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Effect of dissociation energy on Shannon and Rényi entropies

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Abstract

The analytical solutions of the three dimensional Schrödinger equation for the Generalized Morse potential is obtained via parametric Nikiforov−Uvarov method and Formula method. The results are compared with the results obtained from two other methods. The results obtained are found to be in good agreement with the previous results. Thereafter, the position space and momentum space Shannon entropy and Rényi entropy are calculated using a new approach (integral limit) which is more straight forward and less cumbersome. The effect of the dissociation energy on the Shannon entropies is investigated in detail. This is then applied to the Morse potential well. The point of maximum stability of a particle in a system for both Shannon entropy and Rényi entropy are also investigated. The results obtained obey the Heisenberg uncertainty principle and are in agreement with those in the literature.

Keywords: Entropic system; Potential well; Position space; Momentum space; Uncertainty relation

1. Introduction

Quantum information is an important phenomenon in physics and modern communication system which plays an important role in the measurement of uncertainty and other parameters of a system [1]. The quantum information has some basic measures or quantities which are Shannon entropy and Fisher information [2−6]. The basic measures or quantities have numerous applications in different fields of studies such as engineering, computer science, medicine, chemistry and physics. Hence, various research works have been carried out on the quantities with various potential terms in the last few years. Among the research works include, Yañez-Navarro et al. [7], investigated Shannon entropy for position-dependent Schrödinger equation of a particle with non-uniform solitonic mass density in the case of a trival null potential. In their results, the Shannon entropy in position space decreases for narrower mass width while in the momentum space, the Shannon entropy increases for narrower mass width. Najafizade et al. [8,9], investigated the non-relativistic Shannon entropy for both the Kratzer potential and the Killingbeck potential respectively. Their results for the Kratzer potential shows that, the Shannon entropy in

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position space decreases as the potential parameter increases while the momentum space Shannon entropy increases as the potential parameter increases. The results from the Killingbeck potential indicates that $S(\rho)+S(\gamma)\geq D+D\log\pi$ where, D is a spatial dimension. Serrano et al. [10], studied information theoretic measures for solitonic profile mass Schrödinger equation with a squared hyperbolic cosecant potential. In their results, the Shannon entropy in position space decreases as the potential parameter increases while in the momentum space, Shannon entropy increases as the potential parameter increases. Yahya et al. [11], studied quantum information entropies for any $\ell-$ state Pöschl-Teller-type potential. In their study, they investigated the Fisher information based uncertainty relations and Cramer-Rao products for the Pöschl-Teller-type potential model. They however observed that the Heisenberg uncertainty principle for any $\ell-$ state is satisfied for the potential model. Falaye et al. [1], studied Fisher information for the position-dependent mass Schrödinger system with hyperbolic potential. In their results, Fisher information based uncertainty relation and Cramer-Rao inequality and Heisenberg uncertainty principle holds. In this study, we intend to investigate the effect of dissociation energy on Shannon entropy, Rényi entropy and potential well respectively in the field of Generalized Morse potential.

The Generalized Morse potential was proposed by Deng and Fan [12] and was first called simple modified Morse potential to describe diatomic molecular energy spectra and electromagnetic transition. The later name (Generalized Morse) was called by Mesa et al. [13]. The Generalized Morse potential takes the form [14–16].

$$V_{GM}(r)=D_e\left(1-\frac{be^{-\alpha r}}{1-e^{-\alpha r}}\right)^2, \tag{1}$$

where, $0\leq r<\infty$, $b=e^{\alpha r_e}-1$, the parameters D_e denotes the dissociation energy, b is the position of the minimum r_e while α is the range of the potential. This potential is equivalent to the improved Manning-Rosen potential and the Deng-Fan potential model. The Generalized Morse potential has the correct physical boundary conditions at the origin and at infinity [13]. This potential has been studied extensively in both relativistic and non-relativistic quantum mechanics. For instance, Codriansky et al. [17], obtained the eigenvalues and eigenfunctions of the Generalized Morse potential for the case of $\ell=0$ by using $SO\ (2,1)$ algebra method. Zhang et al. [18], obtained approximate solutions of the Schrödinger equation with Generalized Morse potential model including the centrifugal term. Chen et al. [19], obtained the solutions of the Klein–Gordon equation in D dimensions with the Generalized Morse potential. Ikot et al. [20], investigated approximate solutions of the Klein–Gordon equation with the Generalized Morse potential model in D dimensions using SUSY QM. Dong and Gu [21], studied approximate bound state solutions of the Schrödinger equation with the Generalized Morse potential. This potential can be transformed into other useful potentials such as Tietz potential and Morse potential. Its diverse applications also necessitates this study.

