

Position and Momentum Information-Theoretic Measures of the Pseudoharmonic Potential

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In this study, the information-theoretic measures in both the position and momentum spaces for the pseudoharmonic potential using Fisher information, Shannon entropy, Renyi entropy, Tsallis entropy, and Onicescu information energy are investigated analytically and numerically. The results obtained are applied to some diatomic molecules. The Renyi and Tsallis entropies are analytically obtained in position space using Srivastava–Niukkanen linearization formula in terms of the Lauricella hypergeometric function. Also, they are obtained in the momentum space in terms of the multivariate Bell polynomials of Combinatorics. We observed that the Fisher information

increases with n in both the position and momentum spaces, but decreases with ℓ for all the diatomic molecules considered. The Shannon entropy also increases with increasing n in the position space and decreases with increasing ℓ . The variations of the Renyi and Tsallis entropies with ℓ are also discussed. The exact and numerical values of the Onicescu information energy are also obtained, after which the ratio of information-theoretic impetuses to lengths for Fisher, Shannon, and Renyi are obtained. © 2015 Wiley Periodicals, Inc.

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Introduction

Information-theoretic methods have been used extensively to study various systems in Communications,^[1] Physics,^[2,3] Chemistry,^[4–6] and Biology.^[7,8] The various information-theoretic quantities such as Shannon entropy, Fisher information, Renyi entropy, Tsallis entropy, Onicescu information energy have been discussed for different quantum mechanical systems.^[9–19] An interesting and simple method has been used to obtain Fisher information, Shannon, Onicescu, and Tsallis entropies in atoms as functions of the atomic number Z in Ref. [8]. Fractional occupation probabilities of electrons in atomic orbitals were used, instead of the more complicated continuous electron probability densities.

The information-theoretic quantities have also been discussed using scaling properties of the systems.^[15–18,20,21] The relativistic effect have also been considered in the study of the information-theoretic quantities.^[22–27] The Shannon entropy $S[\rho]$ of the electron density, $\rho(\mathbf{r})$, in the coordinate space is defined as^[28,29]

$$S[\rho] = - \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r}, \quad (1)$$

and the corresponding momentum space Shannon entropy $S[\gamma]$ is given by

$$S[\gamma] = - \int \gamma(\mathbf{p}) \ln \gamma(\mathbf{p}) d\mathbf{p}, \quad (2)$$

where $\gamma(\mathbf{p})$ denotes the momentum density. The Shannon entropy measures the uncertainty in the localization of a particle in space.^[9]

The Fisher information is defined in the position space as^[10]

$$I[\rho] = \int \frac{[\nabla \rho(\mathbf{r})]^2}{\rho(\mathbf{r})} d\mathbf{r}, \quad (3)$$

and the corresponding momentum space measure is given by^[22]

$$I[\gamma] = \int \frac{[\nabla \gamma(\mathbf{p})]^2}{\gamma(\mathbf{p})} d\mathbf{p}. \quad (4)$$

The Fisher information in the position space measures the narrowness and the oscillation nature of the probability distribution.^[30]

The Onicescu information energy is defined in the position and momentum spaces, respectively, as^[31]

$$E[\rho] = \int \rho^2(\mathbf{r}) d\mathbf{r}, \quad (5)$$

and

$$E[\gamma] = \int \gamma^2(\mathbf{p}) d\mathbf{p}. \quad (6)$$

The greater the information energy, the more concentrated is the probability distribution, while the information content decreases.^[31] The Renyi position entropy defined as^[11,12,14,32]

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$$R_q[\rho] = \frac{1}{1-q} \log \left[\int \rho(\mathbf{r})^q d\mathbf{r} \right] \quad 0 < q < \infty, q \neq 1, \quad (7)$$

is a generalization of the Shannon entropy. The Renyi entropy in the momentum space is also given as

$$R_q[\gamma] = \frac{1}{1-q} \log \left[\int \gamma(\mathbf{p})^q d\mathbf{p} \right] \quad 0 < q < \infty, q \neq 1. \quad (8)$$

The Tsallis entropy is defined in the position and momentum spaces, respectively, as^[16,18,20,33–35]

$$T_q[\rho] = \frac{1}{q-1} \left(1 - \int \rho(\mathbf{r})^q d\mathbf{r} \right) \quad (9)$$

and

$$T_m[\gamma] = \frac{1}{m-1} \left(1 - \int \gamma(\mathbf{p})^m d\mathbf{p} \right), \quad \frac{1}{q} + \frac{1}{m} = 2. \quad (10)$$

It is important to state that the information theoretical entropic measures described in this work can be used as descriptors of chemical reactivity of molecules.^[30,36,37] The model potentials can be used to simulate the reactivity using information theoretical tools to avoid tedious calculations in those chemical reactions. Suitability testing of the model potentials in describing the bonding in a chosen set of diatomic molecules in terms of the various information theoretical measures is essential.^[38,39]

Apart from the descriptors of chemical reactivity, the information theoretical measures (both global and local) presented, have been found useful in comparing the quantum molecular similarity. In this case, such studies provide valuable knowledge about the interactive information contributing to the molecular drug design.^[40,41]

The information theoretical measures based on the model potential (pseudoharmonic potential) considered in this work have been tested (numerically). The results obtained are found to rigorously satisfy all the characteristic features of information theory paving the way for future studies of chemical reactivity.

The pseudoharmonic potential has been very useful in the area of chemical physics and it has been extensively used to describe interaction of some diatomic molecules as its introduction.^[42–47] This potential is used to describe the roto-vibrational states of diatomic molecules and nuclear rotations and vibrations.^[15] The pseudoharmonic potential can be written as^[42]

$$V(r) = D_e \left(\frac{r}{r_e} - \frac{r_e}{r} \right)^2, \quad (11)$$

where D_e is the dissociation energy between two atoms in a solid and r_e is the equilibrium intermolecular separation. The radial part of the Schrödinger equation for the pseudoharmonic potential is written as $(\hbar = \mu = 1)$ ^[42]:

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \left[2E - 2 \left(\frac{D_e r^2}{r_e^2} + \frac{D_e r_e^2}{r^2} - 2D_e \right) - \frac{\ell(\ell+1)}{r^2} \right] \right\} R_{n,\ell}(r) = 0. \quad (12)$$

By solving Eq. (12), Oyewumi and Sen obtained the wave function as^[42]

$$R_{n,\ell}(r) = N_{n,\ell} r^{\gamma_\ell} e^{-\lambda r^2} L_n^{\gamma_\ell + \frac{1}{2}}(2\lambda r^2), \quad (13)$$

where

$$\gamma_\ell = \frac{1}{2} \left[-1 + \sqrt{(2\ell+1)^2 + 8D_e r_e^2} \right], \quad \lambda = \sqrt{\frac{D_e}{2r_e^2}}, \quad (14)$$

$$N_{n,\ell} = \left[\frac{2(2\lambda^2)^{\frac{1}{2}(2\gamma_\ell+3)} n!}{\Gamma(n+\gamma_\ell+\frac{3}{2})} \right]^{\frac{1}{2}}.$$

