

Information entropies for H₂ and ScF diatomic molecules with Deng- Fan-Eckart potential

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In this paper, the Shannon entropy and Fisher information is investigated with molecular Deng-Fan-Eckart potential for the diatomic molecules H₂ and Shannon entropy and Fisher 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 only two low lying states corresponding to the ground and first excited states. The results are obtained numerically for these diatomic molecules. Localization is observed for the Shannon entropy and delocalization for the Fisher information for the two diatomic molecules considered in position and momentum spaces. The Shannon entropy and the Fisher information measures for the two diatomic molecules satisfied the Bialynicki-Birula and Mycielski and the Stam-Cramer-Rao inequalities uncertainty relation, respectively.

Keywords: Information entropies; Shannon entropy; fisher information; Deng-Fan-Eckart potential; uncertainty relations.

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1. Introduction

The information-theoretic measures have received a great research interest in quantum mechanical systems over the years. These are largely due to its applications in probability density function 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 areas such as communication [4], physical sciences [5], chemical sciences [6], and other disciplines that have connections with quantum information systems [7-8]. Quantum information-theoretic measures quantify uncertainty, and these measures are classified as either global or local measures. 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]. Quantum information theory is a very important tool in the uncertainty measures of atoms and molecules, and of all these quantum information measures, the Shannon entropy and Fisher information have been exhaustively studied than other information-theoretic tools [2, 14]. 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 for chemical bonding [16], and it can also be applied in the

comparison of molecular interactions [17-18]. Several research works have been carried out for information-theoretic measures both analytically and numerically. For instance, Isonguyo *et al.* [19] investigate the different information-theoretic tools for the screened Coulomb potential. On the other hand Onate *et al.* [20] investigated the dissociation energy effect on the Shannon entropy and Renyi entropies. Romera *et al.* [15] studied analytically the behavior of Fisher information for the central potential for a single particle system and established a novel uncertainty relation that is satisfied for any central potential model. Amadi *et al.* [21] analyzed comparatively the screened Coulomb potential and screened Kratzer potential in three dimensions for Shannon entropy and Fisher Information. Another application of the Fisher information is in the study of the Schrödinger equation in the presence of external electrical and magnetic effects in atomic systems [22]. The Shannon and Fisher information has been studied for position-dependent mass within the framework of non-relativistic quantum mechanics [23-25]. This study will offer more information in the applications to semiconductors and quantum dots. Information entropies have been investigated for scaling behavior properties [26-28], confined systems [29-32], shape effect of quantum heterostructures [33], among others [34-41]. In recent times, there are very little research works on information theory with exponential type potentials, and to the best of our knowledge, no application of diatomic molecules for exponential type potential has 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.* [42] studied the DFEP model for some selected diatomic molecules. The choice of this potential stems from the fact that it exhibits an almost exact behavior 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: Section 2 is devoted to the solutions of the Eigen solutions of the DEFP. Section 3 tabulates the spectroscopic values of the diatomic molecules. Section 4 is concerned with the information entropy, where we examine the Shannon entropy and Fisher information. Finally, we give a brief conclusion in Sec. 5.

2. Eigensolution of DFEP

The Deng-Fan-Eckart potential is defined as [42],

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

where, $b = e^{-\delta r_e} - 1$, D_e , r , δ , and r_e are the dissociation energy, internuclear distance, potential range, and molecular bond length, respectively. V_1 and V_2 are potential strengths. Using the Pekeris type approximation [43] for the centrifugal approximation term in the Schrödinger equation [44], Edet *et al.* [42] derived analytical expressions for the energy values and the corresponding wave function for the DFEP using the factorization method [45] as,

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

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

where,

$$v = \frac{1}{2} + \frac{1}{2} \sqrt{(2l+1)^2 + \frac{8\mu D_e b}{\hbar^2 \delta^2} + \frac{8\mu V_2}{\hbar^2 \delta^2}},$$

$$\lambda = \sqrt{\varepsilon + k d_0}, \quad \omega = \frac{1}{2} + \sqrt{\frac{1}{4} + \eta_1 + \beta_2 + k},$$

$$d_0 = \frac{1}{12}, \quad k = l(l+1) \quad \text{and} \quad s = e^{-\delta r}. \tag{4a}$$

Other parameters are defined in Ref. [42], $Y_{l,m}(\Omega)$ is the angular component of the wave function [30]. Using the MATHEMATICA software [45], we obtained the normalization constant for the radial component for the ground state from Eq. (3) in three dimensions as follows [21].