2. The radial Schrödinger equation with the Generalized Morse potential

The three-dimensional time-independent Schrödinger equation in the presence of any physical potential model is given as

$$\left(\frac{p^2}{2\mu}-E_{n,\ell}+V(r)\right)\psi_{n,\ell,m}(r)=0, \tag{2}$$

where μ is the reduced mass, $E_{n,\ell}$ is the non-relativistic energy of the system, $\psi_{n,\ell,m}(r)$ is the wave function and $V(r)$ is the interacting potential. Setting the wave functions $\psi_{n,\ell,m}(r)=U_{n,\ell}(r)Y_{\ell,m}(\theta,\varphi)r^{-1}$, we have the radial Schrödinger equation as

$$\left(\frac{d^2}{dr^2}-\frac{2\mu}{\hbar^2}\left(V(r)+\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right)\right)U_{n,\ell}(r)=-E_{n,\ell}U_{n,\ell}(r). \tag{3}$$

By substituting the potential (1) into Eq. (3), we have the following second order differential equation

$$\frac{d^2U_{n,\ell}(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[E_{n,\ell}-D_e\left(1-\frac{b}{e^{\alpha r}-1}\right)^2-\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]U_{n,\ell}(r)=0. \tag{4}$$

It is noted that Eq. (4) cannot be solved analytically for the case of $\ell = 0$ due to the presence of the centrifugal barrier $\frac{\ell(\ell+1)}{r^2}$. However, Dong and Gu [21], solved approximately Eq. (4) by using the conventional approximation scheme to deal with the centrifugal term. Similarly, Zhang et al. [18,22], solved Eq. (4) approximately using an improved approximation scheme to deal with the centrifugal term. This improved approximation scheme is considered suitable and as such, it is chosen for the purpose of this study. The improved approximation scheme [18] is given as

$$\frac{\ell(\ell+1)}{r^2} \approx \ell(\ell+1)\alpha^2\left(C_0 + \frac{e^{-\alpha r}}{(1-e^{-\alpha r})^2}\right), \tag{5}$$

where the parameter C_0 is a dimensionless constant which is obtained by using the following power series [18].

$$\alpha^2\left(C_0 + \frac{e^{-\alpha r}}{(1-e^{-\alpha r})^2}\right) = \alpha^2\left[C_0 + \frac{1}{(\alpha r)^2} - \frac{1}{12} + \frac{(\alpha r)^2}{240} - \frac{(\alpha r)^4}{6048} + 0\left((\alpha r)^2\right)\right]. \tag{6}$$

On substituting the approximation scheme given in Eq. (5) into Eq. (6), we easily have

$$\left[\frac{d^2}{dr^2} + \frac{2\mu E_{n,\ell} - 2\mu D_e}{\hbar^2} - \ell(\ell+1)C_0\alpha^2 + \frac{\frac{2\mu b D_e(2+b)}{\hbar^2}}{1-e^{-\alpha r}}e^{-\alpha r} + \frac{\frac{-2\mu D_e b^2}{\hbar^2} - \ell(\ell+1)\alpha^2}{(1-e^{-\alpha r})^2}e^{-\alpha r}\right]U_{n,\ell}(r) = 0. \tag{7}$$