The wave function in Eq. (13) is the position space wave function. The momentum space wave function is obtained as

$$R_{n,\ell}(p) = \left[\frac{2n!(2\lambda^2)^{-\frac{1}{2}(2\gamma_\ell+3)}}{\Gamma(n+\gamma_\ell+\frac{3}{2})} \right]^{\frac{1}{2}} p^{\gamma_\ell} e^{-\frac{p^2}{2\lambda}} L_n^{\gamma_\ell + \frac{1}{2}}\left(\frac{p^2}{2\lambda}\right). \quad (15)$$

The probability densities in the position space and the momentum space are therefore written, respectively, as

$$\rho(r) = N_{n,\ell}^2 r^{2\gamma_\ell} e^{-2\lambda r^2} \left[L_n^{\gamma_\ell + \frac{1}{2}}(2\lambda r^2) \right]^2 \quad (16)$$

and

$$\gamma(p) = \frac{2n!(2\lambda)^{-\frac{1}{2}(2\gamma_\ell+3)}}{\Gamma(n+\gamma_\ell+\frac{3}{2})} p^{2\gamma_\ell} e^{-2\frac{p^2}{\lambda}} \left[L_n^{\gamma_\ell + \frac{1}{2}}\left(\frac{p^2}{2\lambda}\right) \right]^2. \quad (17)$$

In this article, we shall study the pseudoharmonic potential using the information-theoretic measures defined above. The article is organized as follows. In Section 2, the Fisher information and Shannon entropy for the pseudoharmonic potential are obtained. Section 3 contains the Renyi entropy, Tsallis entropy and Onicescu information for the pseudoharmonic potential. The information theoretic lengths and impetuses are discussed in Section 4, while the Conclusion is given in the last Section.

Fisher Information and Shannon Entropy for the Pseudoharmonic Potential

Fisher information for the pseudoharmonic potential

From Eq. (3), the Fisher information in the position space can be written as

$$I[\rho] = 4\pi \int_0^\infty \frac{r^2}{\rho(r)} \left(\frac{\partial \rho}{\partial r} \right)^2 dr, \quad (18)$$

where $\rho(r)$ is given in Eq. (16). The integral in Eq. (18) is obtained, after some manipulations, as

$$I[\rho] = \frac{2^{(13-2\gamma_\ell)/4} \pi \lambda}{1+2\gamma_\ell} [(4n+3) + (8n+4)\gamma_\ell]. \quad (19)$$

In the momentum space, the Fisher information is

$$I[\gamma] = 4\pi \int_0^\infty \frac{p^2}{\gamma(p)} \left(\frac{\partial \gamma}{\partial p} \right)^2 dp, \quad (20)$$

where $\gamma(p)$ is as given in Eq. (17). For ground state ($n=0, \ell=0$), Eq. (20) is obtained as

Table 1. Spectroscopic constants of some diatomic molecules.

Molecular state	D_e (eV)	r_e (Å)
$\text{Na}_2 : X^1\Sigma_g^+$	0.746707167	3.079
$\text{Cl}_2 : X^1\Sigma_g^+$	2.513903386	1.987
$\text{O}_2^+ : X^2\Sigma_g^+$	6.780447246	1.116
$\text{N}_2^+ : X^2\Sigma_g^+$	8.848131541	1.116
$\text{NO}^+ : X^1\Sigma^+$	10.99665353	1.063

$$I[\gamma] = \frac{2^{(7-6\gamma_0)/4} \pi (3+4\gamma_0)}{\lambda(1+2\gamma_0)}. \quad (21)$$

The Fisher information for the pseudoharmonic potential is obtained for some diatomic molecules, the results are given in Tables 2 and 3. The values of the dissociation energy D_e and equilibrium intermolecular separation r_e of the diatomic molecules used in this work are given in Table 1, these are obtained from Refs. [42, 47–51]. It can be observed from Tables 2 and 3 that the Fisher information (both in the position and momentum spaces) increase with n for the diatomic molecules considered.

The variations of the Fisher information with orbital angular momentum ℓ are shown in Figure 1 with $n=0$ for five selected diatomic molecules. It is observed from Figure 1 that the Fisher information in the position space decreases with increasing ℓ . The values of the Fisher information for all the diatomic molecules considered tend to 0 for $\ell \gg 1$.

The Shannon entropy of the pseudoharmonic potential

Using Eq. (16), the position space Shannon entropy

$$S[\rho] = -4\pi \int_0^\infty r^2 \rho(r) \ln \rho(r) dr, \quad (22)$$

is obtained as^[9,52]

$$S_{n,\ell}[\rho] = 2n + \gamma_\ell + \frac{3}{2} - \ln \left(\frac{2n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right) - \gamma_\ell \psi \left(n + \gamma_\ell + \frac{3}{2} \right) - \frac{3}{2} \ln(2\lambda) + E \left(\tilde{L}_n^{\gamma_\ell + \frac{1}{2}} \right), \quad (23)$$

where

$$E \left(\tilde{L}_n^{\gamma_\ell + \frac{1}{2}} \right) = \int_0^\infty t^{\gamma_\ell + \frac{1}{2}} e^{-t} \left[\tilde{L}_n^{\gamma_\ell + \frac{1}{2}}(t) \right]^2 \ln \left[\tilde{L}_n^{\gamma_\ell + \frac{1}{2}}(t) \right]^2 dt \quad (24)$$

is the entropic integral of the orthonormal Laguerre polynomials, which can be obtained in one dimension as^[9]

$$E \left(\tilde{L}_n^{\gamma_\ell + \frac{1}{2}} \right) = -2n + \left(\gamma_\ell + \frac{3}{2} \right) \ln n - \left(\gamma_\ell + \frac{1}{2} \right) - 2 + \ln(2\pi) + o(1). \quad (25)$$

The momentum space Shannon entropy

$$S[\gamma] = -4\pi \int_0^\infty r^2 \gamma(p) \ln \gamma(p) dp, \quad (26)$$

is obtained as^[9,52]

Table 2. Fisher information measure for the pseudoharmonic potential for some diatomic molecules with $\ell=0$ in the position space.

n	$I[\rho](\text{Na}_2)$	$I[\rho](\text{Cl}_2)$	$I[\rho](\text{O}_2^+)$	$I[\rho](\text{N}_2^+)$	$I[\rho](\text{NO}^+)$
0	4.03449	8.95359	29.6189	27.4679	29.0007
1	11.6049	25.9150	85.4832	79.6411	84.2456
2	19.1753	42.8764	141.348	131.814	139.490
3	26.7456	59.8378	197.212	183.987	194.735
4	34.3160	76.7992	253.076	236.161	249.980
5	41.8864	93.7605	308.941	288.334	305.225
6	49.4568	110.722	364.805	340.507	360.470
7	57.0272	127.683	420.669	392.680	415.715
8	64.5976	144.645	476.534	444.853	470.960
9	72.1680	161.606	532.398	497.026	526.204
10	79.7383	178.567	588.262	549.199	581.449

