cdots)$ is the used potential with parameters $A, \cdots$, which will be suppressed in the following discussion for simplicity. The suppressed parameters have critical values above which no bound states exist.
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In spherical coordinates $(r,\theta,\varphi)$, the eigenfunction $\Psi(r)$ is defined as:

$$\Psi(r) = R_n^\ell(r)Y_{\ell,m}(\theta,\varphi),$$

where $R_n^\ell(r)$ is the eigenfunction of the nonrelativistic radial Schrödinger equation:

$$\hat{H}R_n^\ell(r) = \left[ \hat{H}_o + \hat{V}(r) \right] R_n^\ell(r) = E_n^\ell R_n^\ell(r)$$

and $Y_{\ell,m}(\theta,\varphi)$ is the spherical harmonics, with $\ell = 0,1,2,3,\cdots$ and $m = -\ell,-\ell+1,\cdots,0,\cdots,\ell-1,\ell$. In Eq(9), $E_n^\ell$ are the eigenvalues of $\hat{H}$, and $\hat{H}_o$ is the reference Hamiltonian.

To find the Harries eigenvalues and radial function $R_n^\ell(r)$, we used the following procedure:

(i) The full Hamiltonian $\hat{H}$ is divided into two parts:

1. The reference Hamiltonian $\hat{H}_o = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2r^2} + \frac{Z}{r}$ and
2. The potential $V \equiv V(r)$

(ii) An appropriate $L^2$ basis, $\{\varphi_n^\ell(\lambda r)\}_{n=0}^{N-1}$, is used to construct the $(\hat{H}_o)$-matrix. Here, $N$ is the dimension of the matrix, and $\lambda$ is a positive length scale parameter. In Laguerre basis set, we define:

$$\varphi_n^\ell(\lambda r) = a_n^\ell(\lambda r) e^{-\lambda r/2}L_n^{2\ell+1}(\lambda r); \quad n = 0,1,2,\cdots N-1$$

where $L_n^{2\ell+1}(\lambda r)$ is the associated Laguerre orthogonal polynomial and $a_n^\ell = \sqrt{\lambda \Gamma(n+1)\Gamma(n+2\ell+2)}$ is the normalization constant, with the 3-term recursion relation for the coefficient of $L_n^{2\ell+1}(x = \lambda r)$, will transfer the reference Hamiltonian $\hat{H}_o$ into tridiagonal matrix form.

(iii) The potential matrix elements $(V)_{nm}$

$$V_{nm} = \lambda^{-1} a_n^\ell a_m^\ell \int_0^\infty x^\ell e^{-\lambda x}L_n^\ell(x)L_m^\ell(x) xV(x/\lambda) dx$$

are calculated numerically using the Gauss quadrature method.

(iv) The full Hamiltonian matrix elements are computed: $(H) = (H_o) + (V)$, or

$$H_{nm} \equiv \begin{cases} (H_o)_{nm} + (V)_{nm} & ; \quad n,m \leq N-1 \\ (H_o)_{nm} & ; \quad n,m > N-1 \end{cases}$$

(v) Finally, the finite Hamiltonian matrix $(N \times N)$ is diagonalised to obtain the eigenvalues $E_n^\ell$ for all $n$, and the corresponding eigenvectors $\{\Omega_n^0,\Omega_n^1,\cdots,\Omega_n^{N-1}\}$ each of dimension $(1 \times N)$ in our matrix, which is called J-matrix, in the function space.

(vi) The above operation results in a set of discrete bound states $(E < 0)$ and a set of discrete points mimicking the continuum.

(vii) With increasing $N$, the stability of the calculations increases.
In our calculation, we need to have \( R'_n(r) \) in the \( r \)-space, rather than the function space \( \phi'_n(r) \). To do so, the wavefunction \( R'_n(r) \), could be constructed by the expansion:

\[
R'_n(r) = \sum_{m=0}^{N-1} Q_{nm}^l \phi'_m(r)
\]  

(13)

Thus, \( \rho(r) \) of the \( n/l/m \)-state can be written as:

\[
\rho(r) = |\Psi(r)|^2 = \rho_{n,l}(r) \rho_{l,m}(\theta, \varphi) = |R'_n(r)|^2 |Y_{l,m}(\theta, \varphi)|^2
\]  