To use the powerful parametric Nikiforov–Uvarov method, it becomes necessary to do transformation of variable. By defining a variable of the form $y = e^{-\alpha r}$ and substituting it into Eq. (7), we obtain

$$\frac{d^2U_{n,\ell}(y)}{dy^2} + \frac{1-y}{y(1-y)}\frac{dU_{n,\ell}(y)}{dr} + \frac{-A_1y^2 + A_2y - A_3}{(y(1-y))^2}U_{n,\ell}(y) = 0, \tag{8}$$

where

$$A_1 = \ell(\ell+1)(C_0+1) + \frac{2\mu[D_e(1+2b+b^2) - E_{n,\ell}]}{\alpha^2\hbar^2}, \tag{9}$$

$$A_2 = 2\ell(\ell+1)C_0 + \frac{4\mu[D_e(1+b) - E_{n,\ell}]}{\alpha^2\hbar^2}, \tag{10}$$

$$A_3 = \ell(\ell+1)C_0 + \frac{2\mu[D_e - E_{n,\ell}]}{\alpha^2\hbar^2}, \tag{11}$$

On comparing Eq. (8) with equation of the form [23,24].

$$\frac{d^2U_{n,\ell}(s)}{ds^2} + \frac{1-s}{s(1-s)}\frac{dU_{n,\ell}(s)}{ds} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{s^2(1-s)^2}U_{n,\ell}(s) = 0, \tag{12}$$

given by Tezcan and Sever [23] as a standard differential equation used to deduce the energy condition,

$$nc_2 - (2n+1)c_5 + [n(n-1) + 2c_8]c_3 + c_7 + \sqrt{4c_8c_9} + (2n+1)(\sqrt{c_9} + c_3\sqrt{c_8}) = 0. \tag{13}$$

and wave function is given as

$$\psi_{n,\ell}(s) = N_{n,\ell}s^{c_{12}}(1-c_3s)^{-c_{12}-\frac{c_{13}}{c_3}}P_n^{\left(c_{10}-1,\frac{c_{11}}{c_3}-c_{10}-1\right)}(1-2c_3s), \tag{14}$$

We deduced the following for c_i $(i = 1, 2, 3, -, 13.)$.

$$c_1 = c_2 = c_3 = 1, c_4 = 0, c_5 = -\frac{1}{2}, c_6 = \frac{1}{4} + A_1, c_7 = -A_2, c_8 = A_3, c_9 = \frac{1}{4}\left[(1+2\ell)^2 + \frac{8\mu D_e b^2}{\alpha^2\hbar^2}\right], c_{10} = 1 + 2\sqrt{\ell(\ell+1)C_0 + \frac{2\mu D_e b}{\alpha^2\hbar^2} - \frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}}, c_{11} = 4c_9 + 2\left(1 + \sqrt{\ell(\ell+1)C_0 + \frac{2\mu D_e b}{\alpha^2\hbar^2} - \frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}}\right), c_{12} = \sqrt{\ell(\ell+1)C_0 + \frac{2\mu D_e b}{\alpha^2\hbar^2} - \frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}}, c_{13} = -c_{12} - \frac{1}{2} - \frac{1}{2}\sqrt{(1+2\ell)^2 + \frac{8\mu D_e b^2}{\alpha^2\hbar^2}}. \tag{15}$$

Substituting the values of c_i $(i = 1, 2, ---, 9)$ in Eq. (15) into the equation for energy condition Eq. (13), the non-relativistic energy equation for the Generalized Morse potential model is obtained as

$$E_{n,\ell} = D_e + \frac{\ell(\ell+1)C_0\alpha^2\hbar^2}{2\mu} - \frac{\alpha^2\hbar^2}{2\mu}\left[\frac{\frac{2\mu D_e b}{\alpha^2\hbar^2} - \frac{1}{2}\left[(2n+1)\sqrt{(1+2\ell)^2 + \frac{8\mu D_e b^2}{\alpha^2\hbar^2}} - 1\right] - n(n+1)}{2n + 1 + \sqrt{(1+2\ell)^2 + \frac{8\mu D_e b^2}{\alpha^2\hbar^2}}}\right]^2. \tag{16}$$

