Information Entropies for Molecular Deng- Fan-Eckart Potential

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Abstract

In this study, the Shannon, Renyi , Tsallis entropies and Fisher Information are investigated with molecular Deng-Fan-Eckart potential for some selected diatomic molecules (H_2, CO, ScN, and ScF) in position and momentum spaces in three dimensions. Due to the difficulty in obtaining the Fourier transform of the wave function in the momentum space, we considered the low lying states corresponding to the ground and first excited states . The effects of the screening parameter α on the Information entropies measures for the selected diatomic molecules were illustrated. We computed numerically the entropies measures for all the diatomic molecules and the corresponding uncertainty relations of the entropies for the selected diatomic molecules were satisfied accordingly..

Keywords: Information entropies, Shannon entropy, Fisher information. Renyi entropy, Tsallis entropy

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1 Introduction

The information-theoretic measures have received a great research interest for quantum mechanical systems over the years. These are largely due to its applications in probability density functional and computation and have provided a broader perspective for various quantum mechanical systems [1-3]. The concepts of information-theoretic measures have been applied in many areas of communication [4], physical sciences [5], chemical sciences [6] and other disciplines that have connections with quantum information systems [7-8].Quantum information-theoretic measures are classified either as global or local measures in order to quantify their uncertainty. The global measures describe the probability density spread in a region [9-10] and these include Shannon entropy [2], Renyi entropy [11], Tsallis entropy [12], and Onicescu information energy [13]. On the other hand, the local measure is the Fisher information [14] and is concerned with the point changes that occur in the probability density [15]. Of all these quantum information measures, the Shannon entropy and Fisher information have been exhaustively studied than others information-theoretic tools. Quantum information theory is very important in the uncertainty measures of atoms and molecules. The entropic densities in the position and conjugate momentum spaces provide the basic description of a molecular and chemical system. In the molecular system, it provides a good narrative measures for chemical bonding [16] and it can also been applied in the comparison of molecular interactions [17-18]. Several kinds of research work have been carried out for information-theoretic measures both analytically and numerically. For instance, Isonguyo et al. [19] investigated the different behaviours for a quantum system using information theoretic tools for the screened Coulomb potential. Onate et al. [20] investigated the dissociation energy effect on the Shannon entropy and Renyi entropies. Romera et al. [15] studied analytically the behaviour of Fisher information with a central potential for a single particle system and established a novel uncertain relation that is satisfied for any central potential model. Another applications of the Fisher information is in the study the external electrical and magnetic effects in atomic systems [21]. The Shannon and Fisher information have been studied for position-dependent mass (PDM) within the framework of non-relativistic quantum mechanics [22-24].Information-theoreric measures finds other applications in semiconductors and quantum dots. For instance, information entropies have been investigated for scaling behaviour properties [25-27], confined systems [28-31], shape effect of quantum heterostructures [32] among others[33-40]. In recent time, there very few research work on information theory with exponential type potentials and to the best of our

knowledge no application of diatomic molecules for exponential type potential have been investigated and hence the motivation of this study. The quantum information-theoretic measure considered in this study is the molecular Deng-Fan-Eckart potential model (DFEP).

Recently, Edet et al. [41] studied DFEP model for some selected diatomic molecules (H_2, CO, ScN, and ScF). The choice of this potential stems from the fact that it exhibits an almost exact behaviour with that of the Morse potential and so makes it a good choice to the study of atomic interaction for diatomic molecules.

The organization of the paper is as follows. In section 2 is devoted to the solutions of the eigen-solutions of the DEFP. Section 3 is the calculations of the quantum information entropies. Section 4 is for the applications of the information entropies for the selected diatomic molecules. Finally, a brief conclusion is given in section 5.

2 Eigensolution of Deng-Fan-Eckart Potential (DFEP)

The Deng-Fan-Eckart potential is defined as [41],

$$V(r) = D_e\left(1 - \frac{b}{e^{\alpha r} - 1}\right)^2 - \frac{V_1 e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{V_2 e^{-\alpha r}}{\left(1 - e^{-\alpha r}\right)^2}, \tag{1}$$

where, $b = e^{-\alpha r_e} - 1$. D_e, r, α, and r_e are the dissociation energy, inter-nuclear distance, potential range, and molecular bond length respectively, V_1 and V_2 are the potential strength. By using the Pekeris type approximation [42] for the centrifugal approximation term in the Schrodinger equation [43], Edet et al. [41] solved and obtained the analytical expressions for the energy values and the corresponding wave function for the DFEP using factorization method [44] as,