The unit of the square of $I[\rho]$ is $\text{eV}/(\text{\AA})^2$.

$$S_{n,\ell}[\gamma] = 2n + \gamma_\ell + \frac{3}{2} - \ln \left(\frac{2n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right) - \gamma_\ell \psi \left(n + \gamma_\ell + \frac{3}{2} \right) + \frac{3}{2} \ln(2\lambda) + E \left(\tilde{L}_n^{\gamma_\ell + \frac{1}{2}} \right). \quad (27)$$

Table 4 contains the numerical values of the Shannon entropy in the position space by making use of Eq. (22). We observe that the Shannon entropy in the position space increases with n . The numerical values of the Shannon entropy in the momentum space are shown in Table 5. The variations of the Shannon entropy with ℓ are shown in the Figure 2 for the diatomic molecules considered. We observe that the Shannon entropy $S[\rho]$ decreases with ℓ and tend to zero for large ℓ .

Renyi Entropy, Tsallis Entropy, and Onicescu Information Energy for the Pseudoharmonic Potential

In this section, we shall calculate the Renyi entropy, Tsallis entropy, and Onicescu information energy for the pseudoharmonic potential in the position and momentum spaces.

Renyi entropy in position space

The Renyi entropy for the pseudoharmonic potential is written in the position space as

Table 3. Fisher information measure for the pseudoharmonic potential for some diatomic molecules with $\ell=0$ in the momentum space.

n	$I[\gamma](\text{Na}_2)$	$I[\gamma](\text{Cl}_2)$	$I[\gamma](\text{O}_2^+)$	$I[\gamma](\text{N}_2^+)$	$I[\gamma](\text{NO}^+)$
0	3.68815	0.62866	0.30859	0.14658	0.09247
1	11.9955	2.28850	1.06359	0.55325	0.36408
2	24.5468	5.10871	2.27526	1.27083	0.86499
3	40.6289	9.05928	3.89987	2.30608	1.61329
4	59.5473	14.0403	5.87902	3.64230	2.60660
5	80.7177	19.9301	8.15580	5.25260	3.83137
6	103.670	26.6080	10.6799	7.10709	5.26891
7	128.032	33.9629	13.4085	9.17643	6.89883
8	153.505	41.8964	16.3058	11.4334	8.70091
9	179.852	50.3228	19.3421	13.8535	10.6560
10	206.884	59.1681	22.4924	16.4150	12.7465

The unit of the square of $I[\gamma]$ is $(\text{\AA})^2/\text{eV}$.

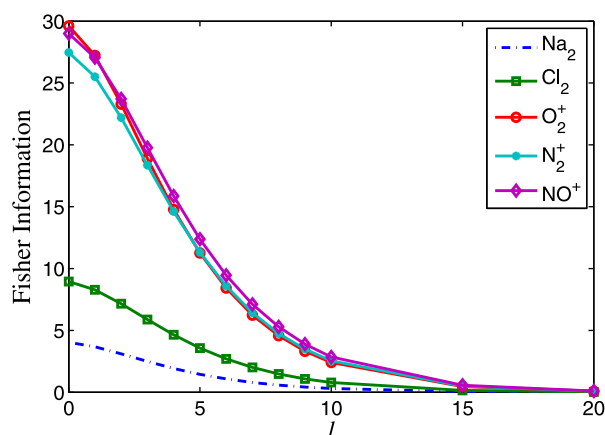


Figure 1. Variation of the Fisher information measure in the position space ($I[\rho]$) with ℓ for Na_2 , Cl_2 , O_2^+ , N_2^+ , and NO^+ .

$$R_q[\rho] = \frac{1}{1-q} \log W_q[\rho], \quad (28)$$

where

$$W_q[\rho] = 4\pi \int_0^\infty r^2 \rho(r)^q dr. \quad (29)$$

If we let $2\lambda r^2 = x$, then $W_q[\rho]$ can be written as

$$W_q[\rho] = \frac{2\pi N_{n,\ell}^{2q}}{(2\lambda)^{q\gamma_\ell + \frac{3}{2}}} \int_0^\infty x^{q\gamma_\ell + \frac{1}{2}} e^{-qx} \left[L_n^{\gamma_\ell + \frac{1}{2}}(x) \right]^{2q} dx = \frac{2\pi N_{n,\ell}^{2q}}{(2\lambda)^{q\gamma_\ell + \frac{3}{2}}} F_q[\rho]. \quad (30)$$

To calculate the integral $F_q[\rho] = \int_0^\infty x^{q\gamma_\ell + \frac{1}{2}} e^{-qx} \left[L_n^{\gamma_\ell + \frac{1}{2}}(x) \right]^{2q} dx$, we make use of the linearization formula of Srivastava-Niukkanen for the products of various Laguerre polynomials given by^[19,53,54]

$$x^\mu L_{m_1}^{(\alpha_1)}(t_1 x) \dots L_{m_r}^{(\alpha_r)}(t_r x) = \sum_{k=0}^\infty \Theta_k(\mu, \beta, r, m_i, \alpha_i, t_i) L_k^{(\beta)}(x), \quad (31)$$

where

n	$S[\rho](\text{Na}_2)$	$S[\rho](\text{Cl}_2)$	$S[\rho](\text{O}_2^+)$	$S[\rho](\text{N}_2^+)$	$S[\rho](\text{NO}^+)$
0	12.4333	7.58285	4.73017	4.07721	3.56137
1	13.5554	8.41921	5.69732	4.83464	4.23386
2	14.3281	8.99397	6.36283	5.35458	4.69475
3	14.9377	9.44880	6.88877	5.76628	5.05992
4	15.4466	9.83007	7.32886	6.11179	5.36671
5	15.8856	10.1602	7.70925	6.41130	5.63298
6	16.2725	10.4522	8.04514	6.67647	5.86899
7	16.6188	10.7145	8.34633	6.91483	6.08136
8	16.9326	10.9527	8.61959	7.13156	6.27465
9	17.2196	11.1711	8.86983	7.33042	6.45214
10	17.4841	11.3729	9.10074	7.51422	6.61633

Table 5. The Shannon entropy for the pseudoharmonic potential for some diatomic molecules with $\ell=0$ in the momentum space.

