

Information and complexity measures for the ring-shaped modified Kratzer potential[†]

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In this study, the Fisher information measure, Shannon entropy, Renyi entropy, Tsallis entropy and Fisher-Shannon complexity of the ring-shaped modified Kratzer potential are investigated. The trends in the variation of the information and complexity measures considered for this model quantum system are discussed.

Keywords: Theoretical chemistry, Fisher information, Shannon entropy, Tsallis entropy, Renyi entropy, Fisher-Shannon complexity, Ring-shaped modified Kratzer potential

There has been an interest in studies on information-theoretic and complexity measures for quantum model systems in the recent years¹⁻¹⁰. The information entropy for the trigonometric Rosen-Morse potential², harmonic oscillator¹¹⁻¹⁴, hydrogenic atoms¹⁵, Morse potential^{16,17}, Yukawa and Hulthen potentials¹⁸ have been investigated.

The Kratzer potential plays an important role in atomic and molecular physics and quantum chemistry¹⁹⁻²². Cheng and Dai²³⁻²⁵ proposed a new potential consisting of the modified Kratzer potential plus a new proposed ring-shaped potential which has possible applications to ring-shaped organic molecules like cyclic polyenes and benzene²³⁻²⁵. In this work, we shall obtain the Fisher information, Fisher length, Shannon entropy, Shannon length, Renyi entropy, Renyi length, Tsallis entropy and the Fisher-Shannon complexity for the ring-shaped modified Kratzer potential. In this section, we present the definition of the information theoretical measures used in this work which are based on the 1-normalized electron density in the position and momentum space. The Shannon information entropy in the position space is given by Eq. (1)^{11,14,26,27}.

$$S(\rho) = - \int (\rho(\mathbf{r})) \log (\rho(\mathbf{r})) d\mathbf{r} \quad \dots (1)$$

The Shannon entropy measures the uncertainty in the localization of a particle in space. The lower the entropy, the more concentrated is the wave function. The smaller the uncertainty, the higher is the accuracy in predicting the localization of the particle. For applications of the Shannon entropy, see Ref. 26. The Shannon length (SL) is defined as Eq. (2)^{1,28,29}.

$$\frac{4}{3} S_L^3 = e^{S(\rho)} \quad \dots (2)$$

The Fisher information measure is defined by Eq. (3)²⁷.

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

The Fisher information measure is used as a tool for characterizing complex signals or systems with applications in geophysics, biology, atomic physics, quantum chemistry and other related areas^{1,4-10,30-41}. The Fisher length (IL) is defined as Eq. (4)^{1,28,29}.

$$I_L = (I(\rho))^{-1/2} \quad \dots (4)$$

The Tsallis entropy is defined as Eq. (5),

$$T_q[\rho] = \frac{1}{q-1} \left(1 - \int (\rho(\mathbf{x}))^q d\mathbf{x} \right), \quad q > 0, \quad q \neq 1 \quad \dots (5)$$

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and describes non-extensive systems. It has been applied to tissue radiation response, solar neutrino problem and image thresholding⁴²⁻⁴⁴. The Renyi entropy defined as Eq. (6),

$$R_q[I] = \frac{1}{1-q} \ln \left(\int (x)^q dx \right), \quad 0 < q < \infty, \quad q \neq 1 \quad \dots (6)$$

is a generalization of the Shannon entropy^{4,45-49}. The Renyi length (R_L) is defined as Eq. (7)^{1,28,29}.

$$\frac{4}{3} R_L^3 = e^{R[I]} \quad \dots (7)$$

The Fisher-Shannon complexity defined as Eq. (8)⁵⁰⁻⁵²,

$$FS = [I][J] \quad \dots (8)$$

is a statistical complexity measure which is built upon a global information measure combined with a local information measure. Here, $[I]$ is the Fisher information measure, and

$$[J] = \frac{1}{2} e^{2S[I]^{1/3}} \quad \dots (9)$$

where $S[I]$ is the Shannon information entropy. The Fisher-Shannon measure grasps the oscillatory nature of the electronic cloud together with its total extent in the configuration space⁵³. Other forms of complexity measures are the algorithmic complexity^{50,54,55}, the statistical measure of complexity C , defined by Lopez-Ruiz, Mancini, Calbet (LMC)^{50,56-59} and the two parameter disorder-order derived measure of complexity Γ , according to Shiner, Davison, Landsberg (SDL)^{50,60,61}. Both C and Γ , are products of two global information measures⁵⁰. They quantify different facets of the internal disorder of a system which are manifest in the diverse and complex three-dimensional geometries of its orbitals⁵³.

In what follows, the solutions of the Klein-Gordon equation with the ring-shaped modified Kratzer potential are given. This is followed by the Fisher information measure and Shannon entropy for the ring-shaped modified Kratzer potential. The Tsallis and Renyi entropies for the ring-shaped modified Kratzer potential are then discussed followed by the Fisher-Shannon complexity and concluding remarks.

Solution of the Schrödinger Equation with the Ring-Shaped Modified Kratzer Potential

The solution of the Schrödinger equation with the Ring-Shaped Modified Kratzer potential has been obtained in Ref. 62. We shall review these solutions

briefly in this section to define our notations. The Schrödinger equation with equal scalar and vector potentials can be written as Eq. (10)⁶².

$$\left[-\frac{\hbar^2}{2m} \nabla^2 \right] \Psi(r, \theta, \phi) = [E - V(r, \theta, \phi)] \Psi(r, \theta, \phi) \quad \dots (10)$$

The potential $V(r, \theta, \phi)$, in this case, is the ring-shaped modified Kratzer potential which is given as Eq. (11)^{23,24,62},

$$V(r, \theta, \phi) = D_e \left(\frac{r - r_e}{r} \right)^2 + \frac{^2 \cos^2}{r^2 \sin^2} \quad \dots (11)$$

where ^{2} is a positive real constant, D_e is the dissociation energy and r_e is the equilibrium internuclear separation.