$$E_{n,l} = \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{2\mu D_e}{\hbar^2\alpha^2} + l(l+1)\,d_0 - \left(\frac{(n+\upsilon)^2 - \frac{2\mu D_e b^2}{\hbar^2\alpha^2} - \frac{4\mu D_e b}{\hbar^2\alpha^2} - \frac{2\mu V_1}{\hbar^2\alpha^2}}{2(n+\upsilon)}\right)^2\right] \tag{2}$$

$$\psi(\bar{r}) = N_{n,l}\, s^{\lambda}(1-s)^{\omega}\ {}_2F_1(-n, n+2(\lambda+\omega); 2\lambda+1; s)\, Y_{l,m}(\Omega) \tag{3}$$

where,

$$\upsilon = \frac{1}{2} + \frac{1}{2}\sqrt{(2l+1)^2 + \frac{8\mu D_e b}{\hbar^2\alpha^2} + \frac{8\mu V_2}{\hbar^2\alpha^2}} \quad (4a)$$

and $\lambda = \sqrt{\varepsilon + \kappa d_0}$, $\omega = \frac{1}{2} + \sqrt{\frac{1}{4} + \eta_1 + \beta_2 + \kappa}$, $d_0 = \frac{1}{12}$, $\kappa = l(l+1)$ and $s = e^{-\alpha r}$. Other parameters are defined in Ref. [41], $Y_{l,m}(\Omega)$ is the angular component of the wave function. Using the MATHEMATICA software, we obtained the normalization constant for the ground state from eq.(3) in three dimensions as follows:

$$N_0 = \sqrt{\frac{\alpha^3\,\Gamma(2\omega+1+2\lambda)}{\sigma\,\Gamma(\lambda)\Gamma(2\lambda+1)}} \quad (4b)$$

where,

$$\sigma = \left(\gamma - H_{2\lambda+\omega} + \psi^{(0)}(2\lambda)\right)^2 + \psi^{(1)}(2\lambda) - \psi^{(1)}(2\lambda+1+2\omega) \quad (5)$$

and $\psi^{(n)} = \frac{\Gamma'(x)}{\Gamma(x)}$ being the polygamma function, H_n is the Harmonic number [9,19] respectively and γ is the Euler Gamma defined by [45], $\gamma = \lim_{n\to\infty}\left(\sum_{k=1}^{n}\frac{1}{k} - \ln n\right)$, where the first term is Harmonic number. The probability densities for the ground and first excited states [46] in the position space are calculated as follows,

$$\rho_0(\vec{r}) = \left[\frac{\alpha^3\,\Gamma(1+2\omega+2\lambda)}{4\pi\sigma\,\Gamma(1+2\omega)\Gamma(\lambda)}\right]\left(e^{-2\alpha r}\right)^{2\lambda}\left(1-e^{-2\alpha r}\right)^{2\omega}\left|Y_{0,0}\right|^2, \quad (6a)$$

$$\rho_1(\vec{r}) = N_1^2\,\frac{s^{2\lambda}s^{2\omega}(1-s+2\lambda-2\lambda s-2\omega s)}{1+2\lambda}\left|Y_{0,0}\right|^2 \quad (6b)$$

The momentum space wave function is obtain by taking the Fourier transformation [47] of the position space wave function and for the ground state the momentum space wave function is given as,

$$\Phi_0(\vec{p}) = N_0^2 \left| \frac{\left(i\,\Gamma[1+2\omega]\,\left(\Gamma\left[-\frac{ip}{\alpha}+\lambda \right] \Gamma\left[\frac{ip}{\alpha}+\lambda+\omega \right] \Omega + \Theta\, X \right) \right)}{\left(\alpha^2 p\,\sqrt{2\pi}\;\Gamma\left[1+\lambda+\omega+\frac{ip}{\alpha} \right] \Gamma\left[1+\omega-\frac{ip}{\alpha}+\lambda \right] \right)} \right|^2 |Y_{0,0}|^2 , \quad (7)$$

where,

$$\Omega = \psi^{(0)}\left[-\frac{ip}{\alpha}+\lambda \right] - \psi^{(0)}\left[-\frac{ip}{\alpha}+\lambda+\omega \right], \quad (8a)$$

$$\Theta = \psi^{(0)}\left[1-\frac{ip}{\alpha}+\lambda+\omega \right] - \psi^{(0)}\left[\frac{ip}{\alpha}+\lambda \right], \quad (8b)$$

$$X = \psi^{(0)}\left(1+\lambda+\omega+\frac{ip}{\alpha} \right) - \psi^{(0)}\left(\lambda+\frac{ip}{\alpha} \right), \quad (8c)$$

However, because of the difficulty and complexity in obtaining the Fourier transform in the momentum space that of the first excited state will be done numerically in this study.