To obtain the wave function, the parametric constant c_i $(i = 10, --, 13)$ in Eq. (15) are substituted into Eq. (14) to have

$$U_{n,\ell}(s) = N_{n,\ell}s^u(1-s)^v P_n^{(2u,2v-1)}(1-2s), \tag{17}$$

where

$$u = \sqrt{\ell(\ell+1)C_0 + \frac{2\mu D_e}{\alpha^2\hbar^2} - \frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}}, \tag{18}$$

$$v = \frac{1}{2} + \frac{1}{2}\sqrt{(1+2\ell)^2 + \frac{8\mu D_e b^2}{\alpha^2\hbar^2}}. \tag{19}$$

2.1. Approximate solutions of the radial Schrödinger equation via the Formula Method (FM)

Using the Formula method for bound state problem proposed by Falaye et al. [25,26], the condition for the energy equation and the wave function are given as

$$\left[\frac{k_4^2 - k_5^2 - \left[\frac{1-2n}{2} - \frac{1}{2c_3}\left(c_2 - \sqrt{(c_2-c_1)^2 + 4A_1}\right)\right]^2}{2\left[\frac{1-2n}{2} - \frac{1}{2c_3}\left(c_2 - \sqrt{(c_2-c_1)^2 + 4A_1}\right)\right]}\right]^2 = k_5^2, \tag{20a}$$

$$U_{n\ell}(s) = N_{n\ell}s^{k_4}(1-c_3 s)^{k_5}{}_2F_1(-n, n + 2(k_4+k_5); 2k_4+1; c_3 s). \tag{20b}$$

where

$$k_4 = \frac{(1-c_1) + \sqrt{(1-c_1)^2 + 4A_3}}{2}, \tag{20c}$$

$$k_5 = \frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3} + \sqrt{\left(\frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3}\right)^2 + \frac{A_1}{c_3} + \frac{A_2}{c_3^2} + A_3}. \tag{20d}$$

Now, substituting for the required parameters into Eqs. (20a) and (20b), we have

$$E_{n,\ell}=\mathbb{Z}-\frac{\alpha^2\hbar^2}{2\mu}\left[\frac{\frac{4\mu D_e b}{\alpha^2\hbar^2}+\ell(\ell+1)+n(n+1)+\frac{1}{2}+\left(\frac{1}{2}-n\right)\sqrt{(1+2\ell)^2+\frac{8\mu D_e b^2}{\alpha^2\hbar^2}}}{2n+1+\sqrt{(1+2\ell)^2+\frac{8\mu D_e b^2}{\alpha^2\hbar^2}}}\right], \tag{20e}$$

$$U_{n\ell}(s)=N_{n\ell}s^u(1-s)^v{}_2F_1(-n,n+2(u+v);2u+1;s). \tag{20f}$$

$$\mathbb{Z}=D_e\left(1+2b+b^2\right)+\frac{\ell(\ell+1)C_0\alpha^2\hbar^2}{2\mu}. \tag{20g}$$

3. Entropic system and the Generalized Morse potential

The concept and application of entropy can be seen in many areas of science. In this study, we limit ourself to entropy in statistical mechanics. The statistical entropy can be defined as the probabilistic measure of uncertainty [27,28]. This entropy has its application mainly in information theory [29−37]. The statistical entropy is categorized as Tsallis entropy, Renyi entropy and Shannon entropy [38−44].

3.1. Shannon entropy and the Generalized Morse potential

The Shannon entropy for a physical system is given as [45−52].

$$S(\rho)=-4\pi\int_0^\infty \rho(r)\log\rho(r)dr. \tag{21}$$

where $\rho(r)$ is the probability density obtained from the wave function of a Schrödinger equation. In this case, it is the squared of the radial wave function of the equation obtained from the three dimensional Schrödinger equation in the presence of any potential. In this study, the probability density is given as

$$\rho(r)=N_{n,\ell}^2e^{-2\alpha ru}\left(1-e^{-\alpha r}\right)^{2v}\left[P_n^{(2u,2v-1)}\left(1-2e^{-\alpha r}\right)\right]^2. \tag{22}$$