Taking the wave functions to be of the form,

$$\Psi(r, \theta, \phi) = \frac{u(r)}{r} H_n(\rho) e^{im\phi}, \quad m = 0, \pm 1, \pm 2, \dots \quad \dots (12)$$

$H_n(x)$ is obtained as Eq. (13),

$$H_n(x) = N_n (1 - x^2)^{-m'/2} \frac{d^{l'-m'}}{dx^{l'-m'}} \left[(x^2 - 1)^{l'} \right] \quad \dots (13)$$

where $H_n(x)$ stands for the associated-Legendre functions $P_l^{-m'}(x)$ and N_n is the normalization constant. The wave function is obtained as Eq. (14),

$$\Psi(r, \theta, \phi) = C_{NL} (2 - r)^L e^{-r} L_N^{2L+1}(2 - r) Y_{\ell'm'}(\Omega) \quad \dots (14)$$

where

$$C_{NL} = \sqrt{\frac{(2 - r)^3 N!}{2(N + L + 1) \Gamma(N + 2L + 2)}}, \quad N = 0, 1, 2, \dots \quad \dots (15)$$

$$L = \sqrt{(2\ell' + 1)^2 + 8 - (D_e(r_e)^2 -)} - 1 \quad \dots (16)$$

$$= \frac{2 - D_e r_e}{N'} \quad \dots (17)$$

$$N' = - \left[2N + 1 + \sqrt{(2\ell' + 1)^2 + 8 - (D_e(r_e)^2 -)} \right] \quad \dots (18)$$

N is the principal quantum number and $Y_{\ell'm'}(\Omega)$ is the spherical harmonics given as Eq. (19),

$$Y_{\ell'm'}(\Omega) = Y_{\ell'm'}(\theta, \phi) = N_{\ell'm'} P_{\ell}^{m'}(\cos \theta) e^{im'\phi} \quad \dots (19)$$

and the normalization constant $N_{\ell'm'}$ is obtained as Eq. (20).

$$N_{\ell m'} = \sqrt{\frac{(2\ell'+1)(\ell'+m')!}{4(\ell'-m')!}} \quad \dots (20)$$

The Fisher and Shannon Information Measures for the Ring-Shaped Modified Kratzer Potential

The Fisher information measures for the ring-shaped modified Kratzer potential

The Fisher information measure for the ring-shaped modified Kratzer potential will be obtained by using Eq. (3). The probability density of this potential model is given as Eq. (21).

$$(\mathbf{r}) = C_{NL}^2 (2-r)^{2L} e^{-2r} \left| I_N^{2L+1}(2-r) \right|^2 |Y_{\ell m'}(\Omega)|^2 \quad \dots (21)$$

Taking into consideration the gradient operator ∇ in polar coordinates and the azimuthal independence of the probability density of the ring-shaped modified Kratzer potential, one has the following expression for the Fisher information measure (Eq. (22)),

$$I(\mathbf{r}) = \int \frac{1}{(\mathbf{r})} \left[\frac{\partial}{\partial r} (\mathbf{r}) \right]^2 d\mathbf{r} + \int \frac{1}{(\mathbf{r})} \left[\frac{1}{r} \frac{\partial}{\partial} (\mathbf{r}) \right]^2 d\mathbf{r} \\ = I_1 + I_2 \quad \dots (22)$$

where

$$I_1 = \int \frac{1}{(\mathbf{r})} \left[\frac{\partial}{\partial r} (\mathbf{r}) \right]^2 d\mathbf{r} \quad \dots (23)$$

and

$$I_2 = \int \frac{1}{(\mathbf{r})} \left[\frac{1}{r} \frac{\partial}{\partial} (\mathbf{r}) \right]^2 d\mathbf{r} \quad \dots (24)$$

The integral I_1 can be decomposed into a sum of five integrals denoted by I_{1i} , ($i = 1-5$). By considering the condition in Appendix (A13) and on using (A1), (A2) and (A13), one has the following integrals:

$$I_{11} = (2)^2 \frac{2L^2}{(N+L+1)(2L+1)} \quad \dots (25)$$

$$I_{12} = -(2)^2 \frac{2L}{N+L+1} \quad \dots (26)$$

$$I_{13} = (2)^2 \quad \dots (27)$$

$$I_{14} = (2)^2 \frac{2N}{N+L+1} \quad \dots (28)$$

$$I_{15} = -(2)^2 \frac{2N}{N+L+1} \quad \dots (29)$$

Therefore, putting together the computed values for I_{1i} , we have

$$I_1 = (2)^2 \frac{2NL+L+N+1}{(2L+1)(N+L+1)} \quad \dots (30)$$

Also, the integral I_2 can be decomposed into the sum of three integrals denoted by I_{2i} , $i = 1-3$. Using equations (A7), (A8) and (A9), we obtain

$$I_{21} = \frac{(2\ell'+1)[(\ell'+m')!]^2}{4[(\ell'-m')!]^2} \frac{\ell'^2(2)^2}{2(N+L+1)(2L+1)} \\ \times \left(\frac{1}{m'} - \frac{2}{2\ell'+1} \right) \quad \dots (31)$$