(14)

In \( p \)-space, to formulate the density \( \gamma(p) \), we have to apply the Fourier transformation to \( \Psi(r) \) in spherical coordinates, i.e.

\[
\Psi(p) = \int e^{i \mathbf{p} \cdot \mathbf{r}} \Psi(r) dr; \quad \gamma(p) = |\Psi(p)|^2.
\]  

(15)

Consequently, we have replaced, in Eq. (5), the subscript \( r \) by \( p, \rho(p) \) by \( \gamma(p) \), integrate and use the normalization condition \( \int \gamma(p) dp = 1 \). Using the definitions of \( \rho(p) \) and \( \gamma(p) \) one can calculate the \( S_q(r) \) and \( S_q(p) \) in the \( r \)- and \( p \)- spaces; respectively.

With the information of \( S_q(r) \) and \( S_q(p) \), we can check the BBM-expression [15], which is given in the three dimensional form as:

\[
S_{total} = S_1(r) + S_1(p) \geq 3(1 + \ln \pi).
\]  

(16)

Eq. (16) represents the relation of the total entropy to the summation of entropies \( S_1(r) \) and \( S_1(p) \).

3. Results and discussion

Table 1 shows, for YP and HP, the variation of the energy eigenvalues and the Tsallis entropy \( S_q \) as a function of \( \mu \), for the 1s-state of the hydrogen atom \( Z = 1 \) in \( r \)- and \( p \)- spaces. For CP [16], where \( \mu = 0 \), the analytical value \( S_1 = 4.1447 \) in the \( r \)- space and \( S_1 = 2.4217 \) in the \( p \)-space.

According to our calculations, from Tables 1, it was found that

\[
S_q(HP) \neq S_q(CP) + S_q(YP).
\]  

(17)

Eq. (17) implies that the Tsallis entropy for Hellmann potential are not additive property of CP and YP, for all values of \( \mu \). Consequently, we will modify Eq. (2) to have the form:

\[
S_q(HP) = S_q(CP) + S_q(YP) + (1 - q') S_q(CP) S_q(YP),
\]  

(18)

and we are going to calculate the value of \( q' \) which satisfy the above equation. In Table 1 and for \( q = 1 \), the value of \( q' \), as a function of \( \mu \), are calculated for the constrain that satisfy by the Eq. (18). The values of \( q' \) are given in the last column in each space. It is noticed that \( q' \) decrease as \( \mu \) increases. The value of \( q' > 1 \) indicates the strong correlations of \( S_q \) in the given system with respect to \( q \) and \( \mu \).

The values given in Table 1 present the following observations:

1. For both YP and HP, the last two columns offer the BBM-expression, that given by Eq(16)The expression \( S_{total} > 6.4342 \), is fulfilled for all values of \( \mu \).

2. Regarding \( S_q \), it goes to Shannon entropy \( S \) as \( q \rightarrow 1 \), which is proven numerically in our case. To facilitate easy comparison, the Shannon entropies have been given in the table.
3. With the meaning of $S_1$, localization-delocalization of $\rho(r)$ corresponds to the smaller-larger values of the $S_1$, which means the delocalization of $\rho(r)$ increases with increasing $\mu$, as shown clearly in table 1.

4. With increasing $\mu$, the $q'$ value decreases from 1.36 to 1.34 in the case of the $r$-space, and decreases from 1.06 to 0.99 in the case of the $p$-space. This implies the correlation is large in the position space but not in momentum space.

5. In the range $\mu = 0$ to 0.5, the values of $S_1$ are additive in the $p$-space, but not in the $r$-space.

Table 1: For YP and HP, the values of the eigenvalues $(-E)$ and Tsallis entropy $S_1$ for the 1s-state of the hydrogen atom ($Z = 1$) in $r$- and $p$-spaces, are given for six values of $\mu$. The Shannon entropies, $S$ [14, 16], were given for comparison.