Substituting for the probability density into Eq. (21), we have the following with the value of the screening parameter taken to be 0.2 except otherwise stated. The Shannon entropy in position space becomes

$$S(\rho)=-62.84\times\frac{\left(2n+\frac{\eta+\lambda+1}{2}\right)\Gamma(n+1)\Gamma\left(\frac{\lambda}{2}+1\right)^2}{2^{\frac{\lambda+\eta+1}{2}}\left(\frac{\eta+1}{2}\right)\Gamma\left(\frac{\lambda}{2}+n+1\right)^2}\times\aleph, \tag{23}$$

$$\aleph=In\left[y^{\frac{\lambda}{2}}(1-y)^{\frac{\eta-1}{2}}\frac{\left(n+\frac{\lambda}{2}\right)!}{\left(n+\frac{\lambda+\eta-1}{2}\right)!}\times\sum_{m=0}^{n}\frac{(n!)^2\left(2n+\frac{\lambda+\eta+1}{2}\right)}{(n-m)!m!\left(\left(n+\frac{\lambda}{2}\right)!\right)^2}\frac{\left(\left(n+\frac{\lambda+\eta-1}{2}\right)!\right)^2}{2^{\frac{\lambda+\eta+1}{2}}\left(n+\frac{\eta-1}{2}\right)!}\right] \tag{24}$$

To obtain the Shannon entropy in momentum space, we define a function of the form $z=1-2s$, and have the Shannon entropy in momentum space as

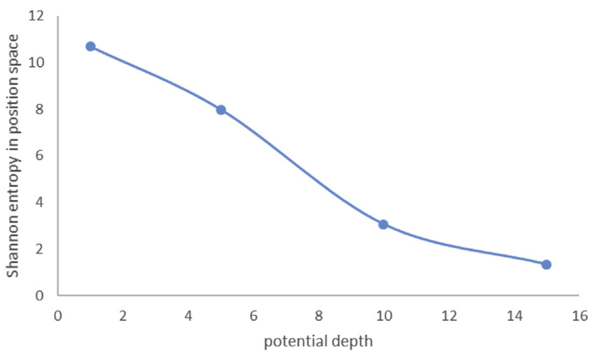

Fig. 1. Shannon entropy in position space for the ground state against the potential depth.

$$S(\gamma) = -31.42 \times \Gamma\left(\frac{\lambda+\eta-1}{2}+n\right) In\left[(0.9608)^{\frac{\lambda}{2}-1}(0.0392)^{\frac{\eta-1}{2}} \times \frac{\left(n+\frac{\lambda}{2}\right)!}{\left(n+\frac{\lambda+\eta-1}{2}\right)!} \times \Re\right], \tag{25}$$

where

$$\Re = \sum_{m=0}^{n} \frac{n!\left(\frac{\lambda}{2}-1\right)\left(\Gamma\left(n+\frac{\lambda+\eta-1}{2}\right)\right)^2}{(n-m)!m!\Gamma\left(n+\frac{\lambda}{2}\right)\Gamma\left(n+\frac{\eta}{2}\right)}. \tag{26}$$

3.2. Reñyi entropy and the Generalized Morse potential

Reñyi entropy $R_q(\rho)$ is given as

$$R_q(\rho) = \frac{1}{1-q}\log 4\pi \int_0^\infty \rho(r)^q dr, \tag{27}$$

Now, substituting for the probability density, we easily have

$$R_q(\rho) = \frac{1}{1-q}\left[\log\frac{12.568}{\alpha} + q\log\frac{n!\alpha\lambda 2^{\lambda+\eta+1}\Gamma(n+\lambda)\Gamma(n+\eta+2)}{(2n+\lambda+\eta)\Gamma(n+1)\Gamma(n+\lambda+1)\Gamma(n+\eta+1)}\right]. \tag{28}$$

To have Reñye entropy in the momentum space, we recall the change of variable $z = 1-2s$ previously made. Thus, the Reñyi entropy in momentum space is obtained as

$$R_q(\gamma) = \frac{1}{1-q}\left[\log 6.284\,\alpha + q\log\frac{2^{\lambda+\eta+1}\lambda\Gamma(n+\lambda+\eta+2)\Gamma(n+\lambda)}{(\lambda-1)\Gamma(n+\lambda+1)\Gamma(n+\eta+1)}\right]. \tag{29}$$

To see the effect of the potential depth on the potential well, we plotted Morse potential for three different values of the potential depth as shown in the Figure below.