$$I_{22} = (\ell'+m')^2 \frac{(2\ell'+1)(\ell'+m')!}{4(\ell'-m')!} \frac{(2)^2}{2(N+L+1)(2L+1)} \\ \times \left(\frac{(\ell'+m'-1)!}{m'(\ell'-m'-1)!} \right) \quad \dots (32)$$

and

$$I_{23} = -2\ell'(\ell'+m') \frac{(2\ell'+1)(\ell'+m')!}{4(\ell'-m')!} \\ \times \frac{(2)^2}{2(N+L+1)(2L+1)} \left(\frac{(\ell'+m'-1)!}{m'(\ell'-m')!} \frac{(\ell'-m')}{m'} \right) \quad \dots (33)$$

Then, the integral I_2 is obtained as

$$I_2 = \frac{(2\ell'+1)[(\ell'+m')!]^2}{4[(\ell'-m')!]^2} \frac{(2)^2}{2(N+L+1)(2L+1)} \\ \times \left(\frac{\ell'^2}{m'} - \frac{2\ell'^2}{2\ell'+1} + \frac{(\ell'+m')(\ell'-m')}{m'} - \frac{2\ell'(\ell'-m')}{m'} \right) \quad \dots (34)$$

Hence, the following expression for the Fisher information measure is obtained (Eq. (35)).

$$I(\mathbf{r}) = I_1 + I_2 = (2)^2 \frac{2LN+L+N+1}{(2L+1)(N+L+1)} \\ + \frac{(2\ell'+1)[(\ell'+m')!]^2}{4[(\ell'-m')!]^2} \frac{(2)^2}{2(N+L+1)(2L+1)} \\ \times \left(\frac{\ell'^2}{m'} - \frac{2\ell'^2}{2\ell'+1} + \frac{(\ell'+m')(\ell'-m')}{m'} - \frac{2\ell'(\ell'-m')}{m'} \right) \quad \dots (35)$$

The graphs of the Fisher length against n , D_e and r_e are plotted in Figs 1, 2 and 3, respectively, for $\ell' = 0$. In Fig. 1, the Fisher length increases as n increases. It can be observed from Fig. 2 that the Fisher length decreases with the dissociation energy D_e , while the Fisher length increases with increasing r_e in Fig. 3 except for the initial decrease from $r_e = 1 \text{ \AA}$ to $r_e = 2 \text{ \AA}$.

The Shannon entropy of the ring-shaped modified Kratzer potential

The Shannon entropy of a hydrogen system in an arbitrary state characterized by the quantum numbers (n, ℓ, m) has been obtained as Eq. (36)^{11,14,27}

$$S(\psi) = S_{NL}(R) + S_{\ell'm'}(Y) \quad \dots (36)$$

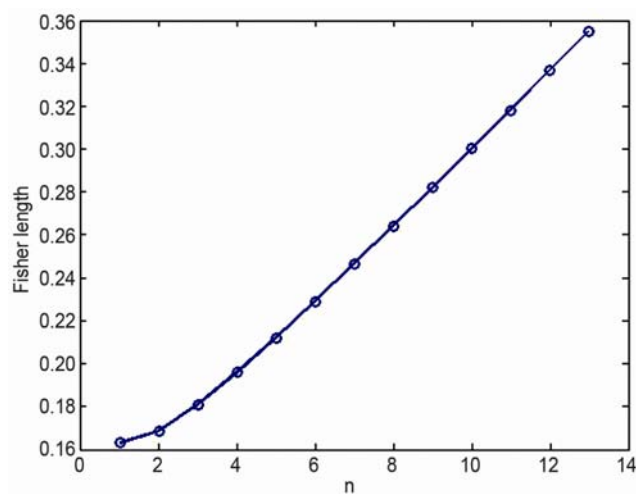


Fig. 1 – Fisher length against n for $\ell' = 0$, $\ell = 1$, $m = 0.5$, $D_e = 6.780447246 \text{ eV}$, $r_e = 1.116 \text{ \AA}$.

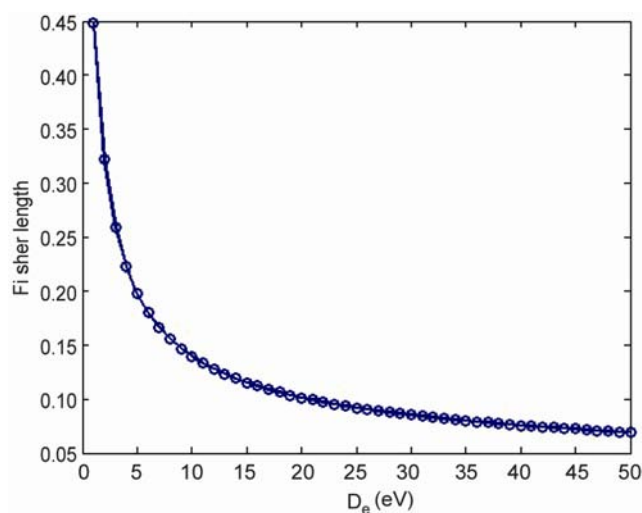


Fig. 2 – Fisher length against D_e for $\ell' = 0$, $\ell = 1$, $m = 0.5$, $n = 2$, $r_e = 1.116 \text{ \AA}$.