3 Information Entropies

In this section, the quantum information-theoretic measures for Shannon entropy, Fisher information, Renyi entropy, Tsallis entropy in position and momentum spaces will be calculated. Shannon entropy which is regarded as a logarithmic probability densities investigate the concentration of the probability densities spread in a quantum system. It is defined in position and momentum spaces as;

$$S_r = -4\pi \int \rho(r) \ln\left[\rho(r) \right] dr \quad (9)$$

$$S_p = -4\pi \int \Phi(p) \ln\left[\Phi(p) \right] dr \quad (10)$$

where S_r and S_p are position and momentum space Shannon entropy respectively. The position and momentum probability densities are $\rho(\vec{r}) = |\psi(\vec{r})|^2$ and $\Phi(\vec{p}) = |\psi(\vec{p})|^2$ The Shannon entropy stipulated that the lower the Shannon entropy the lower the uncertainty and the higher the degree of predicting the particle localization. The Shannon entropy uncertainty relation was established by Berkner, Bialynicki–Birula and Mycieslki (BBM) and is expressed as [48],

$$S_r + S_p \geq D(1 + \ln \pi), \tag{11}$$

where, D is the spatial dimension. The Renyi entropy shared similar characteristics with Shannon entropy and it is a generalization of the Shannon entropy. It is expressed as follows [11,49],

$$R_\alpha(r) = \frac{1}{1-\alpha} \ln\left[4\pi \int (\rho(r))^\alpha dr\right] \tag{12}$$

$$R_\alpha(p) = \frac{1}{1-\alpha} \ln\left[4\pi \int (\Phi(p))^\alpha dp\right] \tag{13}$$

where, $\alpha > 0$ and $\alpha \neq 1$, $R_\alpha(r)$, $R_\alpha(p)$ are the Renyi entropy in the position space and momentum space respectively. The Renyi entropy must satisfied the inequality relation [50,51],

$$R_\alpha(r) + R_\alpha(p) \geq -\left(\frac{1}{1-\alpha} \ln\left(\frac{\alpha}{\pi}\right)\right) \tag{14}$$

Similarly, the Tsallis entropy is another generalization of Shannon entropy and it is defined in position and momentum space defined as [12,51,52],

$$T_\alpha(r) = \frac{1}{1-\alpha}\left(1 - \left[4\pi \int (\rho(r))^\alpha dr\right]\right) \tag{15}$$

$$T_\alpha(p) = \frac{1}{1-\alpha}\left(1 - \left[4\pi \int (\Phi(p))^\alpha dp\right]\right) \tag{16}$$

The Renyi and Tsallis entropies reduces to the Shannon entropy as $\alpha \to 1$. The Fisher Information is a local measure of information entropy as stated before and contains differential which makes it highly sensitive to detect local changes that occur in the

probability density. In Fisher information, the control of localization of the probability density occurs at the nodes and it can be seen as a measure of oscillator degree which has application with the kinetic energy of the system, Sear et al [52]. Thus, Fisher information in position space and momentum space are expressed as [14,37]

$$I_r = 4\pi \int \frac{\left[\rho'(r)\right]^2 r^2}{\rho(r)} dr \tag{17}$$

$$I_p = 4\pi \int \frac{\left[\Phi'(p)\right]^2 p^2}{\Phi(p)} dp \tag{18}$$

Subsequently, in the Fisher information theory the higher the Fisher information the higher the accuracy of predicting the localization of the system and therefore, increasing the Fisher information increases the fluctuation of the system. Just like other quantum information theory, the Fisher information satisfied Stam, Cramer-Rao inequality [15],

$$I_r I_p \geq 9\left(2 - \frac{2l+1}{l(l+1)}|m|\right)^2 \tag{19}$$

4 Applications to Diatomic Molecules

Here, we intend to analysed the applications of the quantum information theories given above for some selected diatomic molecules which are homonuclear and heteronuclear molecules in nature as given in Ref.[41] and other references therein for their classification. These diatomic molecules possess the same properties as each diatomic molecules are made of two atoms only and differs from each other in terms of covalent bonding and their geometric structure which is linear [53-54].. As an input for our computation, we take experimental values of the spectroscopic parameters for each of the diatomic molecules from Ref.[41] and given in Table 1.