4. Discussion

In Figs. 1 and 2, we examined the effects of the potential depth on Shannon entropy. It is observed in Fig. 1 that as the potential depth increases, the Shannon entropy in the position space decreases. This indicates that the potential well becomes narrower as the potential depth increase. Thus, the movement of a particle in the well is reduced thereby making the system more stable. However, in Fig. 2, as the potential depth increases, the Shannon entropy in the momentum space increases. This also shows that the potential well becomes larger as the potential depth increases. Thus, giving more space to a particle in the well to move and as such, more disorderliness occurs which result to instability of the system. The effects in Figs. 1 and 2 respectively, are also obtained in Figs. 3 and 4 respectively for Renyi entropy. It is also deduced here from Figs. 1−3, 4 that as Shannon entropy or Rényi entropy in position space decreases, Shannon entropy or Rényi entropy in momentum space increases, thus obeying Heisenberg uncertainty principle. This agrees with the investigations in the literature. In Fig. 5, we showed Morse potential for three different values of the potential depth. To obtain the maximum stability of a system where Shannon entropy and Rényi entropy are considered simultaneously, we plotted the entropic relations against the potential depth in Fig. 6. The $E1$ stands for the relation $((R_T/S_T)(S_T+R_T))/\pi$ while $E2$ stands for the relation S_T/R_T. The point of intersection of the two relations gives the maximum stability of the system.

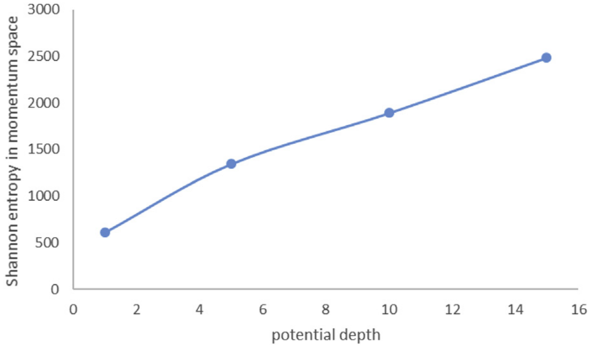

Fig. 2. Shannon entropy in momentum space for the ground state against the potential depth.

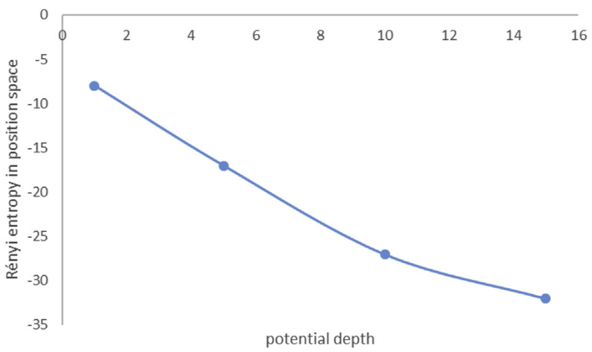

Fig. 3. Rényi entropy in position space for the ground state against the potential depth.

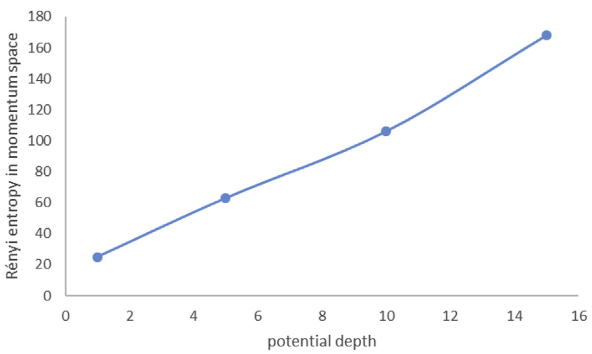

Fig. 4. Rényi entropy in momentum space for the ground state against the potential depth.