For the case of the Kratzer potential, the Shannon entropy for the radial part is

$$S_{NL}(R) = - \int_0^\infty r^2 R_{NL}(r) \ln R_{NL}^2(r) dr \quad \dots (37)$$

Using Eqs (42) and (43) of Yanez *et al.*¹¹ and Eq. (5.1) of Dehesa *et al.*¹⁴, we obtain Eq. (38)

$$\begin{aligned} S_{NL}(R) = & \frac{N!}{2(N+L+1)(N+2L+1)!} \\ & \times \left[\frac{(N+2L+3)!}{N!} + \frac{4(N+2L+2)!}{(N-1)!} + \frac{(N+2L+1)!}{(N-2)!} \right] \\ & - \ln \left[\frac{(2)^3 N!}{2(N+L+1)(N+2L+1)!} \right] \\ & - 2L \left[\frac{2N+1}{2(N+L+1)} + \Psi(N+2L+2) \right] \\ & + \frac{N!}{2(N+L+1)(N+2L+1)!} E_1(L_N^{2L+1}) \end{aligned} \quad \dots (38)$$

This can be simplified into the following form (Eq. (39)):

$$\begin{aligned} S_{NL}(R) = & -3 \ln \left[\frac{N!}{2(N+L+1)(N+2L+1)!} \right] \\ & + 3(L+1) + 3N - 2L \left[\frac{2N+1}{2(N+L+1)} + \Psi(N+2L+2) \right] \\ & + \frac{N!}{2(N+L+1)} E_1(L_N^{2L+1}) \end{aligned} \quad \dots (39)$$

where $\Psi(x) = \Gamma'(x)/\Gamma(x)$, and the symbol $E_1(y_n)$ denotes the entropic integral¹⁵ (Eq. (40)).

$$E_1(y_n) = - \int_0^\infty x \mathcal{Q}_{2L+1}(x) r^2 y_n^2(x) \ln y_n^2(x) dx \quad \dots (40)$$

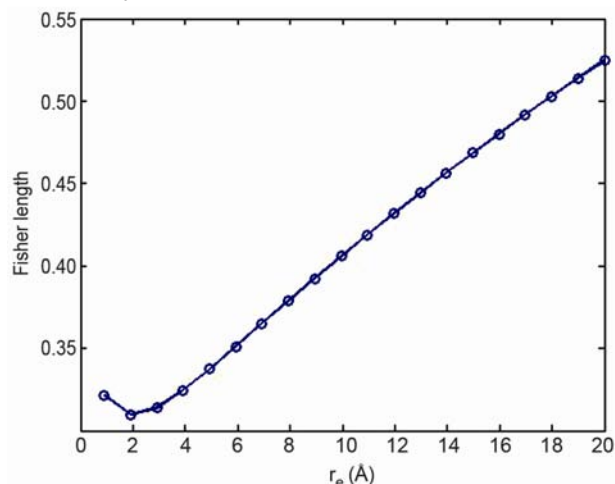


Fig. 3 – Fisher length against r_e for $\ell' = 0$, $\ell = 1$, $m = 0.5$, $n = 2$, $D_e = 2 \text{ eV}$.

To obtain $S_{\ell'm'}(Y)$, we make use of the result (lower bound obtained for the Shannon entropy of the hyperspherical harmonics in 3D) in Eq. (32) of Ref. 63 and the fact that the Shannon entropy has the same value in the states (n, ℓ', m') and $(n, \ell' - m')$ ¹¹. Therefore, $S_{\ell'm'}(Y)$ is obtained as Eq. (41),

$$S_{\ell'm'}(Y) = -\ln \left[\sum_{k=0}^{\ell'-|m'|} C_k(\ell', |m'|) \left[{}_3F_2 \left(\begin{matrix} -\ell' + |m'| + k, \\ |m'| + k + 1/2, \\ \ell' + |m'| + k + 1 \end{matrix} \middle| \begin{matrix} |m'| + k + 1, 2|m'| \\ +2k + 3/2 \end{matrix} \right) \right] \right] \quad \dots (41)$$

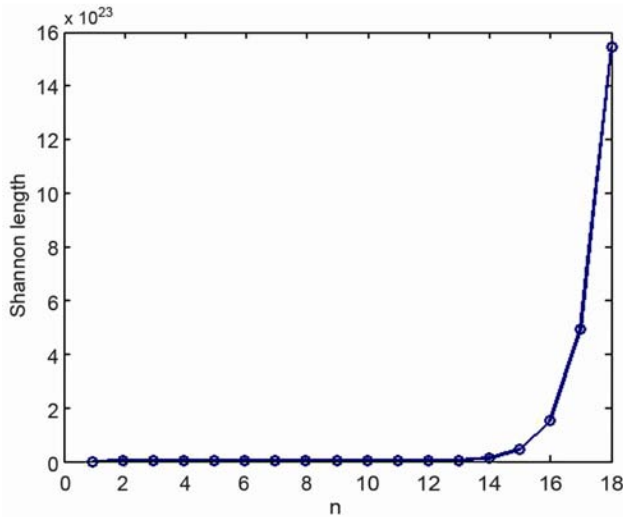


Fig. 4 – Shannon length against n for $\ell' = 0, \ell = 1, \ell = 0.5$, $D_e = 6.780447246$ eV, $r_e = 1.116$ Å.