| $\mu$ | $E$ | $q'$ | $S$ | $E$ | $q'$ | $S$ |
|-------|-----|------|-----|-----|------|-----|
| 0.0   | 4.1447 | 2.0639 | 1.36 | 2.4219 | 4.4994 | 1.06 |
| 0.0   | 0.4071 | 1.9036 | 0.5  | 2.0656 | 6.5666 | 6.5633 |
| 0.0   | 4.1713 | 2.0700 | 1.36 | 2.3974 | 4.4963 | 1.06 |
| 0.0   | 0.4728 | 1.9131 | 0.5  | 2.0656 | 6.5666 | 6.5633 |
| 0.0   | 4.2435 | 2.0793 | 1.36 | 2.3326 | 4.4876 | 1.05 |
| 0.0   | 4.2424 | 2.0793 | 1.36 | 2.3333 | 4.4894 | 1.05 |
| 0.0   | 4.3539 | 2.0945 | 1.36 | 2.2323 | 4.4742 | 1.03 |
| 0.0   | 4.3528 | 2.0941 | 1.36 | 2.3223 | 4.4761 | 1.03 |
| 0.0   | 4.5042 | 2.1136 | 1.35 | 2.0958 | 4.4568 | 1.01 |
| 0.0   | 4.5030 | 2.1132 | 1.35 | 2.0962 | 4.4587 | 1.01 |
| 0.0   | 0.1984 | 1.6532 | 0.1984 | 1.6532 |
| 0.0   | 4.6981 | 2.1350 | 1.34 | 1.9187 | 4.4366 | 0.99 |
| 0.0   | 4.6965 | 2.1238 | 1.34 | 1.9191 | 4.4378 | 0.99 |

The quadratic equations for $S_1$ as a function of $\mu$, for YP and HP in the $r$-space, and their corresponding correlation coefficient $R^2$, are given as follows:

$$S_1(YP, r) = 4.1807\mu^2 + 0.5456\mu + 4.1457, \quad R^2 = 0.9642$$
$$S_1(HP, r) = 0.2928\mu^2 + 0.0147\mu + 2.0639, \quad R^2 = 0.9955$$

In the $p$-space, the quadratic equations, and their corresponding correlation coefficient $R^2$, are given as follows:
The values of $S_1$ for HP are higher than the values of $S_1$ in YP. In both $r$- and $p$- spaces the values of $S_1$ for HP are almost constant and the deviation of $S_1$ for YP at $\mu = 0.5$ is small because we are far from the critical point $\mu_c = 1.18$.

The values of $qSr$, for both YP and HP at different $\mu$ are shown in Table 2.

Table 2 shows the following: for fixed $\mu$, $qSr$ monotonically decreases as the $q$ increases. This behavior indicates that the quantities with the lowest orders are most important for the quantification of the delocalized of $r$ of the system. For fixed $\mu$, $q > 1$, $qSr$ stays constant for all values of $\mu$. This behavior should be expected since the definition of $S_q$ in Eq.1 is a continuous and non-increasing function in $q$.

Moreover, from our study for 1s-state of the hydrogen atom ($Z = 1$) with $\mu = 0.1$ in both YP and HP, the scaling equations that covers the dependence of $S_q(r)$ on $q$ are given in the form:

$$S_q(YP, r) = 3.740q^{-1.752}.$$  
$$S_q(HP, r) = 2.051q^{-1.544}.$$  

For both cases, the correlation coefficient is $R^2 = 0.99$. Equation (21) shows that the values of $S_q$ for HP are smaller than the values $S_q$ of YP for $q = 1, 2$ and 3. The two values start to match with each other for the higher values of $q$, $q > 4$.

4. Conclusion

We have conveyed the outcomes of our numerical studies of Tsallis entropy for 1s-state of the hydrogen atom ($Z = 1$) in the cases CP, YP and HP. The J-matrix method is implemented for the mentioned potentials in spherical coordinates. Many distinctive features have been realized in the case of this study. For example, it was found that the summation of the entropy in $r$ - and $p$ - spaces of the Tsallis entropy fulfills the BBM expression. The scaling laws for the calculated Tsallis entropy are given as a function of the parameters $q$ and $\mu$. The scaling laws clearly show the correlation between the calculated quantities...
and the mentioned parameters. For the given values of $\mu$, it was found that the values of $S_1$ are additive in the $p$-space, but not in the $r$-space. In view of our discussions, it is hoped that this opening study of the nonadditive entropy will motivate stimulating studies, theoretically and experimentally, with other combined potentials in the atomic field.

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