n	$S[\gamma](\text{Na}_2)$	$S[\gamma](\text{Cl}_2)$	$S[\gamma](\text{O}_2^+)$	$S[\gamma](\text{N}_2^+)$	$S[\gamma](\text{NO}^+)$
0	0.316484	0.257021	0.438126	0.269701	0.214067
1	0.581714	0.632060	1.066130	0.737227	0.619039
2	0.699930	1.006880	1.698210	1.287190	1.130940
3	0.677853	1.314390	2.237290	1.826600	1.666120
4	0.557843	1.534280	2.656090	2.304790	2.169300
5	0.382078	1.671710	2.962040	2.703120	2.612640
6	0.181821	1.741740	3.174780	3.021470	2.987110
7	-0.022832	1.760900	3.315330	3.268260	3.294360
8	-0.220225	1.743700	3.401900	3.454700	3.541080
9	-0.404298	1.701700	3.448900	3.591960	3.735720
10	-0.572438	1.643560	3.467290	3.689930	3.886720

$$\Theta_k(\mu, \beta, r, m_i, \alpha_i, t_i) = (\beta+1)_\mu \binom{\alpha_1+m_1}{m_1} \dots \binom{\alpha_n+m_n}{m_n} \times F_A^{(r+1)}[\beta+\mu+1, -m_1, \dots, -m_n, -k; \alpha_1+1, \dots, \alpha_n+1, \beta+1; t_1, \dots, t_n, 1], \quad (32)$$

in terms of Lauricella's hypergeometric functions of $(r+1)$ variables. The Pochhammer symbol $(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}$ and the binomial

number $\binom{a}{b} = \frac{\Gamma(a+1)}{\Gamma(b+1)\Gamma(a-b+1)}$. For the special case $\beta=0, \alpha_1 = \dots = \alpha_r = \gamma_\ell + \frac{1}{2}, m_1 = \dots = m_r = n, x = qt, t_1 = \dots = t_r = \frac{1}{q}, \mu = q\gamma_\ell + \frac{1}{2}, r = 2q$, this general relation yields the following results

$$(qt)^{q\gamma_\ell + \frac{1}{2}} \left[L_n^{\gamma_\ell + \frac{1}{2}}(t) \right]^{2q} = \sum_{k=0}^\infty \Theta_k\left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q}\right) L_k^{(0)}(qt), \quad (33)$$

where

$$\Theta_k\left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q}\right) = \Gamma\left(q\gamma_\ell + \frac{3}{2}\right) \binom{n+\gamma_\ell + \frac{1}{2}}{n}^{2q} \times F_A^{(2q+1)}\left[q\gamma_\ell + \frac{3}{2}, -n, \dots, -n, -k; \gamma_\ell + \frac{3}{2}, \dots, \gamma_\ell + \frac{3}{2}, 1; \frac{1}{q}, \dots, \frac{1}{q}, 1\right]. \quad (34)$$

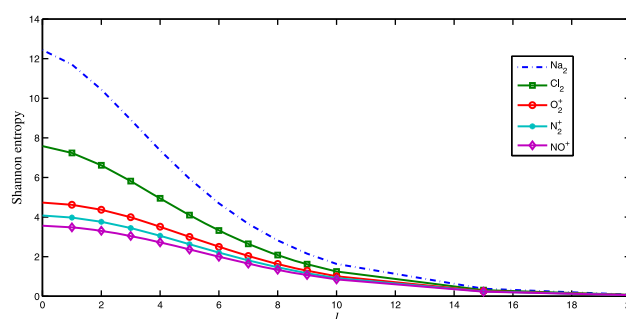


Figure 2. Variation of the Shannon entropy in the position space $S[\rho]$ with ℓ for Na_2 , Cl_2 , O_2^+ , N_2^+ , and NO^+ .

Table 6. Numerical values of the Renyi entropy for the pseudoharmonic potential in the position space for some diatomic molecules with $q = 2$ and $\ell = 0$.

n	$R_2[\rho](\text{Na}_2)$	$R_2[\rho](\text{Cl}_2)$	$R_2[\rho](\text{O}_2^+)$	$R_2[\rho](\text{N}_2^+)$	$R_2[\rho](\text{NO}^+)$
0	4.13494	3.20296	1.27924	1.60833	1.62971
1	4.47401	3.53567	1.61492	1.93919	1.95852
2	4.66934	3.72714	1.80821	2.12949	2.14751
3	4.80869	3.86388	1.94620	2.26543	2.28254
4	4.91756	3.97088	2.05410	2.37185	2.38829
5	5.00708	4.05900	2.14290	2.45953	2.47546
6	5.08315	4.13400	2.21842	2.53419	2.54972
7	5.14932	4.19932	2.28415	2.59923	2.61444
8	5.20788	4.25719	2.34236	2.65688	2.67182
9	5.26040	4.30915	2.39459	2.70865	2.72337
10	5.30801	4.35629	2.44196	2.75564	2.77018

By considering $F_q[\rho]$, Eq. (33) and the orthogonality relation of the Laguerre polynomials, one finds that only the term with $k = 0$ gives a nonvanishing contribution to the summation in Eq. (33), so that

$$F_q[\rho] = \frac{1}{q\gamma_\ell + \frac{3}{2}} \Theta_0\left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q}\right), \quad (35)$$

where

$$\Theta_0\left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q}\right) = \Gamma\left(q\gamma_\ell + \frac{3}{2}\right) \binom{n + \gamma_\ell + \frac{1}{2}}{n}^{2q} \times F_A^{(2q+1)}\left[q\gamma_\ell + \frac{3}{2}, -n, \dots, -n, 0; \gamma_\ell + \frac{3}{2}, \dots, \gamma_\ell + \frac{3}{2}, 1; \frac{1}{q}, \dots, \frac{1}{q}, 1\right]. \quad (36)$$

Hence

$$W_q[\rho] = \frac{2\pi N_{n,\ell}^{2q}}{(2\lambda q)^{q\gamma_\ell + \frac{3}{2}}} \Theta_0\left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q}\right), \quad (37)$$

so that the Renyi entropy for the pseudoharmonic potential in the position space is given by

$$R_q[\rho] = \frac{1}{1-q} \log \left[\frac{2\pi N_{n,\ell}^{2q}}{(2\lambda q)^{q\gamma_\ell + \frac{3}{2}}} \Theta_0\left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q}\right) \right]. \quad (38)$$

Note that the Lauricella function of type A is defined as^[55–57]

$$F_A^{(s)}\left(\begin{matrix} a; b_1, \dots, b_s \\ c_1, \dots, c_s \end{matrix}; x_1, \dots, x_s\right) = \sum_{j_1, \dots, j_s=0}^{\infty} \frac{(a)_{j_1+\dots+j_s} (b_1)_{j_1} \dots (b_s)_{j_s} x_1^{j_1} \dots x_s^{j_s}}{(c_1)_{j_1} \dots (c_s)_{j_s} j_1! \dots j_s!}. \quad (39)$$

Table 6 contains the numerical values of the Renyi entropy in the position space for some diatomic molecules with $q = 2$ and $\ell = 0$. Table 7 shows the variations with the parameter q of the Renyi entropy in the position space for NiC with $\ell = 0$. We observe from Table 6 that the Renyi entropy $R_2[\rho]$ increases

Table 7. Variations of the Renyi entropy for the pseudoharmonic potential in the position space with the q and n for Cl_2 molecule with $\ell = 0$.

n	$q = 3$	$q = 4$	$q = 5$	$q = 6$	$q = 7$
0	3.42934	3.48219	3.49964	3.50566	3.50715
1	3.64938	3.61909	3.58041	3.54859	3.52373
2	3.72728	3.63067	3.55724	3.50571	3.46835
3	3.76441	3.61976	3.52367	3.45939	3.41377
4	3.78507	3.60376	3.49082	3.41689	3.36493
5	3.79775	3.58701	3.46053	3.37873	3.32156
6	3.80610	3.57079	3.43292	3.34443	3.28283
7	3.81188	3.55549	3.40774	3.31340	3.24792
8	3.81605	3.54116	3.38466	3.28514	3.21620
9	3.81915	3.52777	3.36341	3.25921	3.18717
10	3.82153	3.51526	3.34375	3.23529	3.16041

with n . This is not the case when $q > 2$. Figure 3 shows the variation of the position space Renyi entropy with the parameter q and $n = 0$.