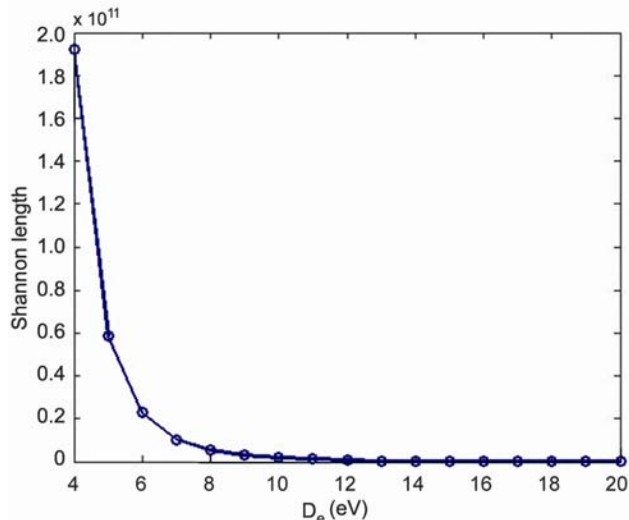


Fig. 5 – Shannon length against D_e for $\ell' = 0, \ell = 1, \ell = 0.5$, $n = 2, r_e = 1.116$ Å.

where

$$C_k(\ell', |m'|) = \frac{(4|m'| + 4k + 1)(2\ell' + 1)^2 \Gamma(k + 1/2) \Gamma(2|m'| + k + 1/2)}{16^{-2} k! (2|m'| + k)!} \times \left[\frac{(\ell' + |m'| + k)! \Gamma(|m'| + k + 1/2)}{(|m'| + k)! (\ell' - |m'| - k)! \Gamma(2|m'| + 2k + 3/2)} \right]^2 \quad \dots (42)$$

The graphs of the Shannon length against n , D_e and r_e are plotted in Figs 4-6 respectively, for $n = 0$; $\ell' = 0$. In Fig. 4, the Shannon length is initially relatively constant with increasing n , but there is an abrupt increase when $n = 15$. The reverse behaviour is observed when the Shannon length is plotted against the dissociation energy D_e . The Shannon length initially decreases with D_e but is relatively constant from $D_e = 10$ eV upwards. The behaviour of the Shannon length against r_e is similar to its behaviour against n as can be observed from Figs 4 and 6.

The Tsallis and Renyi Entropies of the Ring-Shaped Modified Kratzer Potential

Using Eqs (5), (6) and (21), the Tsallis and Renyi entropies are obtained respectively as Eqs (43) and (44).

$$T_q[\] = \frac{1}{q-1} \left\{ 1 - \left[\frac{4 C_{NL}^2}{(2)^2} \int_0^\infty (2r)^{4Lq} e^{-2rq} |L_N^{2L+1}(2r)|^{2q} dr + \int |Y_{\ell'm'}(\ , \)|^{2q} d\Omega \right] \right\} \quad \dots (43)$$

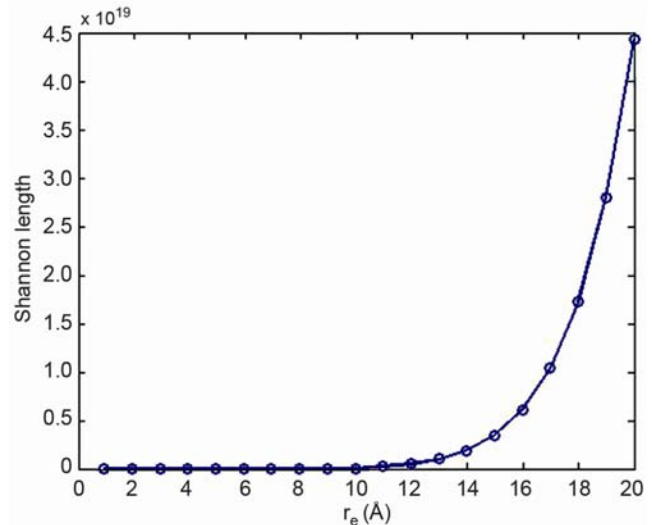


Fig. 6 – Shannon length against r_e for $\ell' = 0, \ell = 1, \ell = 0.5$, $n = 2, D_e = 2$ eV.

and

$$R_q[\] = \frac{1}{1-q} \ln \left[\frac{4 C_{NL}^2}{(2)^2} \times \int_0^\infty (2-r)^{4Lq} e^{-2-rq} \left| L_N^{2L+1}(2-r) \right|^{2q} dr \right] \dots (44)$$

By using the linearization formula of Srivastava-Niukkanen for the products of various Laguerre polynomials^{28,64,65}, we obtain Eq. (45)

$$t^{L_{m_1}^{(1)}}(x_1 t) \dots L_{m_n}^{(n)}(x_n t) = \sum_{k=0}^\infty \Gamma_k(\ ; x_1, \dots, x_n) L_m^{(k)}(t) \dots (45)$$

where

$$\Gamma_k(\ ; x_1, \dots, x_n) = (-1)^k \binom{1+m_1}{m_1} \dots \binom{n+m_n}{m_n} F_A^{(n+1)}[\quad +1, -m_1, \dots, -m_n, -k; \quad +1, \dots, \quad +1, \quad +1; x_1, \dots, x_n, 1] \dots (46)$$