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

where,

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

and $\psi^{(n)} = \Gamma'(x)/\Gamma(x)$ being the polygamma function. H_n is the Harmonic number [9,19] and γ is the Euler Gamma defined by [46], $\gamma = \lim_{n \rightarrow \infty} (\sum_{k=1}^n (1/k) - \ln n)$, where the first term is Harmonic number. The probability density for the ground states [47] in the position space is calculated as follows,

$$\rho_0(\vec{r}) = \left[\frac{\delta^3 \Gamma(1 + 2\omega + 2\lambda)}{\sigma \Gamma(1 + 2\omega) \Gamma(\lambda)} \right] (s)^{2\lambda} (1-s)^{2\omega}. \tag{6}$$

The momentum-space wave function is obtained by taking the Fourier transformation [48] of the position space wave function. For the ground state, the momentum space wave function is given as,

$$\phi_0(\vec{P}) = N_0^2 \left| \frac{(i\Gamma[1 + 2\omega] (\Gamma[-\frac{ip}{\delta} + \lambda] \Gamma[\frac{ip}{\delta} + \lambda + \omega] \Omega + \Theta X))}{(\delta^2 p \sqrt{2\pi} \Gamma[1 + \lambda + \omega + \frac{ip}{\delta}] \Gamma[1 + \omega - \frac{ip}{\delta} + \lambda])} \right|^2, \tag{7}$$

where,

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

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

$$X = \psi^{(0)} \left(1 + \lambda + \omega + \frac{ip}{\delta} \right) - \psi^{(0)} \left(\lambda + \frac{ip}{\delta} \right). \tag{8c}$$

However, due to the difficulty and complexity of the integral expression in the momentum state at the first excited state, we solved for the first excited state in position and momentum spaces numerically.

Figures 1 and 2 shows the characteristic behaviors of the probability densities, which are plotted in position and momentum space, respectively. From the plots, we observed that ScF is more concentrated than H₂ and so shows a higher localization.

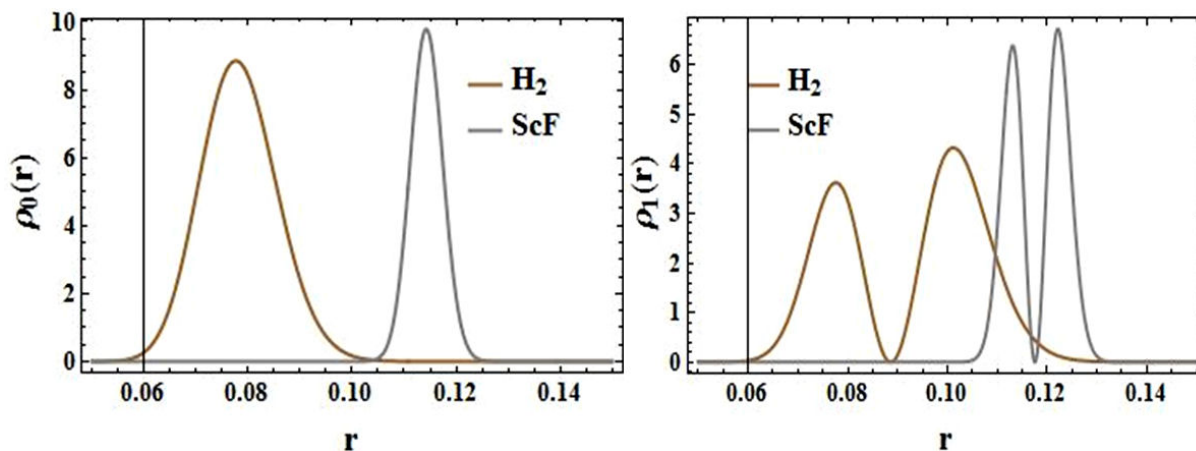


FIGURE 1. Probability densities in the position space for the selected diatomic molecules at the ground and excited state for $l = m = 0$.