Table 1 Spectroscopic parameter of some selected diatomic molecules

Parameters	H_2	CO	ScN	ScF
$D_e\left(cm^{-1}\right)$	38,266	90,540	36,778.88	47,183.43

$r_e\left(\overset{\circ}{\mathrm{A}}\right)$	0.7416	1,1283	1.768	1.794
$\alpha\left(\overset{0}{\mathrm{A}}^{-1}\right)$	1.9426	2.294	1.5068	1.46102
$\mu(amu)$	0.50391	6.860672	10.68277	13.35894

Tables 2 and 3 show the numerical results for the Shannon entropies of the diatomic molecules in the position and momentum spaces for the ground and first excited states respectively where we have taken the magnetic quantum numbers to be zero in all cases. In Table 2, for the position space, one observed striking features at the ground and first excited states as the Shannon entropies are all negative for the various values of the principal and angular momentum quantum number. This behaviour of the negative Shannon entropic value shows that the position Shannon entropy has a characteristic of a high localization [19] which implies a high accuracy in the prediction of the localization of these selected diatomic molecules and the high degree of less uncertainty. Likewise, in Table 3 for the momentum space, it is observed that the momentum space Shannon entropy for all selected diatomic molecules are positive. These affirm the assertion that on entropy must be increasing and the other entropy decreasing but to the extent that their sum stays above the stipulated lower bound of the value $3\left(1+In\left(\pi\right)\right)$ which has been satisfied for all the diatomic molecules. For the selected diatomic molecules, Shannon entropy uncertainty relation is satisfied. In Tables 4 and 5, we displayed the numerical results for the Fisher information in the position and momentum spaces for the different values of the principal and orbital angular momentum quantum numbers for the selected diatomic molecules. We observed in Tables 4 and 5, that in the position space the Fisher information is decreasing while it increases in the momentum space for the ground and first excited states On the other hand, the Fisher information I_r in the position space decreases both at the ground and first excited states and I_p increases also at the ground and first states for all the selected diatomic molecules in such a way that their product $I_r I_p \geq 36$ obeys the Stam-Cramer-Rao inequality relation which has been satisfied for these diatomic molecules investigated. We evaluated for the Renyi entropy

numerically in the position and momentum space for the ground state and first excited state as shown in Tables 6 and 7. One can also observe that the Reny position entropies increases both at the ground and first excited states while the Renyl momentum entropies decreases both at the ground and first excited state. The behaviours of the entropies on the screening parameters α are shown in Figs 1 and 2 for the selected diatomic molecules.

5 Conclusions

In this work, w study the information entropies for Shannon entropy, Fisher information, Renyi entropy and Tsallis entropy for some selected diatomic molecules (H_2, CO, ScN, and ScF) in the position and momentum spaces numerically at the ground and first excited states in three dimensions. Each diatomic molecules investigated satisfied the BBM inequality for the Shannon entropy and Stam-Cramer-Rao inequality relation for the Fisher information. Other information entropies such as Renyi entropies which is a special case of the Shannon entropy was investigated. Interesting, we observed that Renyi and Tsallis entropies shows a similar behaviour. This is not surprising since when $\alpha = 1$ in equations (12-13) and equations (15-16), the Renyl and Tsallis entropies reduced to the Shannon entropy.

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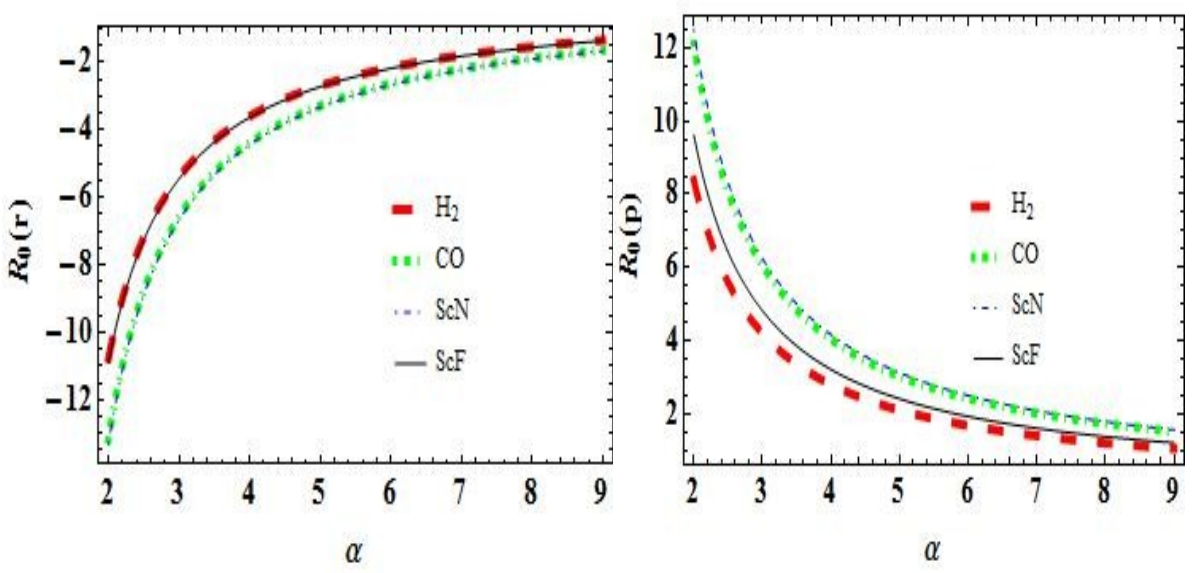