Hence, Tsallis and Renyi entropies are obtained in terms of one of Lauricella's hypergeometric functions of $(n+1)$ variables (Eqs 47 & 48),

$$T_q[\] = \frac{1}{q-1} \left\{ 1 - \left[\left(\frac{4 C_{NL}^2}{(2)^2} \right)^q \sum_{k=0}^\infty \Gamma_k(4Lq; \frac{1}{q}, \dots, \frac{1}{q}) \right] \right\} \dots (47)$$

and

$$R_q[\] = \frac{1}{1-q} \ln \left[\left(\frac{4 C_{NL}^2}{(2)^2} \right)^q \sum_{k=0}^\infty \Gamma_k(4Lq; \frac{1}{q}, \dots, \frac{1}{q}) \right] \dots (48)$$

where

$$\Gamma_k(4Lq; \frac{1}{q}, \dots, \frac{1}{q}) = (4Lq+1) \binom{2L+N+1}{N} F_A^{(2q+1)}[4Lq+1, -N, \dots, -N, -k; 2L+2, \dots, 2L+2, 1; \frac{1}{q}, \dots, \frac{1}{q}, 1] \dots (49)$$

It is known that only the term with $k=0$ is non-vanishing to the integral of the Laguerre polynomials^{28,64,65} and therefore, the Tsalli and Renyi entropies become Eqs (50) and (51),

$$T_q[\] = \frac{1}{q-1} \left\{ 1 - \left[\left(\frac{4 C_{NL}^2}{(2)^2 q^{4Lq+1}} \right)^q \Gamma_0(4Lq; \frac{1}{q}, \dots, \frac{1}{q}) + \int |Y_{\ell'm'}(\ , \)|^{2q} d\Omega \right] \right\} \dots (50)$$

$$R_q[\] = \frac{1}{1-q} \ln \left[\left(\frac{4 C_{NL}^2}{(2)^2 q^{4Lq+1}} \right)^q \Gamma_0(4Lq; \frac{1}{q}, \dots, \frac{1}{q}) + \int |Y_{\ell'm'}(\ , \)|^{2q} d\Omega \right] \dots (51)$$

where

$$\Gamma_0(4Lq; \frac{1}{q}, \dots, \frac{1}{q}) = \Gamma(4Lq+1) \binom{2L+N+1}{N}^{2q} \times F_A^{(2q+1)}[4Lq+1, -N, \dots, -N, 0; 2L+2, \dots, 2L+2, 1; \frac{1}{q}, \dots, \frac{1}{q}, 1] \dots (52)$$

and $(\)_n = \Gamma(\ +n)/\Gamma(\)$.

Consider the case where $q=2$ (due to the wide applications of this for both the Tsallis and Renyi entropies). We then make use of Eqs (14) and (26) of Ref. 63 to evaluate the integral of the spherical harmonics. Finally, the Renyi and Tsallis entropies are obtained respectively as Eqs (53) and (54),

$$T_2[\] = 1 - \left[\left(\frac{4 C_{NL}^2}{(2)^2 q^{8L+1}} \right)^q \Gamma_0(8L; \frac{1}{2}, \dots, \frac{1}{2}) + \sum_{k=0}^{\ell'-|m'|} C_k(\ell', |m'|) \left[{}_3F_2 \left[\begin{matrix} -\ell' + |m'| + k, \\ |m'| + k + 1/2, \\ \ell' + |m'| + k + 1 \\ |m'| + k + 1, 2|m'| \\ +2k + 3/2 \end{matrix} \middle| 1 \right] \right] \right] \dots (53)$$

$$R_2[\] = -\ln \left[\left(\frac{4}{(2)^2} \frac{C_{NL}^2}{q^{8L+1}} \right)^q \Gamma_0(8L; \frac{1}{2}, \dots, \frac{1}{2}) + \sum_{k=0}^{\ell'-|m'|} C_k(\ell', |m'|) \left[{}_3F_2 \left[\begin{matrix} -\ell' + |m'| + k, \\ |m'| + k + 1/2, \\ \ell' + |m'| + k + 1 \\ |m'| + k + 1, 2|m'| \\ +2k + 3/2 \end{matrix} \middle| 1 \right] \right] \right] \quad \dots (54)$$

where

$$\Gamma_0(8L; \frac{1}{2}, \dots, \frac{1}{2}) = \Gamma(8L+1) \binom{2L+N+1}{N}^4 \times F_A^{(5)}[8L+1, -N, \dots, -N, 0; 2L+2, \dots, 2L+2, 1; \frac{1}{2}, \dots, \frac{1}{2}, 1] \quad \dots (55)$$

and $C_k(\ell', |m'|)$ is as given in Ref. 43.

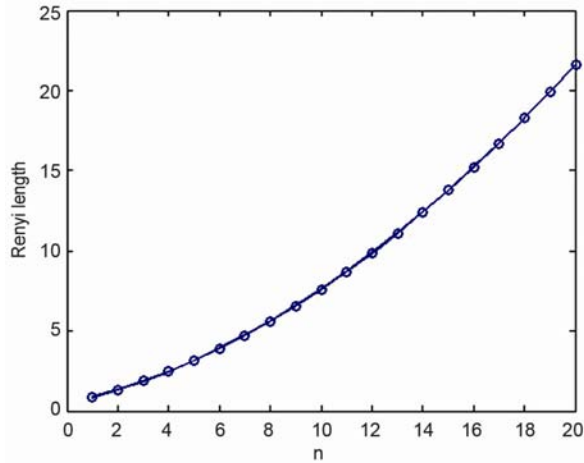


Fig. 7 – Renyi length against n for $\ell' = 0$, $\alpha = 1$, $\beta = 0.5$, $n = 2$, $D_e = 6.780447246$ eV, $r_e = 1.116$ Å.