Renyi entropy in the momentum space

The Renyi entropy in the momentum space is written as

$$R_q[\gamma] = \frac{1}{1-q} \log W_q[\gamma], \quad (40)$$

where

$$W_q[\gamma] = 4\pi \int_0^\infty p^2 \gamma(p)^q dp \quad (41)$$

and $\gamma(p)$ is as given in Eq. (17). If we let $\frac{p^2}{2\lambda} = x$, then we have

$$W_q[\gamma] = 2^{q+1} \pi (2\lambda)^{q\gamma_\ell + \frac{3}{2}} \left((2\lambda^2)^{-\frac{q\gamma_\ell - \frac{3}{2}}{4}} \right)^q \left[\frac{n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right]^q \int_0^\infty x^{q\gamma_\ell + \frac{1}{2}} e^{-4qx} \left[L_n^{\gamma_\ell + \frac{1}{2}}(x) \right]^{2q} dx, \quad (42)$$

which can be written as

$$W_q[\gamma] = 2^{q+1} \pi (2\lambda)^{q\gamma_\ell + \frac{3}{2}} \left((2\lambda^2)^{-\frac{q\gamma_\ell - \frac{3}{2}}{4}} \right)^q \times H_q[\gamma], \quad (43)$$

where

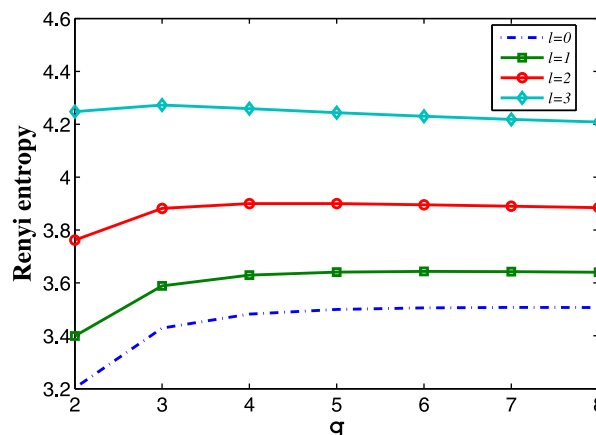


Figure 3. The variation of the Renyi entropy in the position space with q and ℓ when $n = 0$.

$$H_q[\gamma] = \left[\frac{n!}{\Gamma(n + \gamma_\ell + \frac{3}{2})} \right]^q \int_0^\infty x^{q\gamma_\ell + \frac{1}{2}} e^{-4qx} \left[L_n^{\gamma_\ell + \frac{1}{2}}(x) \right]^{2q} dx. \quad (44)$$

$H_q[\gamma]$ will be evaluated using the multivariate Bell polynomials of Combinatorics. We follow the approach similar to Ref. [19], whereby, we consider the explicit expression of the Laguerre polynomials given by

$$\tilde{L}_n^{\gamma_\ell + \frac{1}{2}}(x) = \sum_{k=0}^n c_k^{(n, \gamma_\ell + \frac{1}{2})} x^k \quad (45)$$

with

$$c_k^{(n, \gamma_\ell + \frac{1}{2})} = \sqrt{\frac{\Gamma(n + \gamma_\ell + \frac{3}{2})}{n!}} \frac{(-1)^k}{\Gamma(\gamma_\ell + k + \frac{3}{2})} \binom{n}{k}. \quad (46)$$

The Laguerre polynomials can be written in terms of the multivariate Bell polynomials of Combinatorics as^[19,32]

$$\begin{aligned} \left[\tilde{L}_n^{\gamma_\ell + \frac{1}{2}}(x) \right]^{2q} &= \sum_{k=0}^{2nq} \frac{(2q)!}{(k+2q)!} \\ &\times B_{k+2q, 2q} \left(c_0^{(n, \gamma_\ell + \frac{1}{2})}, 2!c_1^{(n, \gamma_\ell + \frac{1}{2})}, \dots, (k+1)!c_k^{(n, \gamma_\ell + \frac{1}{2})} \right) x^k, \end{aligned} \quad (47)$$

with $c_i^{(n, \gamma_\ell + \frac{1}{2})} = 0$ for $i > n$ and the remaining coefficients are given by Eq. (46). The Bell polynomials are given by^[19,32,58,59]

$$\begin{aligned} B_{m,t}(a_1, a_2, \dots, a_{m-t+1}) &= \sum_{\hat{\pi}(m,t)} \frac{m!}{j_1! j_2! \dots j_{m-t+1}!} \left(\frac{a_1}{1!} \right)^{j_1} \\ &\times \left(\frac{a_2}{2!} \right)^{j_2} \dots \left(\frac{a_{m-t+1}}{(m-t+1)!} \right)^{j_{m-t+1}}, \end{aligned} \quad (48)$$

where the sum runs over all partitions $\hat{\pi}(m, t)$ such that

$$j_1 + j_2 + \dots + j_{m-t+1} = t, \text{ and } j_1 + 2j_2 + \dots + (m-t+1)j_{m-t+1} = m.$$

Therefore,

$$\begin{aligned} H_q[\gamma] &= \sum_{k=0}^{2nq} \frac{(2q)!}{(k+2q)!} B_{k+2q, 2q} \left(c_0^{(n, \gamma_\ell + \frac{1}{2})}, 2!c_1^{(n, \gamma_\ell + \frac{1}{2})}, \dots, (k+1)!c_k^{(n, \gamma_\ell + \frac{1}{2})} \right) \\ &\times \int_0^\infty x^{q\gamma_\ell + k + \frac{1}{2}} e^{-4qx} dx. \end{aligned} \quad (49)$$

On evaluating the integral in Eq. (49), we obtain

Table 8. The numerical values of the Renyi entropy for the pseudoharmonic potential in the momentum space for some diatomic molecules when $q = 2$.