Fig. 1: Variations of the Renyi entwropy with α in the ground state for the different diatomic molecules in the position and momentum space for $l=0$

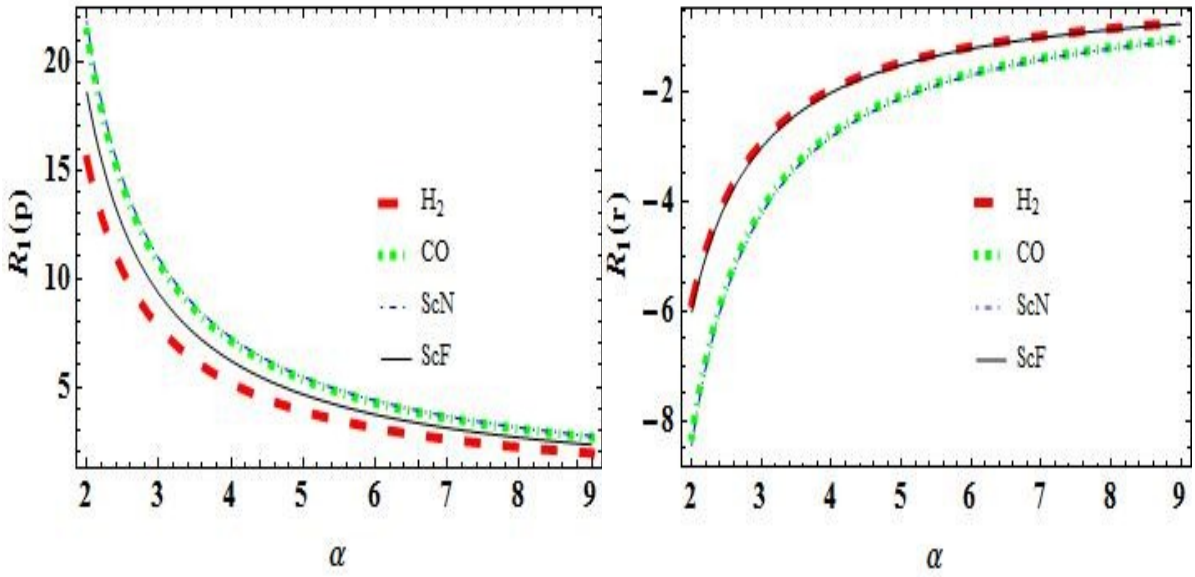


Fig. 2: Variations of the Renyi entropy with α for the first excited state for the different diatomic molecules in the position and momentum space for $l=0$