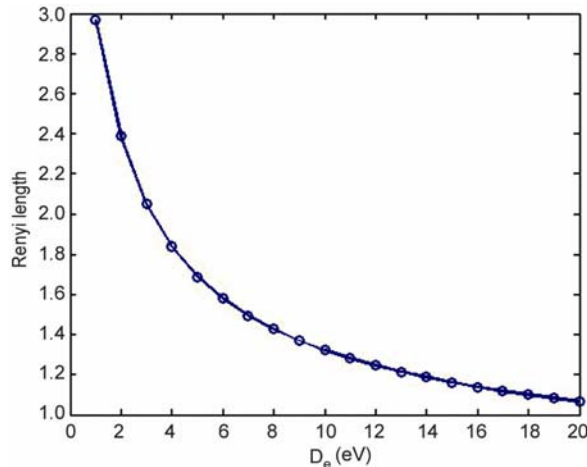


Fig. 8 – Renyi length against D_e for $\ell' = 0$, $\alpha = 1$, $\beta = 0.5$, $n = 2$, $r_e = 1.116$ Å.

The Renyi length is plotted against n , D_e and r_e in Figs 7-9. The Renyi length increases with n and r_e as shown in Figs 7 and 9 while it decreases with r_e as can be observed from Fig. 8.

Fisher-Shannon Complexity

The Fisher-Shannon complexity for the ring-shaped modified Kratzer potential is obtained as Eq. (56),

$$FS = I[\] \frac{1}{2} e^{2S[\]/3} \quad \dots (56)$$

where $I[\]$ is given in Eq. (35) and $S[\] = S_{NL}(R) + S_{\ell'm'}(Y)$. $S_{NL}(R)$ is given in Eq. (39) and $S_{\ell'm'}(Y)$ is given in Eq. (41). We have plotted the graphs of the Fisher-Shannon complexity measure against D_e and r_e , respectively, in Figs 10 and 11. The Fisher-Shannon complexity initially starts to increase

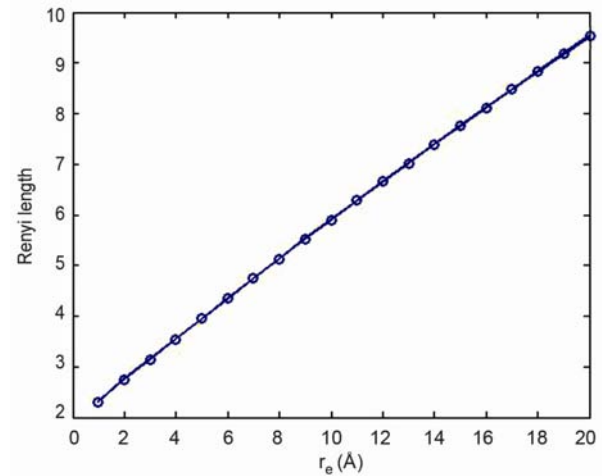


Fig. 9 – Renyi length against r_e for $\ell' = 0$, $\alpha = 1$, $\beta = 0.5$, $n = 2$, $D_e = 2$ eV.

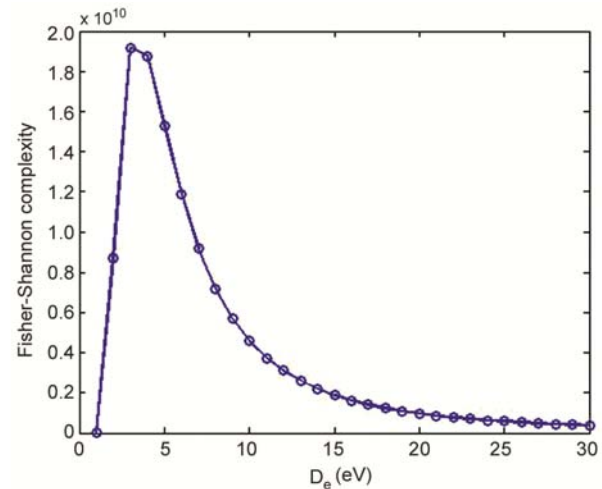


Fig. 10 – Fisher-Shannon complexity against D_e for $\ell' = 0$, $\alpha = 1$, $\beta = 0.5$, $n = 0$, $r_e = 1.0$ Å.

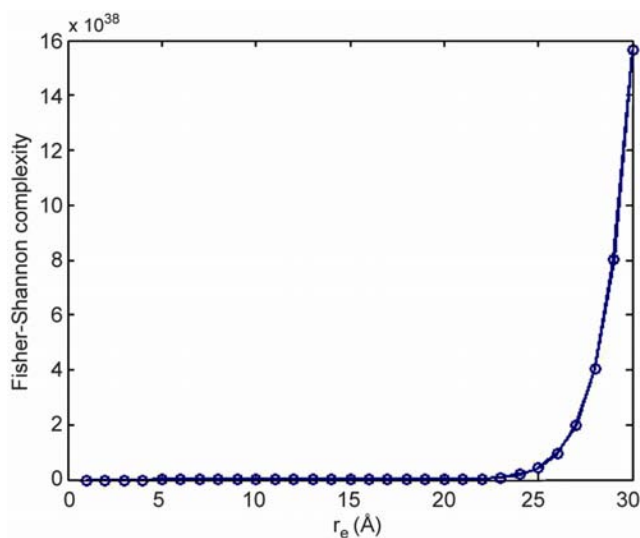


Fig. 11 – Fisher-Shannon complexity against $l' = 0$, $l' = 1$, $n = 0$, $D_e = 2$ eV.

with D_e (from $D_e = 1$ eV to $D_e = 3$ eV) but starts to decrease monotonically when $D_e = 3$ eV, as shown in Fig. 10. In Fig. 11, the Fisher-Shannon complexity initially is relatively constant with increasing r_e but there is an abrupt increase when $r_e = 20$ Å.