Table 1, we numerically compared the eigenvalues result from the parametric method and the Formula method with two other methods previously obtained. The present results agreed with the previous results. In Table 2, we presented the comparison of the experimental results with calculated results. It can be seen that the present results are in better agreement compared to the previous calculated results. In Table 3, we present some results for the relation of Shannon entropy and Rényi entropy. In Tables 4 and 5, we presented the numerical results for the Rényi entropy in position and momentum space and Shannon entropy in position and momentum space respectively for three molecules.

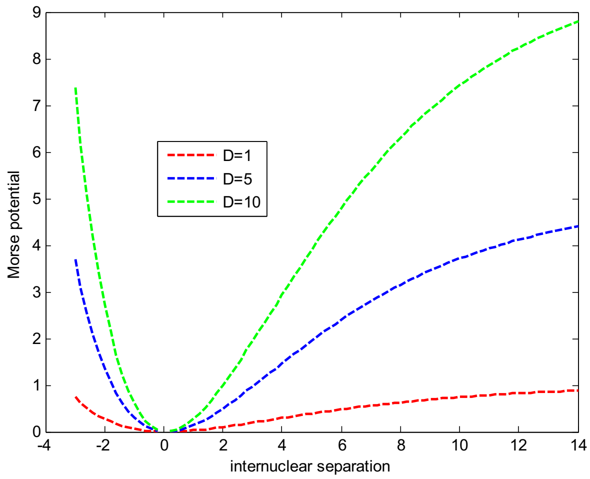

Fig. 5. Morse potential for three values of the potential depth.

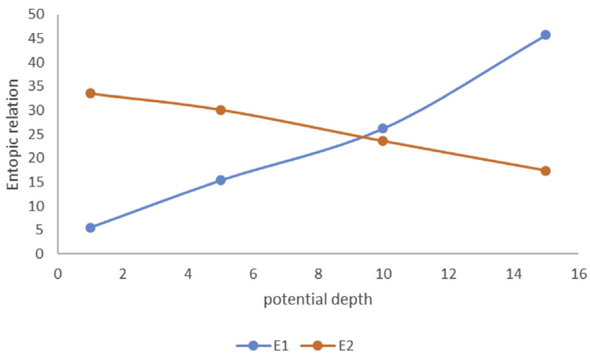

Fig. 6. Entropic relation $(E1 = ((R_T/S_T)(S_T + R_T))/\pi; E2 = (S_T/R_T))$ for the ground state against the potential depth.

Table 1
Comparision of bound State energy eigenvalues in (eV) for various n and ℓ quantum numbers of the Generalized Morse potential for 2p, 3p, 3d, 4p, 4d and 4f with $h = \mu = 1$ and $D_e = 15$.

State	α	Present results		Numerical [53]	SUSY [18]
		NU	FM		
2p	0.05	7.77122	7.86330	7.86280	7.86080
	0.10	7.77577	7.96330	7.95537	7.95330
	0.15	7.78125	8.06760	8.04724	8.04510
	0.20	7.78768	8.17620	8.13842	8.13620
3p	0.05	10.9468	11.0971	10.9998	10.9978
	0.10	11.0628	11.3753	11.1647	11.1626
	0.15	11.1779	11.6650	11.3265	11.3262
	0.20	11.2921	11.9662	11.4851	11.4828
3d	0.05	10.0723	10.2235	10.2165	10.2160
	0.10	10.1725	10.3835	10.3541	10.3535
	0.15	10.2734	10.5569	10.4899	10.4894
	0.20	10.4739	10.7435	10.6240	10.6235
4p	0.05	12.4651	12.6277	12.4992	12.4976
	0.10	12.6344	12.9779	12.6985	12.6968
	0.15	12.7986	13.3415	12.8901	12.8884
	0.20	12.9579	13.7192	13.0740	13.0722
4d	0.05	12.0105	12.1967	12.0981	12.0983
	0.10	12.1143	12.5072	12.2857	12.2850
	0.15	12.2176	12.8382	12.4672	12.4664
	0.20	12.3204	13.1899	12.6432	12.6426
4f	0.05	11.6417	11.8358	11.8209	11.8208
	0.10	11.6456	12.0580	11.9981	11.9980
	0.15	11.6518	12.3067	12.1718	12.1717
	0.20	11.6603	12.5821	12.3421	12.0421

Table 2
Comparison of experimental and calculated rotational transition frequencies for HF with $\alpha = 1.4404$, $r_e = 1.2746$ and $D/hc = 62,773$.