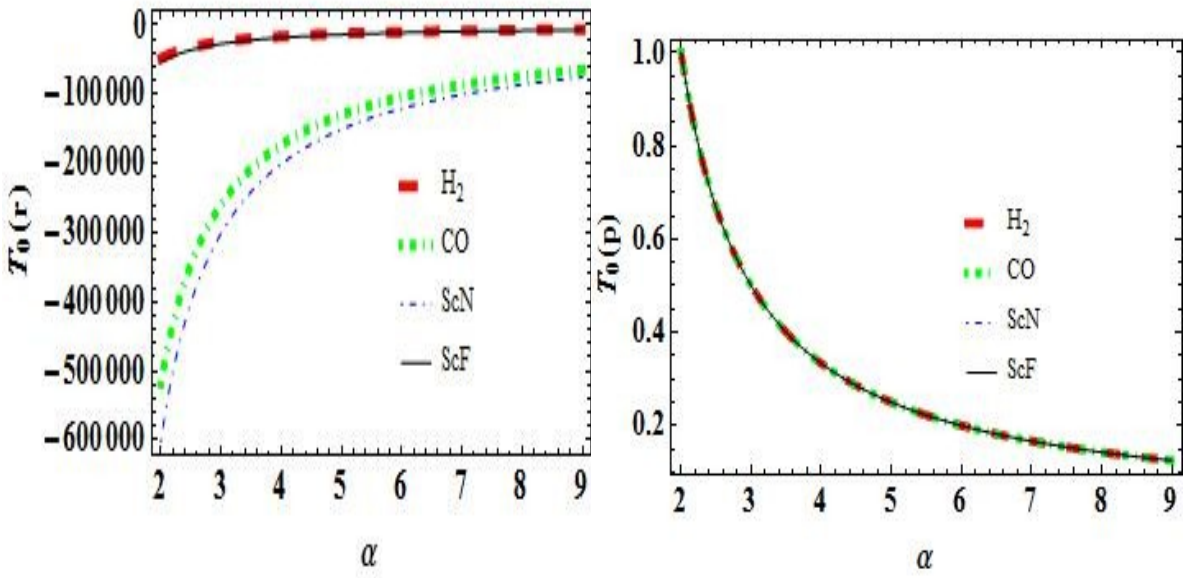


Fig.3:Variations of the Tsallis entropy with α in the ground state for the different diatomic molecules in the position and momentum space for $l=0$

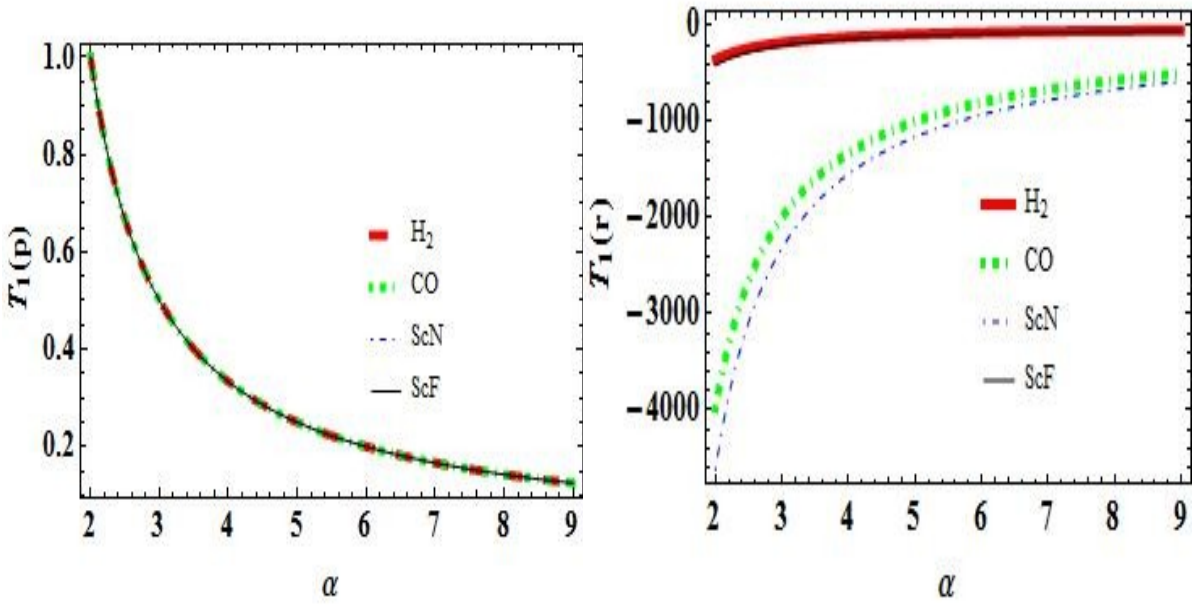


Fig.4:Variations of the Tsallis entropy with α for the first excited state for the different diatomic molecules in the position and momentum space for $l=0$

Table 2. Shannon entropy in the position space for Den- Fang-Eckart potential for the various diatomic molecules

	l	H_2		CO	ScN
ScF					
	0	-82.115042322	-105.744959452	-107.217876133	-83.344323254
	1	-82.024402217	-105.743628984	-107.217349398	-83.342174009
	2	-81.842866707	-105.740967912	-107.216295947	-83.337875178
	3	-81.569919173	-105.736975940	-107.214715672	-83.331426070
	4	-81.204769408	-105.731652636	-107.212608565	-83.322825654
	5	-80.74633463	-105.724997411	-107.209974479	-83.312072559
	6	-80.193213103	-105.717009554	-107.2068133207	-83.299165059
	7	-79.543649138	-105.707688181	-107.2031249737	-83.284101085
	8	-78.795488232	-105.697032282	-107.1989092484	-83.266878227
	9	-77.946120130	-105.685040673	-107.1941659771	-83.247493716
$n=0$	10	-76.992407231	-105.671712068	-107.1888949533	-83.225944431
	0	-5.701934113	-8.150999164	-8.301527637	-5.879527335
	1	-5.692779027	-8.150865754	-8.301473505	-5.879311058
	2	-5.674439804	-8.150595181	-8.301364798	-5.878866689
	3	-5.646870299	-8.150195244	-8.301172034	-5.878185979
	4	-5.609981111	-8.149648376	-8.301010658	-5.877280544
	5	-5.563672328	-8.148962265	-8.300755655	-5.876165201
	6	-5.507794468	-8.148146815	-8.300379328	-5.874837919
	7	-5.442176658	-8.147308940	-8.299999540	-5.873332847
	8	-5.366596980	-8.146153165	-8.299561403	-5.871646811
	9	-5.280793561	-8.144854206	-8.299029761	-5.869695805
$n=1$	10	-5.184447269	-8.143478565	-8.298523251	-5.86744607