Conclusions

We have obtained the Fisher information measure, Shannon entropy, Renyi entropy, Tsallis entropy and Fisher-Shannon complexity for the ring-shaped modified Kratzer potential. The solution of the Fisher information measure has been obtained exactly. The Shannon entropy has been obtained by making use of the lower bound for the Shannon entropy of the hyperspherical harmonics as obtained by Dehesa *et al.*⁶³. It should be noted that (as observed in Ref. 63, the quality of the bound globally decreases with l' , and it increases with $|m'|$ for fixed l' . We also observed that the angular part of the Shannon entropy has the same value in the states (n, l', m') and $(n, l' - m')$ ¹¹.

We have made use of entropy of the Laguerre polynomials, Gegenbauer polynomials, and spherical harmonics. We obtained (for $q = 2$) the Tsallis and Renyi entropies, by making use of the linearization formula of Srivastava-Niukkanen for the Laguerre polynomials in terms of Lauricella hypergeometric functions.

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Appendix

Some properties of the associated Laguerre, associated Legendre polynomials and spherical harmonics are given below.

Associated Laguerre polynomials

The associated Laguerre polynomials are defined as

$$L_n(x) = \frac{d}{dx} L_n(x)$$

where

$$L_n(x) = e^x \frac{d^n}{dx^n} (x^n e^{-x})$$

is the Laguerre polynomials. The associated Laguerre polynomials are known to satisfy the orthogonality properties^{27,28,66}:

$$\int_0^\infty x e^{-x} L_n(x) L_m(x) dx = \frac{\Gamma(n+1)}{n!} \delta_{nm} \quad \dots (A1)$$

$$\int_0^\infty x^s e^{-x} L_n(x) L_m(x) dx = \sum_{r=0}^{\min(n,m)} (-1)^{n+m-r} \begin{pmatrix} s \\ n-r \end{pmatrix} \begin{pmatrix} s \\ m-r \end{pmatrix} \begin{pmatrix} s+r \\ r \end{pmatrix} \quad \dots (A2)$$

The recurrence relation of the associated Laguerre polynomials is given as²⁷

$$x L_k^{+1}(x) = (k+1) L_k(x) - (k+1) L_{k+1}(x) \quad \dots (A3)$$

Spherical harmonics and associated Legendre polynomials

The associated Legendre functions $P_\ell^m(x)$ are defined in terms of the ordinary Legendre polynomials $P_\ell(x)$ as⁵⁷⁻⁵⁹

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} (x^2-1)^\ell \quad \dots (A4)$$

Using the Rodrigues' form of the Legendre polynomials, we have (for $m \geq 0$)

$$P_\ell^m(x) = \frac{(-1)^\ell}{2^\ell \ell!} (1-x^2)^{m/2} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell \quad \dots (A5)$$

and for $m < 0$,

$$P_\ell^{-m}(x) = \frac{(-1)^{\ell-m}}{2^\ell \ell!} (1-x^2)^{-m/2} \frac{d^{\ell-m}}{dx^{\ell-m}} (x^2-1)^\ell \quad \dots (A6)$$

(Contd.)

Appendix (Contd.)

The following relation holds between the associated Legendre polynomials and the Legendre Polynomials

$$P_{\ell}^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_{\ell}^m(x) \quad \dots (A7)$$

Also in the literature, the following notations are being used

$$P_{\ell m}(x) = (-1)^m P_{\ell}^m(x)$$

The associated Legendre polynomials satisfy the following orthonormality condition (for $0 \leq m \leq \ell$).

$$\int_{-1}^1 P_{\ell}^m(x) P_{\ell}^m(x) dx = \frac{2(\ell+m)!}{(2\ell+1)(\ell-m)!} \quad \dots (A8)$$

The associated Legendre polynomials satisfy the orthogonality relation (for fixed ℓ)

$$\int_{-1}^1 \frac{P_{\ell}^m(x) P_{\ell}^n(x)}{(1-x^2)} dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{(\ell+m)!}{m(\ell-m)!} & \text{if } m = n \neq 0 \\ \infty & \text{if } m = n = 0 \end{cases} \quad \dots (A9)$$

The recurrence relation for the associated Legendre polynomials is given as

$$(2\ell+1)xP_{\ell-1}^m(x) = (\ell+m-1)P_{\ell-2}^m(x) + (\ell+m)P_{\ell}^m(x) \quad \dots (A10)$$

The spherical harmonics of order ℓ are defined as⁶⁷

$$Y_{\ell m}(\theta, \phi) = C_{\ell m} P_{\ell}^m(\cos \theta) e^{im\phi} \quad \dots (A11)$$

where the normalization constant $C_{\ell m}$ is given as^{27,67}

$$C_{\ell m} = \sqrt{\frac{(2\ell+1)(\ell-m)!}{4(\ell+m)!}} \quad \dots (A12)$$

The spherical harmonics fulfill the condition

$$\int Y_{\ell m}^*(\Omega) Y_{\ell' m'}(\Omega) d\Omega = \delta_{\ell \ell'} \delta_{m m'} \quad \dots (A13)$$

where $d\Omega = \sin \theta d\theta d\phi$.