$\ell(\to\ell-1)$	Present (cm^{-1})	[54] (cm^{-1})	[51] (cm^{-1})
1	39.92	41.11	41.56
2	80.85	82.07	83.07
3	120.46	122.92	124.48
4	161.08	163.54	165.74
5	201.01	203.93	206.80
6	241.57	243.93	247.62
7	280.99	283.57	288.15
8	319.21	322.85	328.33
9	357.56	361.74	368.13
10	396.14	400.05	407.49

Table 3
Entropic system and entropic ratio for Shannon and Rényi entropies with four values of the potential depth. $S_T = S(\rho) + S(\gamma)$ and $R_T = R_q(\rho) + R_q(\gamma)$.

D	R_T	S_T	R_T/S_T	S_T/R_T	S_T/R_T	S_T/R_T
1	17	570	0.0298	33.529	9690	587
5	46	1387	0.0337	30.152	63,802	1433
10	79	1864	0.0424	23.595	147,256	1943
15	136	2372	0.0573	17.441	322,592	2508

Table 4
Rényi entropy of the Morse potential for three diatomic molecules with $\ell = 1$, $D_e = 0.746707167(eV)$ and $r_e = 3.079(\overset{0}{A})$ for $Na_2(X^1\sum_g^+)$; $D_e = 2.513903386(eV)$ and $r_e = 1.987(\overset{0}{A})$ for $Cl_2(X^1\sum_g^+)$; and $D_e = 10.99665353(eV)$ and $r_e = 1.063(\overset{0}{A})$ for $NO^+(X^1\sum^+)$.

n	Position space $R_2(\rho)$			Momentum space $R_2(\gamma)$		
	Na_2	NO^+	Cl_2	Na_2	NO^+	Cl_2
0	2.4042	5.1234	1.5132	13.8496	15.0568	11.4251
1	2.1926	4.4684	1.3462	14.1689	15.4962	11.8577
2	1.8621	4.8233	1.0941	14.5471	15.9881	12.1435
3	1.4503	4.1429	0.7212	14.9902	16.3960	12.5560
4	1.0070	3.6099	0.4825	15.3147	16.9326	12.9257

Table 5
Shannon entropy of the Morse potential for three diatomic molecules with $\ell = 1$, $D_e = 0.746707167(eV)$ and $r_e = 3.079(\overset{0}{A})$ for $Na_2(X^1\sum_g^+)$; $D_e = 2.513903386(eV)$ and $r_e = 1.987(\overset{0}{A})$ for $Cl_2(X^1\sum_g^+)$ and $D_e 10.99665353(eV)$ and $r_e = 1.063(\overset{0}{A})$ for $NO^+(X^1\sum^+)$.

n	Position space $S(\rho)$			Momentum space $S(\gamma)$		
	Na_2	NO^+	Cl_2	Na_2	NO^+	Cl_2
0	2.8132	5.4138	1.8694	32.6314	38.0499	28.0145
1	2.3462	4.6997	1.6051	39.4701	44.9307	34.9606
2	1.6941	3.7155	1.3384	47.7615	50.3761	41.0009
3	1.0212	2.6999	1.0064	53.8100	57.4613	48.7171
4	0.6843	1.9658	0.4392	61.8146	66.9227	56.5038

5. Conclusion

In this work, we studied the approximate analytical solutions of the 3-dimensional Schrödinger equation with the Generalized Morse potential model via parametric Nikiforov–Uvarov method and Formula method for bound state problem. The theoretical quantities such as Shannon entropy and Rényi entropy are calculated both in position and momentum spaces. Our results for bound state solutions are in good agreement with previous results. The results obtained in each case for Shannon entropy and Rényi entropy obey Heisenberg Uncertainty principle. It is observed that this method is simpler and straight forward.

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