Table 3 Shannon entropy in the momentum space for Den-Fang-Eckart potential for the various diatomic molecules

	l	H_2	CO	ScN	ScF
	0	121.276769869	143.314106524	170.269503852	145.031036395
	1	121.187579759	143.290427687	170.269936680	145.029327771
	2	121.013185383	143.243327291	170.270846509	145.025894486
	3	120.745242151	143.173302507	170.272320473	145.020708780
	4	120.391984086	143.081060723	170.274486997	145.006120654
	5	119.945058796	142.967481250	170.277512968	145.005026906
	6	119.406705442	142.833569514	170.281601186	144.994603363
	7	118.775847060	142.680403570	170.286987645	144.982448359
	8	118.050074195	142.509073083	176.728516488	144.968653046
	9	117.218678570	151.526211472	170.302754660	144.953135497
$n=0$	10	116.296602616	151.309198167	170.313772207	144.937644228
	0	16.453519668	21.563592815	27.424020660	19.114338551
	1	16.444710796	21.562736035	27.421793368	19.113450554
	2	16.426705049	21.561031048	27.417255402	19.111698912
	3	16.399931834	21.558538899	27.410158994	19.109131160
	4	16.364496548	21.555283629	27.400581966	19.105839113
	5	16.321140810	21.551357776	27.387842709	19.101919295
	6	16.265017477	21.546855797	27.371453558	19.097425774
	7	16.202243755	21.541867924	27.351258604	19.087176083
	8	16.129198256	21.532389135	27.326542326	19.080807502
	9	16.047409342	21.526218936	27.296577611	19.076322636
$n=1$	10	15.952870090	18.3968927187	27.261009708	19.072209244

Table 4 Fisher information for Den-Fang-Eckart potential for the various diatomic molecules for $n=0$

	l	H_2	CO	ScN	H_2	CO	ScN	ScF
ScF								
	0	0.184554	6.15177	9.428159473	1.015468418	0.252762476	0.131741055	0.140447318	0.51809012
	1	0.183463	6.15122	9.427826073	1.015322390	0.254338313	0.131752930	0.140452330	0.51816569
	2	0.181297	6.15013	9.427159296	1.015030371	0.257523898	0.131776684	0.140462355	0.51831688
	3	0.178087	6.14848	9.426159180	1.014592442	0.262388498	0.131812327	0.140477395	0.51854378
	4	0.173881	6.14628	9.424825791	1.014008720	0.269039721	0.131859871	0.140497451	0.51884651
	5	0.168739	6.14353	9.423159207	1.013279363	0.277628270	0.131919335	0.140522527	0.51922527
	6	0.162735	6.14024	9.421159535	1.012404566	0.288354810	0.131990742	0.140552627	0.51968028
	7	0.155954	6.1364	9.418826918	1.011384567	0.301479479	0.132074117	0.140587755	0.52021181
	8	0.148490	6.13201	9.416161449	1.010219641	0.317334820	0.132169495	0.140627916	0.52082018
	9	0.140444	6.12707	9.413163339	1.008910100	0.336343244	0.132276910	0.140673116	0.52150576
$n=0$	10	0.131923	6.12159	9.409832765	1.007456299	0.359040623	0.132396403	0.140723363	0.52226895

Note. The numerical values for in the position space are in the order of 10^6

Left: Numerical for position space. **Right:** Numerical for momentum space

Table 5 Fisher information in the position space for Den-Fang-Eckart potential for the various diatomic molecules for $n=1$