n	$R_2[\gamma](\text{Na}_2)$	$R_2[\gamma](\text{Cl}_2)$	$R_2[\gamma](\text{O}_2^+)$	$R_2[\gamma](\text{N}_2^+)$	$R_2[\gamma](\text{NO}^+)$
0	5.93170	9.08768	9.90687	11.4410	12.3349
1	3.69398	6.61131	7.54612	8.88826	9.69331
2	2.38924	5.11855	6.14517	7.33419	8.06709
3	1.51135	4.08903	5.19016	6.25443	6.82777
4	0.87653	3.32961	4.49229	5.45320	6.07661
5	0.39591	2.74501	3.95927	4.83330	5.41436
6	0.01995	2.28109	3.53914	4.33926	4.88398
7	-0.28152	1.90434	3.19998	3.93653	4.44978
8	-0.52805	1.59272	2.92095	3.60229	4.08805
9	-0.73290	1.33107	2.68780	3.32079	3.78235
10	-0.90541	1.10862	2.49045	3.08079	3.52089

$$\begin{aligned} H_q[\gamma] &= \sum_{k=0}^{2nq} \frac{\Gamma(q\gamma_\ell + k + \frac{3}{2})}{2^{2q\gamma_\ell + 2k + 3} q^{q\gamma_\ell + k + \frac{3}{2}}} \frac{(2q)!}{(k+2q)!} \\ &\times B_{k+2q, 2q} \left(c_0^{(n, \gamma_\ell + \frac{1}{2})}, 2!c_1^{(n, \gamma_\ell + \frac{1}{2})}, \dots, (k+1)!c_k^{(n, \gamma_\ell + \frac{1}{2})} \right). \end{aligned} \quad (50)$$

The only nonvanishing terms correspond to those with $j_{i+1} = 0$ so that $(c_i^{(n, \gamma_\ell + \frac{1}{2})})^{j_i+1} = 1$ for every $i > n$. Hence, substituting Eq. (50) into Eq. (43) and then substituting Eq. (43) into Eq. (40) gives the Renyi entropy in the momentum space for the pseudoharmonic potential which can be written as

$$\begin{aligned} R_q[\rho] &= \frac{1}{1-q} \log \left[2^{q+1} \pi (2\lambda)^{q\gamma_\ell + \frac{3}{2}} \left((2\lambda^2)^{-\frac{q\gamma_\ell - 3}{2}} \right)^q \right. \\ &\times \sum_{k=0}^{2nq} \frac{\Gamma(q\gamma_\ell + k + \frac{3}{2})}{2^{2q\gamma_\ell + 2k + 3} q^{q\gamma_\ell + k + \frac{3}{2}}} \frac{(2q)!}{(k+2q)!} \\ &\left. B_{k+2q, 2q} \left(c_0^{(n, \gamma_\ell + \frac{1}{2})}, 2!c_1^{(n, \gamma_\ell + \frac{1}{2})}, \dots, (k+1)!c_k^{(n, \gamma_\ell + \frac{1}{2})} \right) \right]. \end{aligned} \quad (51)$$

The numerical values of the Renyi entropy for the pseudoharmonic potential in the momentum space for some diatomic molecules when $q = 2$ are shown in the Table 8. It is observed that the Renyi entropy for the pseudoharmonic potential in the momentum space, unlike in the position space, decreases with increase in n .

Tsallis entropy for the pseudoharmonic potential

We shall obtain, in this subsection, the Tsallis entropy for the pseudoharmonic potential in the position and momentum spaces.

Tsallis entropy in the position space. The Tsallis entropy in the position space is written as

$$T_q[\rho] = \frac{1}{q-1} [1 - W_q[\rho]], \quad (52)$$

where $W_q[\rho]$ is as given in Eq. (30). Using Eq. (37), the Tsallis entropy in the position space is then obtained as

$$T_q[\rho] = \frac{1}{q-1} \left[1 - \frac{2\pi N_{n,\ell}^{2q}}{(2\lambda q)^{q\gamma_\ell + \frac{3}{2}}} \Theta_0 \left(q\gamma_\ell + \frac{1}{2}, 0, 2q, n, \gamma_\ell + \frac{1}{2}, \frac{1}{q} \right) \right]. \quad (53)$$

The numerical values of the Tsallis entropy in the position space is shown in Table 9 with $q = 2$ and $\ell = 0$. We observe that (See Table 10) the value of the Tsallis entropy for the pseudoharmonic potential in the position space tends to a particular value as ℓ increases for each q and it is independent of ℓ when $q \gg 1$.

Tsallis entropy in the momentum space. The Tsallis entropy in the momentum space can be written as

$$T_m[\gamma] = \frac{1}{m-1} [1 - W_m[\gamma]], \quad (54)$$

where

$$W_m[\gamma] = 4\pi \int_0^\infty p^2 \gamma(p)^m dp = 2^{m+1} \pi (2\lambda)^{m\gamma_\ell + \frac{3}{2}} \left((2\lambda^2)^{-\frac{m\gamma_\ell - 3}{2}} \right)^m \times H_m[\gamma], \quad (55)$$

Table 9. The numerical values of the Tsallis entropy for the pseudoharmonic potential in the position space with $q = 2$ and $\ell = 0$.

n	$T_2[\rho](\text{Na}_2)$	$T_2[\rho](\text{Cl}_2)$	$T_2[\rho](\text{O}_2^+)$	$T_2[\rho](\text{N}_2^+)$	$T_2[\rho](\text{NO}^+)$
0	0.983996	0.959358	0.721752	0.799777	0.804013
1	0.988599	0.970861	0.801094	0.856180	0.858933
2	0.990622	0.975938	0.836053	0.881102	0.883226
3	0.991841	0.979013	0.857184	0.896215	0.897975
4	0.992683	0.981143	0.871792	0.906692	0.908214
5	0.993310	0.982734	0.882685	0.914525	0.915876
6	0.993800	0.983981	0.891219	0.920674	0.921896
7	0.994197	0.984994	0.898139	0.925670	0.926791
8	0.994527	0.985838	0.903899	0.929833	0.930874
9	0.994807	0.986555	0.908790	0.933373	0.934347
10	0.995048	0.987174	0.913010	0.936432	0.937349

$$H_m[\gamma] = \sum_{k=0}^{2nm} \frac{\Gamma(m\gamma_\ell + k + \frac{3}{2})}{2^{2m\gamma_\ell + 2k + 3} m^{m\gamma_\ell + k + \frac{3}{2}} (k + 2m)!} (2m)! \quad (56)$$

$$B_{k+2m, 2m} \left(c_0^{(n, \gamma_\ell + \frac{1}{2})}, 2!c_1^{(n, \gamma_\ell + \frac{1}{2})}, \dots, (k+1)!c_k^{(n, \gamma_\ell + \frac{1}{2})} \right),$$

and

$$\frac{1}{q} + \frac{1}{m} = 2.$$

Table 11 shows the numerical values of the Tsallis entropy for the pseudoharmonic potential in the momentum space for $m = \frac{2}{3}$ and $\ell = 0$.