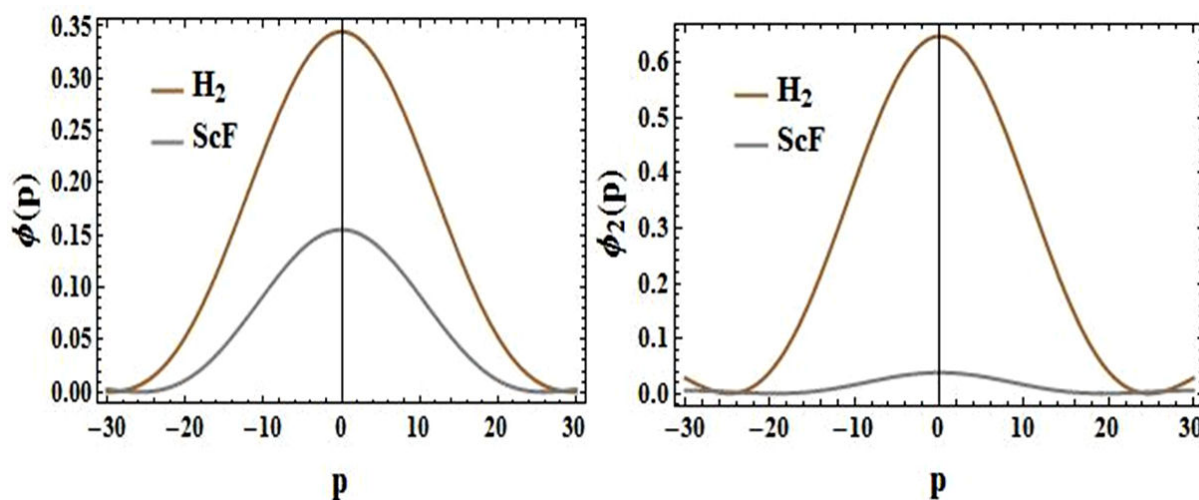


FIGURE 2. Probability density in momentum space for the selected diatomic molecules at ground and excited state for $l = m = 0$.

TABLE I. Spectroscopic parameter of some selected diatomic molecules.

Molecules	D_e (cm^{-1})	r_e (\AA)	α (\AA^{-1})	μ (amu)
H ₂	38,266	0.7416	1.9426	0.50391
ScF	47,183.43	1.794	1.46102	13.35894

3. Spectroscopic values for some diatomic molecules

Many interesting studies have been investigated on Shannon entropies and Fisher information with different potential models in recent times [50-53]. Here, we intend to study the quantum information-theoretic measures for the diatomic molecules of H₂ and ScF. These selected diatomic molecules are homonuclear and heteronuclear, respectively. These diatomic molecules possess the same properties as each diatomic molecule is made of two atoms only and differ from each other in terms of covalent bonding and their geometric structure [54, 55]. Our choice of these two molecules is

based on the available data of their spectroscopic parameters as given in Table I. Hence, we intend to observe their quantum measures in the study. We take the experimental values of the spectroscopic parameters for each of the diatomic molecules from Ref. [42].

4. Information entropies

4.1. Shannon entropy

In this section, the quantum information-theoretic measures for Shannon entropy and Fisher information in position and momentum spaces will be calculated. Shannon entropy, which is regarded as a logarithmic probability density, investigates the concentration of the probability densities spread in a quantum system. It is defined for position and momentum spaces in spherical polar coordinate as [30];

$$S_r = - \int \rho(r) \ln \rho(r) r^2 dr, \quad (9)$$

$$S_p = - \int \phi(p) \ln \phi(p) p^2 dp, \tag{10}$$

$$S_{\theta,\phi} = - \int \gamma(\theta) \ln \gamma(\theta) \sin(\theta) d\theta \tag{11}$$