	l	H_2	CO	ScN	ScF	H_2	CO	ScN	ScF
	0	0.51456	1.86057	2.85697	0.306287	0.0292067911	0.013461699	0.014304760	0.053181433
	1	0.51153	1.86041	2.85687	0.306243	0.0293876876	0.013462911	0.014305272	0.053189198
	2	0.50552	1.86007	2.85666	0.306155	0.0297533558	0.013465331	0.014306297	0.053204713
	3	0.49662	1.85958	2.85635	0.306022	0.0303117102	0.013468978	0.014307789	0.053227956
	4	0.48495	1.85891	2.85597	0.305846	0.0310750450	0.013473836	0.014309928	0.053259012
	5	0.47068	1.85808	2.85547	0.305627	0.0320605769	0.013479909	0.014312520	0.053297935
	6	0.45402	1.85708	2.85485	0. 305363	0.0332912243	0.013487202	0.014315523	0.053344601
	7	0.43519	1.85592	2.85415	0.305055	0.0347966934	0.013495728	0.014319114	0.053399162
	8	0.41447	1.85459	2.85334	0. 304704	0.0366149481	0.013505468	0.014323205	0.053461602
	9	0.39212	1.8531	2.85242	0.304309	0.0387942000	0.013516428	0.014327737	0.053531962
$n=1$	10	0.36844	1.85144	2.85142	0.303870	0.0413955905	0.013528654	0.014332890	0.053610275

Note. The numerical values for in the position space are in the order of 10^6

Left: Numerical for position space. **Right:** Numerical for momentum space

Table 6 Renyi Entropy for Den-Fang-Eckart potential for the various diatomic molecules for $n=0$

	l	H_2	CO	ScN	ScF	H_2	CO	ScN	ScF
	0	-10.776227109	-13.157834276	-13.306782740	-10.888578009	8.386529681	12.103631200	12.490650203	9.626459008
	1	-10.767039556	-13.157699471	-13.30672937	-10.888360243	8.377469559	12.103495972	12.490597728	9.626242231
	2	-10.748638599	-13.157429847	-13.306622632	-10.887924675	8.359324413	12.103225498	12.490492773	9.625808640
	3	-10.720971930	-13.157025373	-13.306462518	-10.887271237	8.332037326	12.102819746	12.490335331	9.625158161
	4	-10.683959533	-13.156486008	-13.306249021	-10.886399825	8.295531110	12.102332316	12.490125389	9.624290683
	5	-10.637491771	-13.155811691	-13.305982132	-10.885310297	8.249693382	12.101658617	12.4898629301	9.623206057
	6	-10.581426706	-13.155002348	-13.305661834	-10.884002481	8.194380364	12.101107504	12.4895479344	9.621904098
	7	-10.515586558	-13.154057892	-13.30528813	-10.882476166	8.129412025	12.100176361	12.4891803741	9.620384588
	8	-10.439753161	-13.15297822	-13.304860988	-10.880731108	8.054567489	12.099111587	12.4887602199	9.618647268
	9	-10.353662199	-13.151763212	-13.304380392	-10.878767026	7.969579230	12.097912919	12.4882874362	9.616675389
$n=0$	10	-10.256995941	-13.150412737	-13.303846324	-10.876583606	7.874125740	12.096580055	12.4877619821	9.614518009

Left: Numerical for position space. **Right:** Numerical for momentum space

Table 7 Renyi Entropy for Den-Fang-Eckart potential for the various diatomic molecules for $n=1$

	l	H_2	CO	ScN	ScF	H_2	CO	ScN	ScF
	0	-5.853999607	-8.288051574	-8.438188357	-6.017036408	15.479048629	21.357388269	21.815316037	18.58273250
	1	-5.844839231	-8.287916572	-8.438135228	-6.016819025	15.470307710	21.357282425	21.815105912	18.58250969
	2	-5.826492682	-8.287645876	-8.438028973	-6.016383490	15.452798697	21.357068995	21.814685519	18.58206467
	3	-5.798907752	-8.287242282	-8.437863369	-6.015728583	15.426466619	21.356740206	21.814060791,	18.58139835
	4	-5.762004566	-8.286703019	-8.437663308	-6.014856867	15.391227465	21.356291085	21.813206395	18.58050778
	5	-5.715673773	-8.286028342	-8.437401832	-6.013769506	15.346966113	21.355710564	21.812148684	18.57939137
	6	-5.659773707	-8.285218739	-8.437072727	-6.012460781	15.293533764	21.354983862	21.810893083	18.57805463
	7	-5.594127023	-8.284275401	-8.436700880	-6.010935186	15.230744154	21.354091572	21.809413729	18.57649256
	8	-5.51851607	-8.283195117	-8.436273859	-6.009190646	15.158368967	21.353014275	21.807721867	18.57470751
	9	-5.432677212	-8.281978164	-8.435783382	-6.007226983	15.076131824	21.241126726	21.805824366	18.57270022
$n=1$	10	-5.336293549	-8.280630373	-8.435254327	-6.005043571	14.983700843	21.236680652	21.803694699	18.57047247

Left: Numerical for position space. **Right:** Numerical for momentum space