Onicescu information energy for the pseudoharmonic potential

Onicescu information energy for the pseudoharmonic potential in the position space. The Onicescu information energy in the position space is written from Eq. (5) as

$$E[\rho] = 4\pi \int_0^\infty \rho^2(r) dr, \quad (57)$$

which is equivalent to $W_2[\rho]$ in Eqs. (29) and (30) when $q = 2$. From Eq. (37), $W_2[\rho]$ is obtained as

$$W_2[\rho] = \frac{2\pi N_{n,\ell}^4}{(4\lambda)^{2\gamma_\ell + \frac{3}{2}}} \Theta_0 \left(2\gamma_\ell + \frac{1}{2}, 0, 4, n, \gamma_\ell + \frac{1}{2}, \frac{1}{2} \right). \quad (58)$$

Therefore, the Onicescu information energy for the pseudoharmonic potential in the position space is given as

Table 10. The numerical values of the Tsallis entropy for the pseudoharmonic potential in the position space as q increases when $\ell = 0$ using NO^+ molecule.					
n	$q = 3$	$q = 4$	$q = 5$	$q = 6$	$q = 10$
0	0.804013	0.485394	0.331782	0.249808	0.111111
1	0.835086	0.488945	0.332277	0.249882	0.111111
2	0.880675	0.493431	0.332818	0.249953	0.111111
3	0.923289	0.496763	0.333139	0.249986	0.111111
4	0.954746	0.498604	0.333272	0.249997	0.111111
5	0.974857	0.499451	0.333316	0.249999	0.111111
6	0.986594	0.499797	0.333329	0.250000	0.111111
7	0.993050	0.499928	0.333332	0.250000	0.111111
8	0.996466	0.499975	0.333333	0.250000	0.111111
9	0.998227	0.499991	0.333333	0.250000	0.111111
10	0.999119	0.499997	0.333333	0.250000	0.111111

Table 11. The numerical values of the Tsallis entropy in the momentum space for $m = \frac{2}{3}$ when $\ell = 0$.

n	$T_m[\gamma](\text{Na}_2)$	$T_m[\gamma](\text{Cl}_2)$	$T_m[\gamma](\text{O}_2^+)$	$T_m[\gamma](\text{N}_2^+)$	$T_m[\gamma](\text{NO}^+)$
0	-2.07110	-1.97990	-0.83715	-1.39502	-1.55384
1	-1.30571	-0.95051	1.14771	0.32431	0.10281
2	-0.71571	-0.01585	2.81766	1.96173	1.76714
3	-0.29502	0.75581	4.10632	3.37149	3.26865
4	-0.00556	1.36370	5.06124	4.52435	4.54838
5	0.18981	1.83168	5.75521	5.44275	5.60653
6	0.31935	2.18773	6.25382	6.16456	6.46739
7	0.40295	2.45664	6.60820	6.72764	7.16158
8	0.45433	2.65835	6.85627	7.16459	7.71844
9	0.48290	2.80833	7.02563	7.50188	8.16349
10	0.49521	2.91834	7.13635	7.76048	8.51776

$$E[\gamma] = \frac{2\pi N_{n,\ell}^4}{(4\lambda)^{2\gamma_\ell + \frac{3}{2}}} \Theta_0 \left(2\gamma_\ell + \frac{1}{2}, 0, 4, n, \gamma_\ell + \frac{1}{2}, \frac{1}{2} \right). \quad (59)$$

Onicescu information energy for the pseudoharmonic potential in the momentum space. The Onicescu information energy in the momentum space is written from Eq. (6) as

$$E[\gamma] = 4\pi \int_0^\infty \gamma^2(p) dp, \quad (60)$$

which is equivalent to $W_2[\gamma]$ in Eqs (41–43) when $q = 2$. $W_2[\gamma]$ is obtained from Eq. (43) as

$$W_2[\gamma] = 2^3 \pi (2\lambda)^{2\gamma_\ell + \frac{3}{2}} \left((2\lambda^2)^{-\frac{2\gamma_\ell}{2} - \frac{3}{4}} \right)^2 \times H_2[\gamma], \quad (61)$$

where

$$H_2[\gamma] = \sum_{k=0}^{4n} \frac{\Gamma(2\gamma_\ell + k + \frac{3}{2})}{2^{4\gamma_\ell + 2k + 3} 2^{2\gamma_\ell + k + \frac{3}{2}} (k + 4)!} B_{k+4, 4} \left(c_0^{(n, \gamma_\ell + \frac{1}{2})}, 2!c_1^{(n, \gamma_\ell + \frac{1}{2})}, \dots, (k+1)!c_k^{(n, \gamma_\ell + \frac{1}{2})} \right). \quad (62)$$

The numerical values of the Onicescu information energy for the pseudoharmonic potential in the position and momentum spaces are shown in Table 12. The Onicescu information energy for the pseudoharmonic potential decreases with

Table 12. The numerical values of the Onicescu information energy for the pseudoharmonic potential in the position and momentum spaces when $\ell = 0$.				
n	$E[\rho](\text{O}_2^+)$	$E[\rho](\text{NO}^+)$	$E[\gamma](\text{O}_2^+)$	$E[\gamma](\text{NO}^+)$
0	0.278248	0.195987	0.000049831	0.000004395
1	0.198906	0.141067	0.000528157	0.000061695
2	0.163947	0.116774	0.002143820	0.000313693
3	0.142816	0.102025	0.005571110	0.000980189
4	0.128208	0.091786	0.011195000	0.002295950
5	0.117315	0.084124	0.019077100	0.004452190
6	0.108781	0.078104	0.029038400	0.007566820
7	0.101861	0.073209	0.040763000	0.011681100
8	0.096101	0.069126	0.053882700	0.016771900
9	0.091210	0.065653	0.068030600	0.022769100
10	0.086990	0.062651	0.082872600	0.029573100

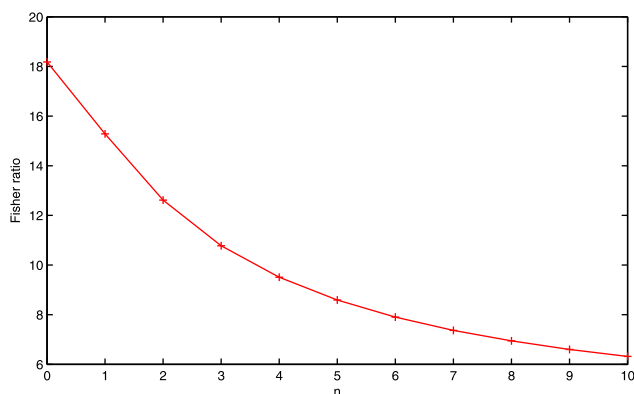


Figure 4. The graph of the ratio of Fisher impetus to length for the pseudoharmonic potential against n using NO^+ .

increase in n for the position space and increases with increasing n for the momentum space.

Information-Theoretic Lengths and Impetuses

We shall obtain, in this section, the ratio of the information-theoretic impetuses to lengths for the Fisher information, the Shannon entropy, and the Renyi information entropy for the pseudoharmonic potential.