$$S_T = 2\pi[S_r + S_p + S_{\theta,\phi}] \tag{12}$$

where S_r , S_p , and $S_{\theta,\phi}$ are position Shannon entropy, momentum Shannon entropy, the angular component of Shannon entropy, and S_T is the total Shannon entropy, respectively. The probability densities are $\rho(r) = |\psi(r)|^2$, $\Phi(r) = |\psi(p)|^2$, and $\gamma(\theta) = |\Theta(\theta)|^2$. The angular component of Shannon entropy is constant for both spaces. Now using Eqs. (10-12), we obtain the numerical values of the Shannon entropies for the two diatomic molecules, which validate the BBM uncertainty relation [30] as shown in Tables II and III. One of the consequences of the BBM inequality is that it represents the lower bound values of the Shannon entropy sum [30, 49] such that, if the position entropy increases, then the momentum entropy will decrease in such a way that their sum bounds above (BBM) inequality. The Shannon entropy uncertainty relation was established by Berkner, Bialynicki-Birula, and Mycielski (BBM) and is expressed as [49-51],

$$S_t = 2\pi[S_r + S_p + S_{\theta,\phi}] \geq D(1 + \ln \pi) \tag{13}$$

where, D is the spatial dimension.

Tables II and III show the numerical results for the Shannon entropies of the two diatomic molecules of and ScF for the ground and excited states in the position and momentum spaces. In Table II, we observed that the Shannon entropies in the position space are all negative in the ground and excited state. This behavior 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 and less uncertainty. More so, in the first excited state, there is a decrease in the Shannon entropy values in the position space, which reaffirms its delocalization of H₂ diatomic molecules. Similarly, in Table III,

high localization is observed for ScF diatomic molecule in the position space as its Shannon entropy values dropped for increasing angular momentum quantum number l . In the momentum space, we observed a decreasing Shannon entropic value for both diatomic molecules at the first excited state, and hence there is an occurrence of localization for the two diatomic molecules. Subsequently, the computed Shannon entropies in the position and momentum spaces for the two diatomic molecules satisfied the BBM uncertainty relation.

4.2. Fisher information

On the other hand, the Fisher Information is a local measure of information entropy and has a differential component which makes it very sensitive to detect local changes that occur in the probability density. Fisher information, usually regarded as the measure of information entropy [14, 38], is the control of localization of the probability density. It can be seen as a measure of oscillator degree, which has applications in quantum mechanical kinetic energy of the system [54]. Thus, Fisher information in position space and momentum space is expressed as [14,38]

$$I_r = \int \frac{\nabla \rho(\vec{r})}{\rho(\vec{r})} d\vec{r}, \tag{14}$$

$$I_p = \int \frac{\nabla \phi(\vec{r})}{\phi(\vec{r})} d\vec{r}. \tag{15}$$

In the theory of Fisher information, the higher the Fisher information, the higher the accuracy of predicting the localization of the system and thus increasing the Fisher information increased the fluctuation of the system. Generally, for an arbitrary angular momentum quantum number l of any central potential model, the two products of the Fisher information must satisfy the the Stam, Cramer-Rao inequality [15],

$$I_r I_p \geq 4 \langle r^2 \rangle \langle p^2 \rangle \left[2 - \frac{2l+1}{l(l+1)} |m| \right]^2, \tag{16}$$

where $m = 0, \pm 1, \pm 2 \dots$ is the magnetic quantum number.

TABLE II. Shannon entropy in the position space for H₂ diatomic molecules

n	l	S_r	S_p	$S_{\varphi,\theta}$	S_t
0	0	-8.5615577582	12.0463422727	2.5310242469	53.7013355814
1	0	-8.2329583587	13.9224628761	2.5310242469	67.5539999101
	1	-8.2238032731	13.9136537663	2.0990786246	62.1281849644

TABLE III. Shannon entropy for ScF diatomic molecule.

n	l	S_r	S_p	$S_{\varphi,\theta}$	S_t
0	0	-8.6861099573	14.4531162093	2.5310242469	68.0409576704
1	0	-8.4105519485	16.5893973167	2.5310242469	83.1949897682
	1	-8.4103361211	16.5885734544	2.0990786246	77.7631805966

TABLE IV. Fisher Information for the diatomic molecules.

		H ₂		ScF	
n	l	I_r	I_p	I_r	I_p
0	0	7.2812768317	18699.31566	40.0634648239	102888.46210
1	0	20.0364861998	51456.43944	119.2641535616	306286.67286
	1	19.9186301824	51153.76904	119.2470271964	306242.69001

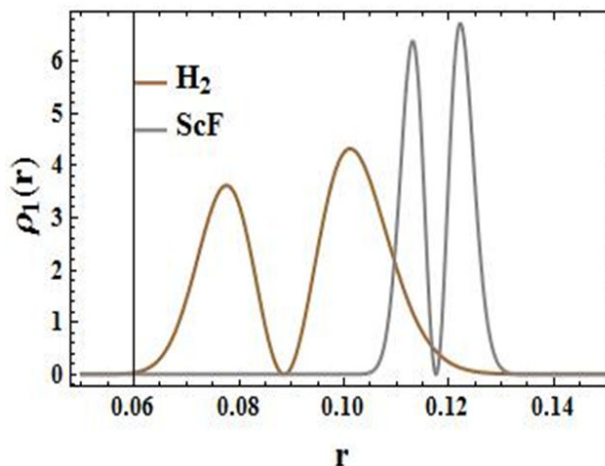
In Tables IV, we compute numerically the Fisher information in the position and momentum spaces for the diatomic molecules of H₂ and ScF at the ground and excited states for different quantum numbers. We observed that the Fisher information values increase as it transits from the ground state to the excited state. At the excited state, Fisher information decreases as the orbital angular momentum quantum l is increased. This behavior is observed for the two diatomic molecules, which indicate the presence of fluctuation and delocalization in the diatomic molecules. Finally, the Stam-Cramer-Rao inequality relation is satisfied for the two diatomic molecules.

5. Conclusions

In this work, we have studied the quantum information measures for Shannon entropy and Fisher information for the two selected diatomic molecules of H₂ and ScF in the position and momentum spaces numerically at the ground and first excited states. Each diatomic molecule investigated satisfied the BBM inequality for the Shannon entropy and Stam-Cramer-Rao inequality relation for the Fisher information. In this study, we have shown that H₂ that ScF satisfied the uncertainty relations for Shannon and Fisher information at the ground and excited states.

6. Graphical abstract text and image

In this study, the Shannon entropy and Fisher information is investigated with molecular Deng-Fan-Eckart potential for the diatomic molecules H₂ and ScF in position and momentum spaces in three dimensions. Localization is observed for the Shannon entropy and delocalization for the Fisher information for the two diatomic molecules considered in position and momentum spaces. The Shannon entropy and the Fisher information measures for the two diatomic molecules satisfied the Bialynicki-Birula and Mycielski (BBM) and the Stam-Cramer-Rao inequalities uncertainty relation respectively.