Ratio of the Fisher impetus to length for the pseudoharmonic potential

The ratio of the Fisher impetus to length is defined as^[22]:

$$\frac{F_I}{F_L} = \frac{\sqrt{I[\rho]}}{\sqrt{I[\gamma]}} \quad (63)$$

$I[\rho]$ and $I[\gamma]$ are given by Eqs. (19) and (21), respectively.

Ratio of the Shannon impetus to length for the pseudoharmonic potential

The ratio of the Shannon impetus to length is defined as^[22]:

$$\frac{S_I}{S_L} = \left[e^{S[\gamma] - S[\rho]} \right]^{\frac{1}{3}} \quad (64)$$

$S[\rho]$ and $S[\gamma]$ are given by Eqs. (23) and (27), respectively.

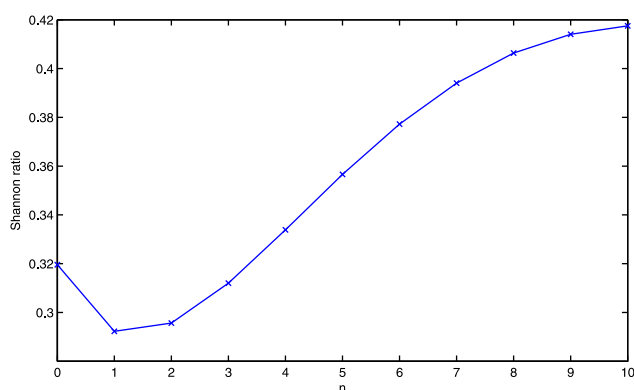


Figure 5. The graph of the ratio of Shannon impetus to length for the pseudoharmonic potential against n using NO^+ .

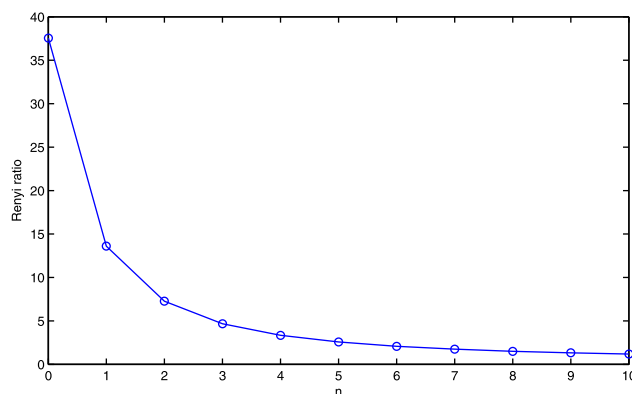


Figure 6. The graph of the ratio of Renyi impetus to length for the pseudoharmonic potential against n using NO^+ .

The ratio of the Renyi impetus to length for the pseudoharmonic potential

The ratio of the q th-order Renyi impetus length is defined as^[22]:

$$\frac{R_I}{R_L} = \left[e^{R_q[\gamma] - R_q[\rho]} \right]^{\frac{1}{3}} \quad (65)$$

$R_q[\rho]$ and $R_q[\gamma]$ are given by Eqs (38) and (51), respectively. The graphs of the ratio of the information impetuses to lengths of Fisher information $\left(\frac{F_I}{F_L}\right)$, Shannon entropy $\left(\frac{S_I}{S_L}\right)$, and Renyi entropy $\left(\frac{R_I}{R_L}\right)$ for the pseudoharmonic potential when $q=2$ are shown in the Figures 4–6. From Figure 4, it is observed that the Fisher ratio $\left(\frac{F_I}{F_L}\right)$ decreases exponentially with increasing n . It is observed from Figure 5 that the Shannon ratio $\left(\frac{S_I}{S_L}\right)$ starts to decrease from $n=0$ to $n=1$ but increases with n afterwards. Also, from Figure 6, the Renyi ratio $\left(\frac{R_I}{R_L}\right)$ for $q=2$ decreases exponentially with increasing n .

Conclusion

We have studied, both analytically and numerically, the information-theoretic measures for the pseudoharmonic potential using Fisher information, Shannon entropy, Renyi entropy, Tsallis entropy, and Onicescu information energy in both the position and momentum spaces. Using the values of D_e and r_e of some diatomic molecules, we have obtained the numerical values of the information-theoretic measures for the pseudoharmonic potential. Using the linearization formula of Srivastava–Niukkanen, we have obtained the Renyi and Tsallis entropies in the position space in terms of the Lauricella hypergeometric function.

To obtain the Renyi and Tsallis entropies in the momentum space, we made use of the, multivariate Bell polynomials of Combinatorics. We observed that the Fisher information increases with n in both the position and momentum spaces, but decreases with increasing ℓ for all the diatomic molecules considered. The Shannon entropy also increases with n in the position space and decreases with increasing ℓ .

The Renyi entropy increases with the parameter q but the Tsallis entropy decreases with increase in the parameter q . We also observed that as n increases, the Tsallis entropy tends to a particular value for each q . For large value of q , the Tsallis

entropy is constant with change in n . The analytical and numerical values of the Onicescu information energy have also been obtained and we finally obtained the ratio of the information-theoretic impetuses to lengths of Fisher, Shannon, and Renyi.

Information theoretical entropic measures such as those described in this work can be used as descriptors of chemical reactivity of molecules.^[30,36,37] In those chemical reactions where full *ab initio* calculations are tedious, the model potentials can be used to simulate the reactivity using information theoretical tools. It is, therefore, essential to first test the suitability of the model potentials to describe bonding in a chosen set of diatomic molecules in terms of the various information theoretical measures.^[38,39]

Such tests have been presented here using both global and local information theoretical measures. In addition to the descriptors of chemical reactivity, such measures have been found useful in comparing the quantum molecular similarity. Such studies provide valuable insights in to the host-guest interactions contributing to the molecular drug design.^[40,41] The information theoretical measures based on the model potentials considered in this work have been numerically tested and found to rigorously satisfy all the characteristic features of information theory paving the way for future studies of chemical reactivity.

An example of the application of the study is the calculation of $1-S[\rho]$, the 1-normalized Shannon entropy can be similarly performed for the spherically confined pseudoharmonic potential where in the potential in Eq. (11) is confined within the impenetrable cavity of radius R . The quantitative relationship of mean ionization energy, I_m , to $1-S[\rho]$ can be used to draw valuable information on how the I_m changes on confinement.^[60,61] The value of I_m increases as $1-S[\rho]$ decreases. A calculation of $1-S[\rho]$ for N_2^+ suggests a 7% decrease in $1-S[\rho]$ in going from the free state to the spherically confined state at $R=4$ a.u.. For NO^+ , this change amounts to about 9%. In other words, the measure of disorder in terms of $1-S[\rho]$ can be related to the electronic property of ionization.

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Keywords: pseudoharmonic potential • information-theoretic measures • impetus • diatomic molecules

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