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1. R.G. Parr, and W. Yang, *Density-Functional Theory of Atoms and Molecules*, (Oxford University Press, New York, 1989).
2. C.E. Shannon, *Bell Syst. Tech. J.* **27** (1948) 623. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>
3. M.A. Nielsen, and I.L. Chuang, *Quantum Computation and Quantum Information*, (Cambridge University Press, Cambridge, 2000).
4. M. Wilson, *Nanotechnology, Basic Science and Emerging Technologies*, (CRC Press, New York 2003).
5. J. S. Dehesa, S. Lopez-Rosa, A. Martínez-Finkelshtein, and R. J. Yañez, *Int. J. Quantum Chem.* **110** (2010) 1529. <https://doi.org/10.1002/qua.22244>
6. P. Karafiloglou, and C. P. Panos, *Chem. Phys. Lett.* **389** (2004) 400. <https://doi.org/10.1016/j.cpllett.2004.03.118>
7. F. Franchini, A. R. Its, and V. E. Korepin, *J. Phys. A: Math. Theor.* **41** (2008) 025302. <https://doi.org/10.1088/1751-8113/41/2/025302>
8. E. Romera, and F. de Los Santos, *Phys. Rev. A* **78** (2008) 013837. <https://doi.org/10.1103/PhysRevA.78.013837>
9. S. Dong, G. H Sun, S. H, Dong, and J P. Draayer, *Phys. Lett. A.* **378** (2014) 124. <https://doi.org/10.1016/j.physleta.2013.11.020>
10. Pooja, R. Kumar, G. Kumar, R. Kumar, and A. Kumar, *Int. J. Quantum Chem.* **116** (2016) 1413. <https://doi.org/10.1002/qua.25197>
11. A. Renyi, in *Proc. 4th Symp. on Mathematics, Statistics and Probability*, (Berkeley University Press, Berkeley 1960).
12. C. Tsallis, *J. Stat. Phys.* **54** (1988) 479. <https://doi.org/10.1007/BF01016429>
13. O. Onicescu, *C. R. Acad. Sci. Paris. A*, **263** (1966) 25.
14. R. A. Fisher, *Proc. Camb. Philos. Soc.* **22** (1925) 700. <https://doi.org/10.1017/S0305004100009580>
15. E. Romera, P. Sánchez-Moreno, and J. S. Dehesa, *Chem. Phys. Lett.* **414** (2005) 468. <https://doi.org/10.1016/j.cpllett.2005.08.032>
16. R. O. Esquivel *et al.*, *J. Phys. Chem. A* **114** (2010) 1906. <https://doi.org/10.1021/jp908898w>
17. A. Nagy, *Int. J. Quantum Chem.* **115** (2015) 1392.
18. D. Chakraborty and P. W. Ayers, in *Statistical Complexity: Applications in Electronic Structure*, (K. D. Sen (Ed.), Springer, 2012).
19. C. N. Isonguyo, K. J. Oyewumi, and O. S. Oyun, *Int. J. Quant. Chem.* **118** (2018) 025620. <https://doi.org/10.1002/qua.25620>
20. C.A. Onate, A.N. Ikot, M.C. Onyeaju, O. Ebomwonyi, and J.O.A. Idiodi, *J. Mod Sci* **4** (2018) 134e142. <https://doi.org/10.1016/j.kijoms.2017.12.004>
21. P.O. Amadi, Ikot, A. T. Ngiangia, U. S. Okorie, G. J. Rampho, and H. Y. Abdullah, *Int. J. Quant. Chem.* **120** (2020) e26246. <https://doi.org/10.1002/qua.26246>
22. R. González-Férez, and J.S. Dehesa, *Eur. Phys. J. D* **32** (2005) 39. <https://doi.org/10.1140/epjd/e2004-00182-3>
23. B. J.Falaye, F. A. Serrano, and S. H. Dong, *Physics Letters A.* **380** (2016) 267. <https://doi.org/10.1016/j.physleta.2015.09.029>
24. D. X. Macedo, and I. Guedes, *Phys A* **434** (2015) 211. <https://doi.org/10.1063/1.4962923>
25. S. Guo-Hua, P. Du ˘san, C. N. Oscar, and S. H. Dong, *Chin Phys B* **24** (2015) 10.
26. A. Abdel-Hady, and I. Nasser, *Appl. Math. Inf. Sci.* **4** (2018) 12. DOI:10.18576/amis/120406
27. I. Nasser, M. S. Abdelmonem, and A. Abdel-Hady, *Phys. Scr.* **84** (2011) 045001. <https://doi.org/10.1088/0031-8949/84/04/045001>
28. M. S. Abdelmonem, A. Abdel-Hady, and I. Nasser, *Mol. Phys.* **115** (2017) 1480. <https://doi.org/10.1080/00268976.2017.1299887>
29. L. G. Jiao, R. Z. Li, Z. Z. Yong, and K. H. Yew, *Int. J. Quant. Chem* **13** (2017) 117.
30. N. Mukherjee, and A. K. Roy, *Int. J. Quant. Chem* **21** (2018) 118. <https://doi.org/10.1002/qua.25596>
31. N. Mukherjee, and A. K. Roy, *J. Math. Chem* **7** (2019) 57. <https://doi.org/10.1007/s10910-019-01039-8>
32. D. Munjal, K. D Sen, and V. Prasad, *J. Phys. Commun.* **2** (2017) 2. <https://doi.org/10.1063/1.5008949>
33. C. A. Onate, M. C. Onyeaju, A. N. Ikot, O. Ebomwonyi, and J. O. A. Idiodi, *Int J Quant Chem.* **19** (2019) 119. <https://doi.org/10.1002/qua.25991>
34. N. Sobrino-Coll, D. Puertas-Centeno, I. V. Toranzo, and J. S. Dehesa, *J. Stat. Mech.* **8** (2017) 083102. <https://doi.org/10.1088/1742-5468/aa7df4>
35. A. K. Roy, *Mod. Phys. Lett. A* **29** (2014) 1450042. <https://doi.org/10.1142/S0217732314500424>
36. Etebong E. Ibekwe, Alalibo T. Ngiangia, Uduakobong S. Okorie, Akpan N. Ikot, and Hewa Y. Abdullah, *IRAN J SCI TECH-NOL A.* (2020).
37. A. Ghosal, N. Mukherjee, and A. K. Roy, *Ann. Phys.* **528** (2016) 796. <https://doi.org/10.1002/andp.201600121>
38. W. A. Yaha, K. J. Oyewumi, and K. D. Sen, *Int. J. Quantum Chem.* **115** (2015) 1543.
39. S. A. Najafizade, H. Hassanabadi, and S. Zarrinkamar, *Chin. Phys. B.* **25** (2016) 4. <https://doi.org/10.1088/1674-1056/25/4/040301>
40. N. Sobrino-Coll, D. Puertas-Centeno, I. V. Toranzo, and J. S. Dehesa, *J. Stat. Mech.* **8** (2017) 083102.
41. C.A Onate, L. S. Adebisi, and D. T. J. Bankole, *Theor. and Comp Chem*, **2** (2020)19 2050007.
42. C. O. Edet, U. S. Okorie, G. Osobonye, A. N. Ikot, G. J. Rampho, and R. Sever, *J. Math Chem* **58**, (2020) 989. <https://doi.org/10.1007/s10910-020-01107-4>
43. M. Hamzavi, S. M. Ikhdair, and K. E. Thylwe, *J. Math Chem* **51** (2013) 227. <https://doi.org/10.1007/s10910-012-0075-x>

44. S. H. Dong, I. (Springer-Verlag, Berlin. 2007).
45. Wolfram Research, Inc., Mathematica, Version 9.0, Champaign, IL (2012).
46. R. L. Graham, D. E. Knuth, and O. Patash, *Concrete Mathematics: A Foundation for Computer Science*, 2nd Ed. Reading, MA: Addison-Wesely, 1994.
47. W. Greiner, *Quantum Mechanics an Introduction*, 4th ed., (Springer-Verlag Berlin, Heidelberg, New York 2000).
48. C. Brown, M. *Ford Standard Level Chemistry* (2nd ed.). (Prentice Hall. 2014).
49. I. N. Levine, *Quantum Chemistry*; 5th Edition; (Pearson/Prentice Hall; 2009).
50. N. Mukherjee, S. Majumdar, and A. K. Roy, *Chem. Phys. Lett.* **691** (2018) 449. <https://doi.org/10.1016/j.cplett.2017.11.059>
51. I. Bialynicki-Birula, and J. Mycielski, *Commun. Math. Phys.* **44** (1975) 129. <https://doi.org/10.1007/BF01608825>
52. S. B. Sears, R. G. Parr, and U. Dinur, *Israel J. Chem.* **19** (1980) 165. <https://doi.org/10.1002/ijch.198000018>
53. Y. J. Shi, G. H. Sun, Jian Jing, and S. H. Dong, *Laser Phys.* **27** (2017) 125201. <https://doi.org/10.1088/1555-6611/aa8bbf>
54. A. J. Torres-Arenas, Q. Dong, G. H. Sun, and S. H. Dong, *Phys Letters A* **26** (2018) 382. <https://doi.org/10.1016/j.physletb.2018.12.010>
55. Q. Dong, A. J. Torres-Arenas, G. H. Sun, and S. H. Dong, *Laser Phys. Lett.* **15** (2018) 115202. <https://doi.org/10.1007/s11467-018-0876-x>